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Tricyclic xanthine derivatives containing a basic substituent: effects on adenosine receptor affinity and drug-related properties

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Appendix A

Metabolic stability of selected compounds.

The metabolic stability of compounds **27** and **36** was initially examined by*in silico* tools. The computational procedure MetaSite 4.1.1 provided by Molecular Discovery Ltd was used to determine the potential sites of metabolism as well as the most probable structures of metabolites. The plot of MetSite predictions for the most probable sites of **27** and **36** metabolism by a computational liver model is shown below (Fig. S1).

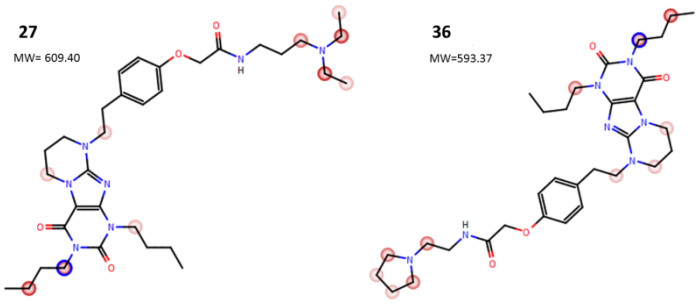


Figure S1. The plot of MetaSite predictions for sites of metabolism of compounds **27** and **36**. The darker red color of the marked functional group indicates its higher probability to be involved in the metabolism pathway. The blue circle marks the site involved in metabolism with highest probability.

Metabolic stability was additionally evaluated *in vitro* using human (HLMs) or rat (RLMs) liver microsomes. UPLC-MS analysis of the reaction mixture after 120 minutes of incubation of **27** with HLMs led to the identification of three main metabolites with the following molecular masses of their quasimolecular ions $[M+H]^+$: *m/z* = 582.64 (**M1**), *m/z* = 626.72 (**M2**), *m/z* = 569.54 (**M3**). The analysis of the reaction mixture after incubation of **27** with RLMs showed similar results indicating the presence of the same metabolites: **M1**, **M2**, **M3** and an additional metabolite **M4** (*m/z* = 554.65). Moreover, as was indicated by the UPLC spectra shown below, compound **27** seems to be a metabolically rather unstable molecule because about 50% (in the presence of HLMs) or 70% (in the presence of RLMs) of **27** were metabolized (Fig S2):

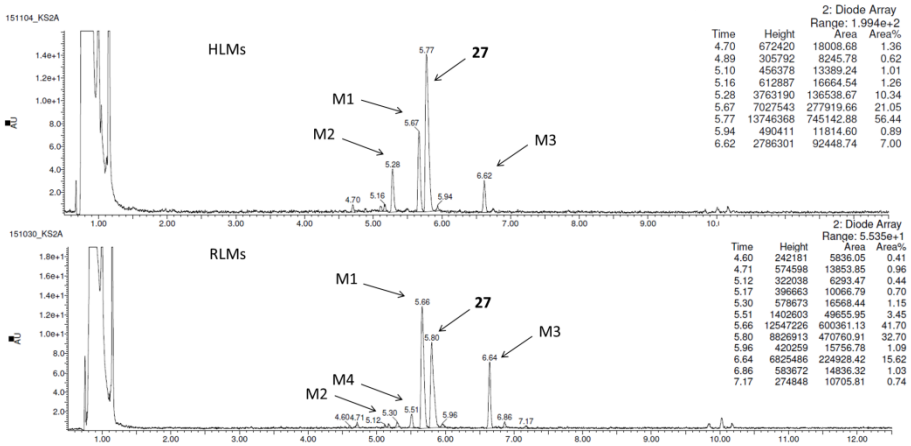


Figure S2. UPLC spectrum after 120 minutes reaction of **27** with HLMs and RLMs.

The metabolite structures generated on the basic of *in silico* studies corresponded to the masses of quasimolecular ions from MS analyses and suggested the following metabolic pathways of **27**: (i) dealkylation (**M1**, **M4**), (ii) hydroxylation (**M2**), (iii) dealkylation and deamination followed by oxidation (**M3**). The most probable structures of the metabolites of **27** are shown below (Fig. S3).

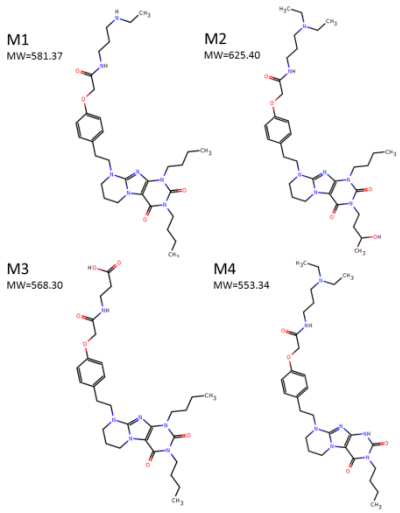


Figure S3. Proposed structures of the metabolites formed from **27, M1**, **M2**, **M3** and **M4.**

Compound **36** produced five metabolites after 120 minutes of incubation with HLMs, and MS analysis gave the following molecular masses of the metabolites' quasimolecular ions $[M+H]^+$: *m/z* = 610.63 (**M1**), *m/z* = 540.56 (**M2**), *m/z* = 592.61 (**M3**), *m/z*=555.52 (**M4**), *m/z*=610.63 (**M5**). UPLC-MS analysis of the metabolites obtained by RLMs and its comparison to results from HLMs showed the presence of similar metabolites, **M1** – **M5**, and an additional product with a molecular mass of *m/z*=610.70 (**M6**). However, the various concentrations of metabolites **M1** – **M5** obtained by HLMs or RLMs, and the presence of the additional metabolite **M6**, only obtained by RLMs in relatively high concentration, indicate some differences between the metabolism of **36** in rat versus human (Fig. S4). Moreover, the analysis of the obtained chromatograms showed that compound **36** appears to be more stable than **27** (Fig. S2)(Fig. S4).

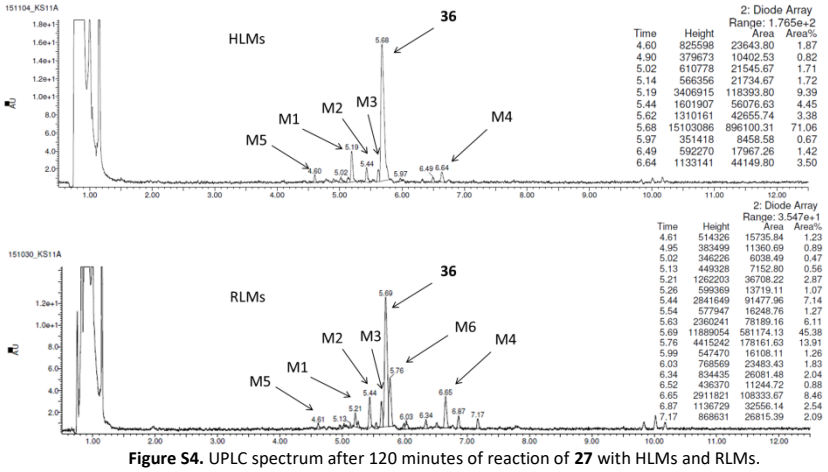


Figure S4. UPLC spectrum after 120 minutes of reaction of **27** with HLMs and RLMs.

According to the MS analysis and *in silico* results, the following metabolic pathways of compound **36** probably occurred: (i) hydroxylation (**M1**, **M5**, **M6**), (ii) dealkylation (**M2**), (iii) dehydrogenation (**M3**), (iv) dealkylation and deamination followed by oxidation (**M4**). The most probable structures of metabolites of **36** are shown below (Fig. S5). However, due to different possibilities for the site of hydroxylation, only one hydroxylated structure, predicted by MetaSite with the highest probability (score 100%), was included in figure S5.

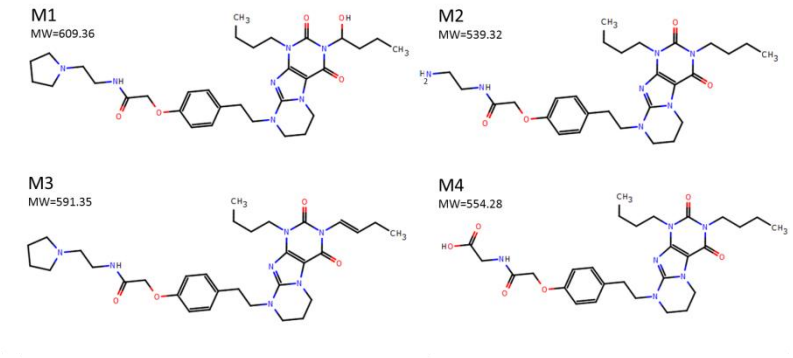


Figure S5. Proposed structures of metabolites of **36**, M1, M2, M3 and M4.

Appendix B
Chemistry

Synthesis of methyl 2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (10) or methyl 2-(4-(2-(2,4-dioxo-1,3-dibutyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (11).

A mixture of 9 mmol of 9-(4-hydroxyphenethyl)-1,3-dipropyl-6,7,8,9-tetrahydropyrimido[2,1-*f*]purine-2,4(1*H*,3*H*)-dione (**6**) or 9-(4-hydroxyphenethyl)-1,3-dibutyl-6,7,8,9-tetrahydropyrimido[2,1-*f*]purine-2,4(1*H*,3*H*)-dione (**7**), 9 mmol of anhydrous K2CO3, 19 mmol of methyl bromoacetate, a catalytic amount of TEBA and 95.00 ml of butan-2-one was refluxed for 17 h. The solvent was removed and the residue was treated with water. A precipitate was filtered off. To purify the products they were crystallized from ethanol. The precipitate was filtered off and dried.

Methyl 2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyri-mido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (10)

Yield: 4.3 g, 99 % , mp: 126-128 °C; ^{1}H NMR (300 MHz, CHLOROFORM-*d*) δ ppm: 0,96 (m, 6H, 2 x C$\underline{H}_3$CH$_2$CH$_2$); 1,62-1,82(m, 4H, 2 x CH$_3$C$\underline{H}_2$CH$_2$); 2,00-2,17 (m, 2H, C7$\underline{H}_2$); 2,89 (t, J=7,18Hz, 2H, C$\underline{H}_2$C6H4); 3,20 (t, J=5,64Hz, 2H, N9C$\underline{H}_2$); 3,69 (t, J=7,33Hz, 2H, C8$\underline{H}_2$); 3,81 (s, 3H, OC$\underline{H}_3$); 3,90-3,95 (m, 2H, N3C$\underline{H}_2$); 4,01 (t, J=7,31Hz, 2H, N1C$\underline{H}_2$); 4,17 (t, J=6,03Hz, 2H, N5C$\underline{H}_2$); 4,62 (s, 2H, OC$\underline{H}_2$CO); 6,82-6,87 (m, 2H, Ar); 7,11-7,16 (m, 2H, Ar). ^{13}C NMR (CHLOROFORM-*d*) δ ppm: 11,27, 11,37, 21,38, 21,43, 21,49, 32,99, 41,51, 42,46, 44,82, 45,41, 51,68, 52,24, 65,41, 102,80, 114,78, 129,91, 132,15, 148,49, 151,06, 151,27, 153,86, 156,52,169,37. IR [KBr] 1696, 1654 (C=O), 1240 (C-O$_{Ar}$)[cm^{-1}]. LC-MS: purity 99,14 %, t$_R$ = 7,28, (ESI) m/z 484 [M$^+$+1].Anal. for $C_{25}H_{33}N_5O_5$: Calcd: C, 62,09; H, 6,89; N, 14,48. Found: C, 61,83; H, 6,76; N, 14,47.

Methyl 2-(4-(2-(2,4-dioxo-1,3-dibutyl-1,2,3,4,7,8-hexahydropyri-mido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (11)

Yield: 4.18 g, 91%, mp: 88-91 °C; ^{1}H NMR (300 MHz, CHLOROFORM-*d*) δ ppm: 0,91-1,00 (m, 6H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$); 1,25-1,47 (m, 4H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$); 1,57-1,79 (m, 4H, 2 x CH$_3$CH$_2$C$\underline{H}_2$CH$_2$); 2,00-2,17 (m, 2H, C7$\underline{H}_2$); 2,89 (t, J=7,32Hz, 2H, C$\underline{H}_2$C6H4); 3,20(t, J=5,64Hz, 2H, N9C$\underline{H}_2$); 3,68 (t, J=7,31Hz, 2H, C8$\underline{H}_2$); 3,81 (s, 3H, OC$\underline{H}_3$); 3,96 (t, J=7,57Hz, 2H, N3C$\underline{H}_2$); 4,05 (t, J=7,31Hz, 2H, N1C$\underline{H}_2$); 4,15 (t, J=5,85Hz, 2H, N5C$\underline{H}_2$); 4,60 (d, J=6,67Hz, 2H, OC$\underline{H}_2$CO); 6,82-6,87 (m, 2H, Ar); 7,13 (d, J=8,46Hz, 2H, Ar). ^{13}C NMR (CHLOROFORM-*d*) δ ppm: 13,83, 13,85, 19,97, 20,31, 21,32, 30,22, 30,34, 33,01, 40,86, 41,53, 43,25, 45,43, 51,81, 52,24, 65,40, 102,77, 114,79, 129,92, 132,07, 150,76, 151,15, 153,83, 156,54, 169,35. IR [KBr] 1697, 1655 (C=O), 1241 (C-O$_{Ar}$)[cm^{-1}]. LC-MS: purity 100 %, t$_R$ = 8,24, (ESI) m/z 512 [M$^+$+1]. Anal. for $C_{27}H_{37}N_5O_5$: Calcd: C, 63,39; H, 7,30; N, 13,69. Found: C, 63,68; H, 7,37; N, 13,75.

General procedure for the synthesis of N-(substituted)-2-(4-(2-(1,3-dipropyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (14-25) and N-(substituted)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (26-38)

Table S1.

Microwave irradiation

Compound	Power and Time	Compound	Power and Time
13	450 W - 2 x 3 min	26	450 W- 2 x 3 min
14	450 W - 2 x 3 min	27	450 W- 3 x 3 min
15	450 W - 2 x 3 min and 1 x 2 min	28	450 W - 3 x 3 min
16	450 W - 2 x 3 min	29	450 W - 2 x 3 min
17	450 W- 2 x 3 min and 1 x 2 min	30	450 W - 3 x 3 min
18	450 W- 2 x 3 min and 1 x 2 min	31	450 W - 2 x 3 min

19	450 W - 2 x 3 min and 2 x 1 min	32	450 W - 2 x 3 min and 1 x 2 min
20	450 W - 2 x 3 min	33	450 W - 2 x 3 min
21	450 W - 2 x 3 min	34	450 W - 2 x 3 min
22	450 W- 2 x 3 min and 1 x 2 min	35	450 W - 2 x 3 min
23	450 W- 2 x 3 min and 2 x 2 min	36	450 W - 2 x 3 min
24	450 W- 2 x 3 min	37	450 W - 2 x 3 min and 600W - 2 min
25	450 W- 2 x 2 min	38	450 W- 1 x 3 min and 1 x 2 min

The mixture of 1 mmol methyl 2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (**10**) or methyl 2-(4-(2-(2,4-dioxo-1,3-dibutyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (**11**) and 2 mmol of appropriate amine was melted using a domestic microwave oven (power and time in **Table 1**). The residue was treated with 10 ml of ethanol. The precipitate was filtered off and the product was purified by crystallization from EtOH in the presence of charcoal or column chromatography (DCM/MeOH 9:1).

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-ylo)ethyl)phenoxy)-N-(2-morpholinoethyl)acetamide (14)

Used amine: 2-morpholinoethan-1-amine

Yield: 0.26 g, 44 %; mp: 148-150 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.88 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.43 - 1.58 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.58 - 1.72 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.93 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.29 - 2.36 (m, 6 H, C$\underline{H}_2$NCH$_2$CH$_2$O, 2 x NC$\underline{H}_2$CH$_2$O) 2.80 (t, *J*=7.18 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.17 - 3.30 (m, 4 H, NHC$\underline{H}_2$CH$_2$, N9C$\underline{H}_2$) 3.48 - 3.53 (m, 4 H, 2 x NCH$_2$C$\underline{H}_2$O) 3.60 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.72 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.40 (s, 2 H, OC$\underline{H}_2$CO) 6.86 (d, *J*=8.46 Hz, 2 H, Ar) 7.15 (d, *J*=8.72 Hz, 2 H, Ar) 7.87 (t, *J*=5.51 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 11.52, 11.63, 21.22, 21.31, 21.44, 32.53, 35.86, 41.75, 41.88, 44.31, 44.65, 51.18, 53.60, 57.51, 66.65, 67.57, 102.27, 115.15, 130.13, 132.26, 148.65, 150.98, 151.74, 152.94, 156.63, 168.02. IR [KBr] 3431 (N-H$_r$); 2965 (C-H); 1652 (C=O); 1611 (N-H$_d$); 1527 (C=C$_{Ar}$); 1241 (C-O$_{Ar}$)[cm^{-1}]. LC-MS: purity 100.00 %, t_R = 4.70, (ESI) m/z 582.57 [M$^+$+1]. Anal. for $C_{30}H_{43}N_7O_5$: Calcd: C, 61.94; H, 7.45; N, 16.85. Found: C, 61.70; H, 7.19; N, 16.65.

N-(2-(diethylamino)ethyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (15)

Used amine: N^1,N^1-diethylethane-1,2-diamine

Yield: 0.15 g, 26 %; mp: 140-143 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.93 (m, 12 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$, 2 x C$\underline{H}_3$CH$_2$N) 1.43 - 1.57 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.58 - 1.72 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.93 - 2.01 (m, 2 H, C7$\underline{H}_2$) 2.38 - 2.45 (m, 6 H, 2 x NC$\underline{H}_2$CH$_3$, NHCH$_2$C$\underline{H}_2$N) 2.80 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.11 - 3.19 (m, 2 H, NHC$\underline{H}_2$CH$_2$N) 3.24 - 3.28 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.71 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.00 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.39 (s, 2 H, OC$\underline{H}_2$CO) 6.85 (d, *J*=8.72 Hz, 2 H, Ar) 7.14 (d, *J*=8.46 Hz, 2 H, Ar) 7.82 (t, *J*=5.64 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 11.52, 11.62, 12.27, 21.21, 21.31, 21.44, 32.52, 36.88, 41.74, 41.88, 44.30, 44.64, 47.02, 51.16, 51.73, 67.57, 102.27, 115.11, 130.14, 132.25, 148.64, 150.98, 151.73, 152.93, 156.60, 167.95. IR [KBr]: 3393 (N-H$_r$); 2965 (C-H); 1659 (C=O); 1618 (N-H$_d$); 1529 (C=C$_{Ar}$); 1237 (C-O$_{Ar}$)[cm^{-1}]. LC-MS: purity 99.25 %, t_R = 4.96, (ESI) m/z 568 [M$^+$+1]. Anal. for $C_{30}H_{45}N_7O_4$: Calcd: C, 63.46; H, 7.99; N, 17.27. Found: C, 63.24; H, 7.59; N, 16.8.

N-(3-(diethylamino)propyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (16)

Used amine: N^1,N^1-diethylpropane-1,3-diamine

Yield: 0.30 g, 52 %; mp: 95-98 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.93 (m, 12 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$, 2 x C$\underline{H}_3$CH$_2$N) 1.43 - 1.57 (m, 4 H, CH$_3$C$\underline{H}_2$CH$_2$N1, NHCH$_2$C$\underline{H}_2$CH$_2$N) 1.58 - 1.72 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.92 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.28 - 2.41 (m, 6 H, 2 x NC$\underline{H}_2$CH$_3$, NHCH$_2$CH$_2$C$\underline{H}_2$N) 2.80 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.09 - 3.17 (m, 2 H, NHC$\underline{H}_2$CH$_2$CH$_2$N) 3.25 -

3.30 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.71 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.00 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H}_2$) 4.38 (s, 2 H, OC$\underline{H}_2$CO) 6.84 (d, *J*=8.46 Hz, 2 H, Ar) 7.14 (d, *J*=8.72 Hz, 2 H, Ar) 8.16 (t, *J*=5.26 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d_6) δ ppm: 11.52, 11.63, 12.06, 21.21, 21.31, 21.44, 26.76, 32.52, 37.88, 41.74, 41.88, 44.30, 44.64, 46.76, 50.87, 51.15, 67.58, 102.27, 115.04, 130.13, 132.18, 148.64, 150.98, 151.74, 152.94, 156.64, 167.83. IR [KBr]: 3406 (N-H$_r$); 2966 (C-H); 1651 (C=O); 1613 (N-H$_d$); 1528 (C=C$_{Ar}$); 1173 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 98.54 %, t_R = 4.90, (ESI) m/z 582 [M$^+$+1]. Anal. for $C_{30}H_{45}N_7O_4$: Calcd: C, 63.02; H, 8.19; N, 16.60. Found: C, 63.47; H, 8.30; N, 16.32.

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(3-methoxybenzyl)acetamide (17)

Used amine: 3-methoxybenzylamine

Yield: 0.11 g, 19 %; mp: 158-160 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.83 (dt, *J*=9.49, 7.44 Hz, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.43 - 1.57 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.59 - 1.73 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.92 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.80 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.25 - 3.30 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H}_2$) 3.69 (s, 3 H, OCH$_3$) 3.71 - 3.79 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.28 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.49 (s, 2 H, OC$\underline{H}_2$CO) 6.74 - 6.81 (m, 3 H, Ar) 6.88 (d, *J*=8.72 Hz, 2 H, Ar) 7.11 - 7.22 (m, 3 H, Ar) 8.58 (t, *J*=6.28 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d_6) δ ppm: 11.52, 11.63, 21.21, 21.32, 21.44, 32.55, 41.75, 41.88, 42.18, 44.32, 44.68, 51.21, 55.40, 67.53, 102.29, 112.65, 113.27, 115.15, 119.81, 129.70, 130.11, 132.20, 141.38, 148.67, 150.99, 151.75, 152.95, 156.69, 159.73, 168.28. IR [KBr]: 3418 (N-H$_r$); 2961 (C-H); 1650 (C=O); 1614 (N-H$_d$); 1527 (C=C$_{Ar}$); 1232 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 100 %, t_R = 7.30, (ESI) m/z 589 [M$^+$+1]. Anal. for $C_{32}H_{40}N_6O_5$: Calcd: C, 65.28; H, 6.85; N, 14.27. Found: C, 64.98; H, 6.74; N, 14.08.

N-(3-chlorobenzyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (18)

Used amine: 3-chlorobenzylamine

Yield: 0.11 g, 19 %; mp: 164-167 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.89 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.43 - 1.57 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.59 - 1.73 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.92 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.81 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.24 - 3.30 (m, 2 H, N9C$\underline{H}_2$) 3.61 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.72 - 3.79 (m, 2 H, N3C$\underline{H}_2$) 3.88 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H}_2$) 4.31 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.50 (s, 2 H, OC$\underline{H}_2$CO) 6.88 (d, *J*=8.72 Hz, 2 H, Ar) 7.12 - 7.20 (m, 3 H, Ar) 7.22 - 7.34 (m, 3 H, Ar) 8.65 (t, *J*=6.28 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d_6) δ: 11.53, 11.63, 21.22, 21.33, 21.44, 32.55, 41.72, 41.88, 44.31, 44.68, 51.21, 67.51, 102.29, 115.14, 126.34, 127.14, 127.39, 130.13, 130.51, 132.23, 142.43, 148.67, 150.98, 151.74, 152.94, 156.62, 168.50 ppm. IR [KBr]: 3416 (N-H$_r$); 2961 (C-H); 1652 (C=O); 1618 (N-H$_d$); 1529 (C=C$_{Ar}$); 1238 (C-O$_{Ar}$); [cm^{-1}]. LC-MS: purity 99.5 %, t_R = 7.74, (ESI) m/z 594 [M$^+$+1]. Anal. for $C_{31}H_{37}ClN_6O_4$: Calcd: C, 62.77; H, 6.28; N, 14.17. Found: C, 62.88; H, 6.11; N, 14.10.

N-(3-(cyclohexylamino)propyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (19)

Used amine: N1-cyclohexylpropane-1,3-diamine

Yield: 0.25 g, 41 %; mp: 221-224 °C; ^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.78 - 1.22 (m, 10 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$, 2 x C$\underline{H}_2$ cyclohexane) 1.43 - 1.78 (m, 12 H, N3CH$_3$C$\underline{H}_2$CH$_2$, N1CH$_3$C$\underline{H}_2$CH$_2$, 3 x C$\underline{H}_2$ cyclohexane, NHCH$_2$C$\underline{H}_2$CH$_2$NH) 1.93 - 2.01 (m, 2 H, C7$\underline{H}_2$) 2.19 - 2.29 (m, 1 H, C$\underline{H}$cyclohexane) 2.80 (t, *J*=7.03 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.15 (q, *J*=6.45 Hz, 2 H, NHCH$_2$CH$_2$C$\underline{H}_2$NH) 3.24 - 3.33 (m, 5 H, CH$_2$N$\underline{H}$CH cyclohexane, N9C$\underline{H}_2$, NHC$\underline{H}_2$CH$_2$CH$_2$NH) 3.60 (t, *J*=7.33 Hz, 2 H, C8$\underline{H}_2$) 3.71 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.03 Hz, 2 H, N1C$\underline{H}_2$) 4.00 (t, *J*=5.86 Hz, 2 H, N5C$\underline{H}_2$) 4.38 (s, 2 H, OC$\underline{H}_2$CO) 6.85 (d, *J*=8.79 Hz, 2 H, Ar) 7.14 (d, *J*=8.79 Hz, 2 H, Ar) 8.14 (t, *J*=5.57 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d_6) δ ppm: 11.52, 11.62, 21.23, 21.31, 21.44, 24.93, 26.37, 29.99, 32.55, 33.46, 37.55,41.75, 41.88, 44.31, 44.55, 44.70, 51.19, 56.55, 67.68, 102.28, 115.15, 130.10, 132.22, 148.67, 151.00, 151.76, 152.95, 155.72, 156.71, 156.72 167.90. IR [KBr]: 3416 (N-H$_r$); 2961 (C-H); 1652 (C=O); 1618 (N-H$_d$); 1529 (C=C$_{Ar}$); 1238 (C-O$_{Ar}$); [cm^{-1}]. LC-MS: purity 100 %, t_R = 5.42,

(ESI) m/z 608 [M^++1]. Anal. for $C_{33}H_{49}N_7O_4$: Calcd: C, 60.66; H, 7.85; N, 15.01. Found: C, 60.43; H, 7.86; N, 15.09.

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(pyridin-2-yl)ethyl)acetamide (20)

Used amine: 2-(pyridin-2-yl)ethan-1-amine

Yield: 0.07 g, 12 %; mp: 136-139 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.88 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.42 - 1.57 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.58 - 1.72 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.92 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.76 - 2.91 (m, 4 H, C$\underline{H}_2$C$_6$H$_4$, NHCH$_2$C$\underline{H}_2$C$_5$H$_4$N) 3.24 - 3.29 (m, 2 H, N9C$\underline{H}_2$) 3.42 - 3.51 (m, 2 H, NHC$\underline{H}_2$CH$_2$C$_5$H$_4$N) 3.61 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.71 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.00 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.38 (s, 2 H, OC$\underline{H}_2$CO) 6.80 - 6.89 (m, 2 H, Ar) 7.10 - 7.22 (m, 4 H, Ar) 7.61 - 7.70 (m, 1 H, Ar) 8.16 (t, *J*=5.64 Hz, 1 H, N$\underline{H}$CH$_2$) 8.44 - 8.48 (m, 1 H, Ar). ^{13}C NMR (DMSO d$_6$) δ ppm: 11.52, 11.63, 21.20, 21.31, 21.44, 32.54, 37.53, 38.60, 41.74, 41.88, 44.31, 44.68, 51.19, 67.52, 102.28, 115.11, 121.93, 123.55, 130.12, 132.18, 136.91, 148.66, 149.46, 150.98, 151.74, 152.94, 156.63, 159.48, 168.03. IR [KBr]: 3413 (N-H$_r$); 2958 (C-H); 1655 (C=O); 1618 (N-H$_d$); 1530 (C=C$_{Ar}$); 1249 (C-O$_{Ar}$); [cm^{-1}]. LC-MS: purity 100 %, t_R = 4.94, (ESI) m/z 574.29 [M^++1]. Anal. for $C_{30}H_{37}N_7O_4$: Calcd: C, 64.90; H, 6.85; N, 17.09. Found: C, 64.50; H, 7.13; N, 16.81.

N-benzyl-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (21)

Used amine: benzylamine

Yield: 0.31 g, 55 %; mp: 155-156 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.88 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.43 - 1.57 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.59 - 1.73 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.92 - 2.01 (m, 2 H, C7$\underline{H}_2$) 2.80 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.24 - 3.29 (m, 2 H, N9C$\underline{H}_2$) 3.61 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.72 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H}_2$) 4.31 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.49 (s, 2 H, OC$\underline{H}_2$CO) 6.88 (d, *J*=8.72 Hz, 2 H, Ar) 7.11 - 7.31 (m, 7 H, Ar) 8.60 (t, *J*=6.03 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 11.53, 11.63, 21.21, 21.32, 21.44, 32.55, 41.75, 41.89, 42.23, 44.32, 44.68, 51.21, 67.53, 102.29, 115.17, 127.18, 127.65, 128.64, 130.10, 132.21, 139.78, 148.67, 150.98, 151.75, 152.94, 156.67, 168.26. IR [KBr]: 3408 (N-H$_r$); 2963 (C-H); 1648 (C=O); 1616 (N-H$_d$); 1527 (C=C$_{Ar}$); 1234 (C-O$_{Ar}$); [cm^{-1}]. LC-MS: purity 97.7 %, t_R = 7.33, (ESI) m/z 559 [M^++1]. Anal. for $C_{31}H_{38}N_6O_4$: Calcd: C, 66.64; H, 6.86; N, 15.04. Found: C, 66.35; H, 6.91; N, 14.89.

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-fluorobenzyl)acetamide (22)

Used amine: 4-fluorobenzylamine

Yield: 0.3 g, 52 %; mp: 172-174 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.88 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.43 - 1.56 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.59 - 1.72 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.92 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.80 (t, *J*=7.18 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.24 - 3.29 (m, 2 H, N9C$\underline{H}_2$) 3.61 (t, *J*=7.44 Hz, 2 H, C8$\underline{H}_2$) 3.72 - 3.78 (m, 2 H, N3C$\underline{H}_2$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.29 (d, *J*=6.16 Hz, 2 H. NHC$\underline{H}_2$C$_6$H$_4$) 4.47 (s, 2 H, OC$\underline{H}_2$CO) 6.87 (d, *J*=8.72 Hz, 2 H, Ar) 7.05 - 7.17 (m, 4 H, Ar) 7.22 - 7.30 (m, 2 H, Ar) 8.61 (t, *J*=6.16 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 11.52, 11.63, 21.22, 21.31, 21.44, 32.55, 41.55, 41,74, 41.88, 44.31, 44.68, 51.21, 67.53, 102.28, 115.17, 115.23, 115.45, 129.63, 129.71, 130.11, 132.23, 136.02, 148.66, 150.98, 151.74, 152.94, 156.64, 160.40, 162.80, 168.28. IR [KBr]: 3415 (N-H$_r$); 2962 (C-H); 1648 (C=O); 1616 (N-H$_d$); 1528 (C=C$_{Ar}$); 1235 (C-O$_{Ar}$); [cm^{-1}]. LC-MS: purity 97.8 %, t_R = 7.37, (ESI) m/z 577 [M^++1]. Anal. for $C_{31}H_{37}FN_6O_4$: Compound contains Fluor atom - analysis didn't perform.

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-sulfamoylphenethyl)acetamide (23)

Used amine: 4-(2-aminoethyl)benzenesulfonamide

Yield: 0.17 g, 26.00 %; mp: 223-226 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.88 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$) 1.43 - 1.57 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N1) 1.58 - 1.72 (m, 2 H, CH$_3$C$\underline{H}_2$CH$_2$N3) 1.93 -

2.02 (m, 2 H, C7$\underline{H_2}$) 2.80 (t, *J*=7.05 Hz, 4 H, 2 x C$\underline{H_2}C_6H_4$) 3.25 - 3.30 (m, 2 H, N9C$\underline{H_2}$) 3.32 - 3.40 (m, 2 H, NHC$\underline{H_2}CH_2C_6H_4$) 3.61 (t, *J*=7.31 Hz, 2 H, C8$\underline{H_2}$) 3.72 - 3.78 (m, 2 H, N3C$\underline{H_2}$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H_2}$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H_2}$) 4.38 (s, 2 H, OC$\underline{H_2}$CO) 6.83 (d, *J*=8.72 Hz, 2 H, Ar) 7.14 (d, *J*=8.72 Hz, 2 H, Ar) 7.27 (s, 2 H, $SO_2N\underline{H_2}$) 7.35 (d, *J*=8.46 Hz, 2 H, Ar) 7.71 (d, *J*=8.21 Hz, 2 H, Ar) 8.13 (t, *J*=5.90 Hz, 1 H, N$\underline{H}CH_2$). ^{13}C NMR (DMSO d_6) δ ppm: 11.54, 11.64, 21.22, 21.32, 21.44 32.54, 35.23, 41,75, 41.89, 44.32, 44.67, 51.19, 67.54, 102.27, 115.13, 126.15,129.54, 130.14, 132.23, 142.53, 143.97, 148.67, 150.98, 151.75, 152.94, 156.67, 168.15. IR [KBr]: 3301 (N-H_r); 2961 (C-H); 1655 (C=O); 1626 (N-H_d); 1530 (C=C_{Ar}); 1226 (C-O_{Ar}); [cm^{-1}]. LC-MS: purity 97.1 %, t_R = 6.15, (ESI) m/z 653 [M^++1]. Anal. for $C_{32}H_{41}N_7O_6S$: Calcd: C, 57.98; H, 6.69; N, 14.79. Found: C, 57.77; H, 6.75; N, 14.65.

N-(4-chlorobenzyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (24)

Used amine: 4-chlorobenzylamine

Yield: 0.31 g, 52.00 %; mp: 168-171 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.77 - 0.88 (m, 6 H, 2 x C$\underline{H_3}CH_2CH_2$) 1.43 - 1.57 (m, 2 H, $CH_3C\underline{H_2}CH_2$N1) 1.58 - 1.72 (m, 2 H, $CH_3C\underline{H_2}CH_2$N3) 1.92 - 2.01 (m, 2 H, C7$\underline{H_2}$) 2.81 (t, *J*=7.44 Hz, 2 H, C$\underline{H_2}C_6H_4$) 3.24 - 3.29 (m, 2 H, N9C$\underline{H_2}$) 3.61 (t, *J*=7.31 Hz, 2 H, C8$\underline{H_2}$) 3.72 - 3.79 (m, 2 H, N3C$\underline{H_2}$) 3.87 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H_2}$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H_2}$) 4.29 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H_2}C_6H_4$) 4.48 (s, 2 H, OC$\underline{H_2}$CO) 6.84 - 6.91 (m, 2 H, Ar) 7.11 - 7.17 (m, 2 H, Ar) 7.21 - 7.26 (m, 2 H, Ar) 7.30 - 7.36 (m, 2 H, Ar) 8.63 (t, *J*=6.16 Hz, 1 H, N$\underline{H}CH_2$). ^{13}C NMR (DMSO d_6) δ ppm: 11.53, 11.64, 21.23, 21.32, 21.44, 32.55, 41.61, 41,74, 41.89, 44.32, 44.69, 51.22, 67.52, 102.28, 115.17, 128.57, 129.56, 130.11, 131.76, 132.25, 138.88, 148.66, 150.98, 151.74, 152.94, 156.63, 168.38. IR [KBr]: 3411 (N-H_r); 2963 (C-H); 1652 (C=O); 1627 (N-H_d); 1527 (C=C_{Ar}); 1174 (C-O_{Ar}); [cm^{-1}]. LC-MS: purity 98.5 %, t_R = 7.77, (ESI) m/z 594 [M^++1]. Anal. for $C_{31}H_{37}ClN_6O_4$: Calcd: C, 62.77; H, 6.29; N, 14.17. Found: C, 62.99; H, 6.72; N, 14.10.

N-(3-(1H-imidazol-1-yl)propyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (25)

Used amine: 3-(1H-imidazol-1-yl)propan-1-amine

Yield: 0.24 g, 42.00 %; mp: 185-189 °C; 1H NMR (300 MHz, DMSO-d6) δ ppm 0.76 - 0.89 (m, 6 H, 2 x CH3CH2CH2) 1.43 - 1.57 (m, 2 H, CH3CH2CH2N1) 1.58 - 1.72 (m, 2 H, CH3CH2CH2N3) 1.83 (quin, J=6.86 Hz, 2 H, NHCH2CH2CH2N) 1.92 - 2.01 (m, 2 H, C7H2) 2.80 (t, J=7.18 Hz, 2 H, CH2C6H4) 3.07 (q, J=6.50 Hz, 2 H, NHCH2CH2CH2N) 3.23 - 3.29 (m, 2 H, N9CH2) 3.60 (t, J=7.31 Hz, 2 H, C8H2) 3.71 - 3.78 (m, 2 H, N3CH2) 3.88 (q, J=6.33 Hz, 4 H, N1CH2, NHCH2CH2CH2N) 4.00 (t, J=5.90 Hz, 2 H, N5CH2) 4.42 (s, 2 H, OCH2CO) 6.83 - 6.90 (m, 3 H, Ar) 7.11 - 7.17 (m, 3 H, Ar) 7.55 - 7.57 (m, 1 H, Ar) 8.12 (t, J=5.77 Hz, 1 H, NHCH2). 13C NMR (DMSO d6) δ: 11.52, 11.63, 21.20, 21.31, 21.44, 31.20, 32.54, 36.05, 41,74, 41.88, 44.04, 44.31, 44.68, 51.19, 67.56, 102.27, 115.14, 119.73, 128.82, 130.13, 132.21, 137.70, 148.66, 150.98, 151.73, 152.94, 156.67, 168.31 ppm. IR [KBr]: 3326 (N-Hr); 2907 (C-H); 1657, (C=O); 1613 (N-Hd); 1529 (C=CAr); 1195 (C-OAr) [cm-1]. LC-MS: purity 98.41 %, tR = 4.83, (ESI) m/z 577.28 [M++1]. Anal. for C30H40N8O4: Calcd: C, 62.48; H, 6.99; N, 19.43. Found: C, 61.99; H, 6.86; N, 18.93.

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(diethylamino)ethyl)acetamide (26)

Used amine: N^1,N^1-diethylethane-1,2-diamine

Yield: 0.17 g, 57.5 % mp: 107-110 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.78 - 0.95 (m, 12 H, 2 x C$\underline{H_3}CH_2CH_2CH_2$, 2 x C$\underline{H_3}CH_2$N) 1.19 - 1.32 (m, 4 H, 2 x $CH_3C\underline{H_2}CH_2CH_2$) 1.41 - 1.51 (m, 2 H, C$\underline{H_2}CH_2$N1) 1.57 - 1.67 (m, 2 H, C$\underline{H_2}CH_2$N3) 1.93 - 2.02 (m, 2 H, C7$\underline{H_2}$) 2.37 - 2.46 (m, 6 H, C$\underline{H_2}$N(C$\underline{H_2}CH_3)_2$) 2.80 (t, *J*=7.31 Hz, 2 H, C$\underline{H_2}C_6H_4$) 3.15 (q, *J*=7.20 Hz, 2 H, NHC$\underline{H_2}$) 3.25 - 3.28 (m, 2 H, N9C$\underline{H_2}$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H_2}$) 3.78 (t, *J*=7.40 Hz, 2 H, N3C$\underline{H_2}$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H_2}$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H_2}$) 4.40 (s, 2 H, OC$\underline{H_2}$CO) 6.85 (d, *J*=8.72 Hz, 2 H, Ar) 7.14 (d, *J*=8.72 Hz, 2 H, Ar) 7.81 (t, *J*=5.39 Hz, 1 H, N$\underline{H}CH_2$). ^{13}C NMR (DMSO d_6) δ: 12.34, 14.05,

14.19, 19.80, 20.11, 21.23, 30.04, 30.34, 32.53, 36.95, 41.74, 42.42, 44.64, 47.02, 51.20, 51.77, 67.59, 102.30, 115.11, 130.11, 132.23, 148.62, 150.90, 151.72, 152.91, 156.60, 167.91 ppm. IR [KBr]: 3419 (N-H_r); 2957 (C-H); 1653 (C=O); 1615 (N-H_d); 1532 (C=C_{Ar}); 1236 (C-O_{Ar}); [cm^{-1}]. LC-MS: purity 100 %, t_R = 5.68, (ESI) m/z 596.7 [M^++1]. Anal. for $C_{32}H_{49}N_7O_4$: Calcd: C, 64.51; H, 8.29; N, 16.46. Found: C, 64.60; H, 7.84; N, 16.57.

N-benzyl-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (28)

Used amine: benzylamine

Yield: 0.56 g, 63.6 %, mp: 146-148 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.83 - 0.93 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$) 1.18 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$) 1.40 - 1.53 (m, 2 H, C$\underline{H}_2$CH$_2$N1) 1.57 - 1.68 (m, 2 H, C$\underline{H}_2$CH$_2$N3) 1.93 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.81 (t, *J*=7.44 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.25 - 3.30 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H}_2$) 3.79 (t, *J*=7.20 Hz, 2 H, N3$\underline{H}_2$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.32 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.49 (s, 2 H, OC$\underline{H}_2$CO) 6.88 (d, *J*=8.72 Hz, 2 H, Ar) 7.15 (d, *J*=8.72 Hz, 2 H, Ar) 7.19 - 7.31 (m, 5 H, Ar) 8.59 (t, *J*=6.03 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 14.06, 14.20, 19.80, 20.12, 21.23, 30.05, 30.34, 32.55, 41.75, 42.23, 42.43, 44.68, 51.26, 67.53, 102.31, 115.17, 127.18, 127.65, 128.63, 130.07, 132.18, 139.78, 148.64, 150.91, 151.72, 152.92, 156.68, 168.25. IR [KBr]: 3288 (N-H_r); 2953 (C-H); 1655 (C=O); 1612 (N-H_d); 1527 (C=C_{Ar}); 1227 (C-O_{Ar}) [cm^{-1}]. LC-MS: purity 98.93 %, t_R = 8.26, (ESI) m/z 587.69 [M^++1]. Anal. for $C_{33}H_{42}N_6O_4$: Calcd: C, 67.55; H, 7.22; N, 14.32. Found: C, 67.18; H, 6.77; N, 14.61.

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-morpholinoethyl)acetamide (29)

Used amine: 2-morpholinoethan-1-amine

Yield: 0.29 g, 47.62 % mp: 157-161 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.83 - 0.93 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$) 1.18 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$) 1.46 (dt, *J*=14.68, 7.41 Hz, 2 H, N3CH$_2$C$\underline{H}_2$) 1.62 (quin, *J*=7.25 Hz, 2 H, N1CH$_2$C$\underline{H}_2$) 1.93 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.28 - 2.36 (m, 6 H, 2 x NC$\underline{H}_2$CH$_2$O, NHCH$_2$C$\underline{H}_2$N) 2.80 (t, *J*=7.18 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.17 - 3.30 (m, 4 H, N9C$\underline{H}_2$, NHC$\underline{H}_2$CH$_2$N) 3.50 (t, *J*=4.60 Hz, 4 H, 2 x NCH$_2$C$\underline{H}_2$O) 3.60 (t, *J*=7.31 Hz, 2 H, C8$\underline{H}_2$) 3.78 (t, *J*=7.20 Hz, 2 H, N3C$\underline{H}_2$) 3.91 (t, *J*=6.92 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H}_2$) 4.41 (s, 2 H, OC$\underline{H}_2$CO) 6.86 (d, *J*=8.72 Hz, 2 H, Ar) 7.15 (d, *J*=8.72 Hz, 2 H, Ar) 7.88 (t, *J*=5.51 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 14.06, 14.19, 19.80, 20.11, 21.23, 30.04, 30.34, 32.53, 35.86, 41.74, 42.43, 44.66, 51.23, 53.60, 57.51, 66.65, 67.58, 102.30, 115.15, 130.11, 132.24, 148.62, 150.90, 151.72, 152.92, 156.63, 168.01. IR [KBr]: 3298 (N-H_r); 2952, (C-H); 1655 (C=O); 1609 (N-H_d); 1529 (C=C_{Ar}); 1227 (C-O_{Ar}) [cm^{-1}]. LC-MS: purity 100.0 %, t_R = 5.48, (ESI) m/z 610.7 [M^++1]. Anal. for $C_{32}H_{47}N_7O_5$: Calcd: C, 63.03; H, 7.77; N, 16.08. Found: C, 62.84; H, 7.49; N, 16.27.

N-(3-chlorobenzyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (30)

Used amine: 3-chlorobenzylamine

Yield: 0.51 g, 54.8 % mp: 148-153 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.83 - 0.94 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$) 1.18 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$) 1.41 - 1.52 (m, 2 H, N3CH$_2$C$\underline{H}_2$) 1.57 - 1.68 (m, 2 H, C$\underline{H}_2$CH$_2$N1) 1.93 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.81 (t, *J*=7.57 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.25 - 3.30 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H}_2$) 3.79 (t, *J*=7.20 Hz, 2 H, N3C$\underline{H}_2$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H}_2$) 4.31 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.51 (s, 2 H, OC$\underline{H}_2$CO) 6.88 (d, *J*=8.72 Hz, 2 H, Ar) 7.12 - 7.21 (m, 3 H, Ar) 7.23 - 7.34 (m, 3 H, Ar) 8.65 (t, *J*=6.16 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 14.07, 14.20, 19.80, 20.12, 21.23, 30.05, 30.34, 32.56, 41.72, 42.44, 44.69, 51.25, 67.51, 102.31, 115.14, 126.34, 127.14, 127.39, 130.11, 130.51, 132.22, 133.41, 142.43, 148.64, 150.91, 151.72, 152.92, 156.63, 168.49. IR [KBr]: 3321 (N-H_r); 2950 (C-H); 1655 (C=O); 1618 (N-H_d); 1530 (C=C_{Ar}); 1249 (C-O_{Ar}) [cm^{-1}]. LC-MS: purity 100.0 %, t_R = 8.63, (ESI) m/z 622.6 [M^++1]. Anal. for $C_{33}H_{41}N_6O_4Cl$: Calcd: C, 63.80; H, 6.65; N, 13.53. Found: C, 63.82; H, 6.50; N, 13.62.

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(3-methoxybenzyl)acetamide (31)

Used amine: 3-methoxybenzylamine

Yield: 0.39 g, 64.3 % mp: 110-114 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.82 - 0.93 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$) 1.17 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$) 1.40 - 1.52 (m, 2 H, C$\underline{H}_2$CH$_2$N3) 1.57 - 1.68 (m, 2 H, C$\underline{H}_2$CH$_2$N1) 1.92 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.80 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.23 - 3.30 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H}_2$) 3.69 (s, 3 H, OC$\underline{H}_3$) 3.79 (t, *J*=7.40 Hz, 2 H, N3C$\underline{H}_2$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H}_2$) 4.29 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.49 (s, 2 H, OC$\underline{H}_2$CO) 6.74 - 6.81 (m, 3 H, Ar) 6.88 (d, *J*=8.72 Hz, 2 H, Ar) 7.11 - 7.22 (m, 3 H, AR) 8.57 (t, *J*=6.16 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 14.05, 14.19, 19.80, 20.12, 21.23, 30.05, 30.34, 32.55, 41.74, 42.18, 42.43, 44.68, 51.25, 55.39, 67.53, 102.31, 112.63, 113.27, 115.15, 119.81, 129.69, 130.08, 132.18, 141.38, 148.64, 150.90, 151.72, 152.92, 156.70, 159.72, 168.27. IR [KBr]: 3408 (N-H$_r$); 2953 (C-H); 1653 (C=O); 1614 (N-H$_d$); 1530 (C=C$_{Ar}$); 1236 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 98.26 %, t_R = 8.19, (ESI) m/z 617.68 [M$^+$+1]. Anal. for $C_{34}H_{44}N_6O_5$: Calcd: C, 66.21; H, 7.19; N, 13.63. Found: C, 66.21; H, 6.89 N, 13.58.

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-fluorobenzyl)acetamide (32)

Used amine: 4-fluorobenzylamine

Yield: 0.37 g, 61.21% mp: 162-164 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.81 - 0.94 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$) 1.17 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$) 1.40 - 1.52 (m, 2 H, C$\underline{H}_2$CH$_2$N3) 1.62 (quin, *J*=7.18 Hz, 2 H, C$\underline{H}_2$CH$_2$N1) 1.93 - 2.02 (m, 2 H, C7$\underline{H}_2$) 2.81 (t, *J*=7.31 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.24 - 3.30 (m, 2 H, N9C$\underline{H}_2$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H}_2$) 3.79 (t, *J*=7.40 Hz, 2 H, N3C$\underline{H}_2$) 3.91 (t, *J*=6.92 Hz, 2 H, N1C$\underline{H}_2$) 4.01 (t, *J*=6.03 Hz, 2 H, N5C$\underline{H}_2$) 4.29 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H}_2$C$_6$H$_4$) 4.48 (s, 2 H, OC$\underline{H}_2$CO) 6.87 (d, *J*=8.72 Hz, 2 H, Ar) 7.05 - 7.18 (m, 4 H, Ar) 7.21 - 7.30 (m, 2 H, Ar) 8.61 (t, *J*=6.16 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 14.05, 14.19, 19.80, 20.12, 21.23, 30.04, 30.34, 32.55, 41.55, 41.74, 42.43, 44.68, 51.26, 67.54, 102.31, 115.17, 115.23, 115.45, 129.63, 129.71, 130.08, 132.21, 136.02, 148.64, 150.91, 151.72, 152.92, 156.65, 160.40, 162.80, 168.28. IR [KBr]: 3278 (N-H$_r$); 2954 (C-H); 1655 (C=O); 1616 (N-H$_d$); 1529 (C=C$_{Ar}$); 1243 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 100.0 %, t_R = 8.29, (ESI) m/z 605.64 [M$^+$+1].Anal. for $C_{33}H_{41}N_6O_4F$: Calcd: C, 65.54; H, 6.83; N, 13.89. Found: C, 65.99; H, 6.73 N, 13.28.

N-(3-(cyclohexylamino)propyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (33)

Used amine: N1-cyclohexylpropane-1,3-diamine

Yield: 0.29 g, 45.56 % mp: 102-108 °C; ^{1}H NMR (300 MHz, DMSO-d_6) ? ppm 0.82 - 1.35 (m, 16 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$, 3 x C$\underline{H}_{2\ cyclohexane}$) 1.40 - 1.78 (m, 10 H, C$\underline{H}_2$CH$_2$N3, C$\underline{H}_2$CH$_2$N1, 2 x C$\underline{H}_{2\ cyclohexane}$) 1.92 - 2.02 (m, 2 H, C$\underline{H}_2C_6H_4$) 2.19 - 2.30 (m, 1 H, C$\underline{H}_{cyclohexane}$) 2.80 (t, *J*=7.03 Hz, 2 H, C$\underline{H}_2$C$_6$H$_4$) 3.11 - 3.19 (m, 2 H, NHCH$_2$CH$_2$C$\underline{H}_2$NH) 3.28 (d, *J*=4.69 Hz, 5 H, CH$_2$N$\underline{H}$CH$_{cyclohexane}$, N9C$\underline{H}_2$, NHC$\underline{H}_2$CH$_2$CH$_2$NH) 3.59 (t, *J*=7.33 Hz, 2 H, C8$\underline{H}_2$) 3.78 (t, *J*=7.33 Hz, 2 H, N3C$\underline{H}_2$) 3.90 (t, *J*=7.03 Hz, 2 H, N1C$\underline{H}_2$) 4.00 (t, *J*=5.86 Hz, 2 H, N5C$\underline{H}_2$) 4.39 (s, 2 H, OC$\underline{H}_2$CO) 6.85 (d, *J*=8.79 Hz, 2 H, Ar) 7.14 (d, *J*=8.79 Hz, 2 H, Ar) 8.16 (t, *J*=5.57 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ: 14.05, 14.18, 19.79, 20.11, 21.19, 24.90, 26.32, 29.83, 30.01, 30.32, 32.51, 33.29, 37.47, 41.70, 42.39, 44.45, 44.65, 51.21, 56.55, 63.85, 67.57, 102.27, 115.09, 130.06, 132.12, 148.59, 150.87, 151.67, 152.88, 156.65, 167.93 ppm. IR [KBr]: 3306 (N-H$_r$); 2929 (C-H); 1655 (C=O); 1614 (N-H$_d$); 1528 (C=C$_{Ar}$); 1276 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 98.87 %, t_R = 6.00, (ESI) m/z 636.44 [M$^+$+1]. Anal. for $C_{35}H_{53}N_7O_4$: Calcd: C, 66.11; H, 8.40; N, 15.42. Found: C, 66.19; H, 8.25 N, 15.22.

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(pyridin-2-yl)ethyl)acetamide (34)

Used amine: 2-(pyridin-2-yl)ethan-1-amine

Yield: 0.067 g, 11.13 % mp: 116-119 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.83 - 0.93 (m, 6 H, 2 x C$\underline{H}_3$CH$_2$CH$_2$CH$_2$) 1.18 - 1.34 (m, 4 H, 2 x CH$_3$C$\underline{H}_2$CH$_2$CH$_2$) 1.41 - 1.52 (m, 2 H, C$\underline{H}_2$CH$_2$N3)

1.57 - 1.68 (m, 2 H, C$\underline{H_2}$CH$_2$N1) 1.93 - 2.02 (m, 2 H, C7$\underline{H_2}$) 2.77 - 2.91 (m, 4 H, C$\underline{H_2}$C$_6$H$_4$, C$\underline{H_2}$C$_5$H$_4$N) 3.25 - 3.30 (m, 2 H, N9C$\underline{H_2}$) 3.43 - 3.51 (m, 2 H, NHC$\underline{H_2}$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H_2}$) 3.78 (t, *J*=7.20 Hz, 2 H, N3C$\underline{H_2}$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H_2}$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H_2}$) 4.38 (s, 2 H, OC$\underline{H_2}$CO) 6.84 (d, *J*=8.72 Hz, 2 H, Ar) 7.11 - 7.21 (m, 4 H, Ar) 7.62 - 7.69 (m, 1 H, Ar) 8.15 (t, *J*=5.64 Hz, 1 H, 1H, N$\underline{H}$CH$_2$) 8.44 - 8.48 (m, 1 H, Ar). ^{13}C NMR (DMSO d$_6$) δ: 14.06, 14.20, 19.80, 20.11, 21.22, 30.04, 30.33, 32.55, 37.53, 38.60, 41.74, 42.44, 44.68, 51.23, 67.53, 102.30, 115.12, 121.94, 123.55, 130.10, 132.18, 136.91, 148.64, 149.46, 150.91, 151.73, 152.92, 156.64, 159.48, 168.02 ppm. IR [KBr]: 3304 (N-H$_r$); 2952 (C-H); 1653 (C=O); 1612 (N-H$_d$); 1530 (C=C$_{Ar}$); 1251 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 98.1 %, t$_R$ = 5.87, (ESI) m/z 602 [M$^+$+1]. Anal. for C$_{33}$H$_{43}$N$_7$O$_4$: Calcd: C, 65.86; H, 7.20; N, 16.29. Found: C, 66.07 H, 7.03 N, 16.26.

N-(3-(1*H*-imidazol-1-yl)propyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (35)

Used amine: 3-(1H-imidazol-1-yl)propan-1-amine

Yield: 0.13 g, 21.1 % mp: 173-175 °C; 1H NMR (300 MHz, DMSO-d6) δ ppm 0.82 - 0.93 (m, 6 H, 2 x CH3CH2CH2CH2) 1.17 - 1.35 (m, 4 H, 2 x CH3CH2CH2CH2) 1.40 - 1.52 (m, 2 H, CH2CH2N3) 1.56 - 1.67 (m, 2 H, CH2CH2N1) 1.77 - 1.88 (m, 2 H, NHCH2CH2CH2N) 1.92 - 2.01 (m, 2 H, C7H2) 2.80 (t, J=7.18 Hz, 2 H, CH2C6H4) 3.07 (q, J=6.67 Hz, 2 H, NHCH2CH2CH2N) 3.24 - 3.29 (m, 2 H, N9CH2) 3.59 (t, J=7.18 Hz, 2 H, 2H, C8H2) 3.75 - 3.82 (m, 2 H, 2H, N3CH2) 3.85 - 3.94 (m, 4 H, CH2N, N1CH2) 4.00 (t, J=5.77 Hz, 2 H, N5CH2) 4.42 (s, 2 H, OCH2CO) 6.84 - 6.90 (m, 3 H, Ar) 7.10 - 7.17 (m, 3 H, Ar) 7.55 - 7.58 (m, 1 H, Ar) 8.12 (t, J=5.77 Hz, 1 H, NHCH2). 13C NMR (DMSO d6) δ ppm: 14.06, 14.20, 19.79, 20.11, 21.22, 30.03, 30.33, 31.20, 32.54, 36.05, 41,74, 42.43, 44.03, 44.68, 51.24, 67.57, 102.30, 115.14, 119.73, 128.82, 130.11, 132.21, 137.70, 148.64, 150.91, 151.73, 152.92, 156.67, 168.31. IR [KBr]: 3251 (N-Hr); 2954 (C-H); 1651, (C=O); 1614 (N-Hd); 1574 (C=CAr); 1248 (C-OAr) [cm-1]. LC-MS: purity 97.01 %, tR = 5.60, (ESI) m/z 605.64 [M++1]. Anal. for C32H44N8O4: Calcd: C, 63.55; H, 7.33; N, 18.53. Found: C, 63.26 H, 6.99 N, 18.60.

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-sulfamoylphenethyl)acetamide (37)

Used amine: 4-(2-aminoethyl)benzenesulfonamide

Yield: 0.26 g, 37.2 % mp: 217-220 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.82 - 0.93 (m, 6 H, 2 x C$\underline{H_3}$CH$_2$CH$_2$CH$_2$) 1.18 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H_2}$CH$_2$CH$_2$) 1.40 - 1.52 (m, 2 H, C$\underline{H_2}$CH$_2$N3) 1.62 (quin, *J*=7.18 Hz, 2 H, C$\underline{H_2}$CH$_2$N1) 1.93 - 2.02 (m, 2 H, C7$\underline{H_2}$) 2.77 - 2.85 (m, 4 H, 2 x C$\underline{H_2}$C$_6$H$_4$) 3.26 - 3.29 (m, 2 H, NHC$\underline{H_2}$CH$_2$C$_6$H$_4$) 3.32 - 3.41 (m, 2 H, N9C$\underline{H_2}$) 3.61 (t, *J*=7.31 Hz, 2 H, C8$\underline{H_2}$) 3.78 (t, *J*=7.20 Hz, 2 H, N3C$\underline{H_2}$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H_2}$) 4.01 (t, *J*=5.77 Hz, 2 H, N5C$\underline{H_2}$) 4.39 (s, 2 H, OC$\underline{H_2}$CO) 6.83 (d, *J*=8.72 Hz, 2 H, Ar) 7.14 (d, *J*=8.46 Hz, 2 H, Ar) 7.28 (s, 2 H, SO$_2$N$\underline{H_2}$) 7.35 (d, *J*=8.46 Hz, 2 H, Ar) 7.71 (d, *J*=8.46 Hz, 2 H, Ar) 8.14 (t, *J*=5.90 Hz, 1 H, N$\underline{H}$CH$_2$). ^{13}C NMR (DMSO d$_6$) δ ppm: 14.07, 14.20, 19.80, 20.11, 21.22, 30.03, 30.33, 32.54, 35.22, 41.73, 42.43, 44.67, 51.23, 67.54, 102.30, 115.13, 126.15, 129.54, 130.11, 132.21, 142.53, 143.96, 148.64, 150.90, 151.73, 152.92, 156.67, 168.14. IR [KBr]: 3304 (N-H$_r$); 2961 (C-H); 1655 (C=O); 1626 (N-H$_d$); 1530 (C=C$_{Ar}$); 1225 (C-O$_{Ar}$) [cm^{-1}]. LC-MS: purity 100.0 %, t$_R$ = 7.08, (ESI) m/z 680.64 [M$^+$+1]. Anal. for C$_{34}$H$_{45}$N$_7$O$_6$S: Calcd: C, 60.06; H, 6.67; N, 14.42. Found: C, 59.97 H, 7.14 N, 14.47.

N-(4-chlorobenzyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (38)

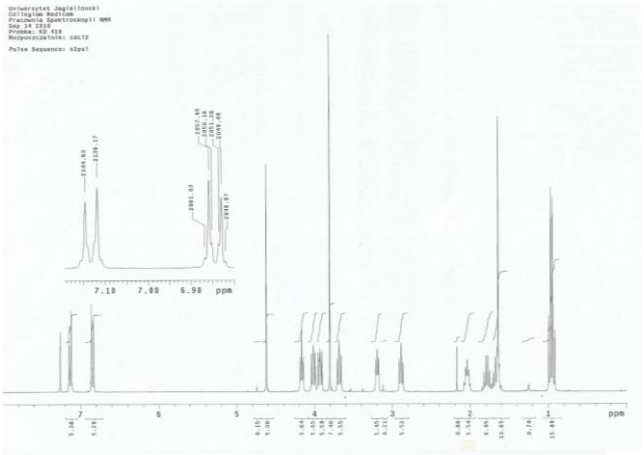
Used amine: 4-chlorobenzylamine

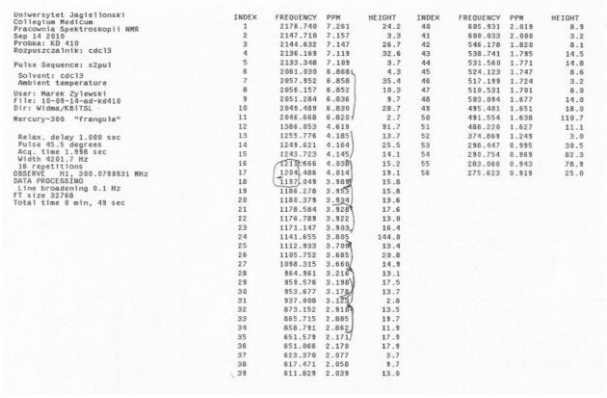
Yield: 0.28 g, 45.1% mp: 162-164 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ ppm 0.83 - 0.93 (m, 6 H, 2 x C$\underline{H_3}$CH$_2$CH$_2$CH$_2$) 1.17 - 1.35 (m, 4 H, 2 x CH$_3$C$\underline{H_2}$CH$_2$CH$_2$) 1.40 - 1.52 (m, 2 H, C$\underline{H_2}$CH$_2$N3) 1.63 (quin, *J*=7.18 Hz, 2 H, C$\underline{H_2}$CH$_2$N1) 1.92 - 2.02 (m, 2 H, C7$\underline{H_2}$) 2.77 - 2.85 (m, 2 H, C$\underline{H_2}$C$_6$H$_4$) 3.24 - 3.30 (m, 2 H, N9C$\underline{H_2}$) 3.60 (t, *J*=7.44 Hz, 2 H, C8$\underline{H_2}$) 3.79 (t, *J*=7.40 Hz, 2 H, N3C$\underline{H_2}$) 3.91 (t, *J*=7.05 Hz, 2 H, N1C$\underline{H_2}$) 4.01 (t, *J*=5.90 Hz, 2 H, N5C$\underline{H_2}$) 4.29 (d, *J*=6.16 Hz, 2 H, NHC$\underline{H_2}$) 4.48 (s, 2 H, OC$\underline{H_2}$CO) 6.87 (d, *J*=8.72

Hz, 2 H, Ar) 7.15 (d, *J*=8.46 Hz, 2 H, Ar) 7.21 - 7.26 (m, 2 H, Ar) 7.30 - 7.36 (m, 2 H, Ar) 8.63 (t, *J*=6.16 Hz, 1 H, N*H*CH_2). ^{13}C NMR (DMSO d_6) δ ppm: 14.05, 14.19, 19.80, 20.12, 21.23, 30.04, 30.34, 32.56, 41.61, 41.74, 42.43, 44.70, 51.27, 67.53, 102.31, 115.17, 128.57, 129.55, 130.08, 131.76, 132.23, 138.88, 148.64, 150.90, 151.71, 152.92, 156.64, 168.37. IR [KBr]: 3279 (N-H_r); 2954 (C-H); 1655 (C=O); 1614 (N-H_d); 1529 (C=C_{Ar}); 1246 (C-O_{Ar}) [cm^{-1}]. LC-MS: purity 98.56 %, t_R = 8.66, (ESI) m/z 621,6 [M^++1]. Anal. for $C_{33}H_{41}N_6O_4Cl$: Calcd: C, 63.80; H, 6.65; N, 13.53. Found: C, 64.19 H, 7.03 N, 13.7.

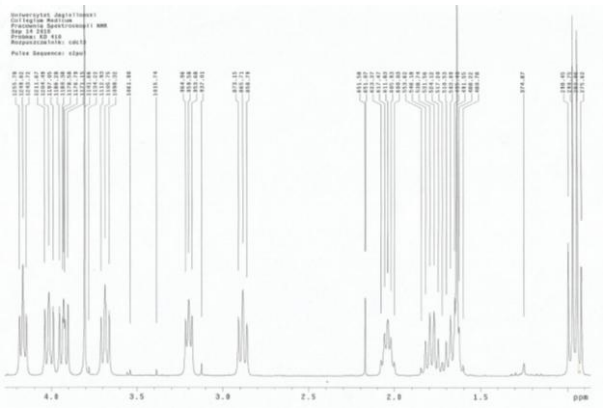
^{1}H-NMR and ^{13}C-NMR Spectra

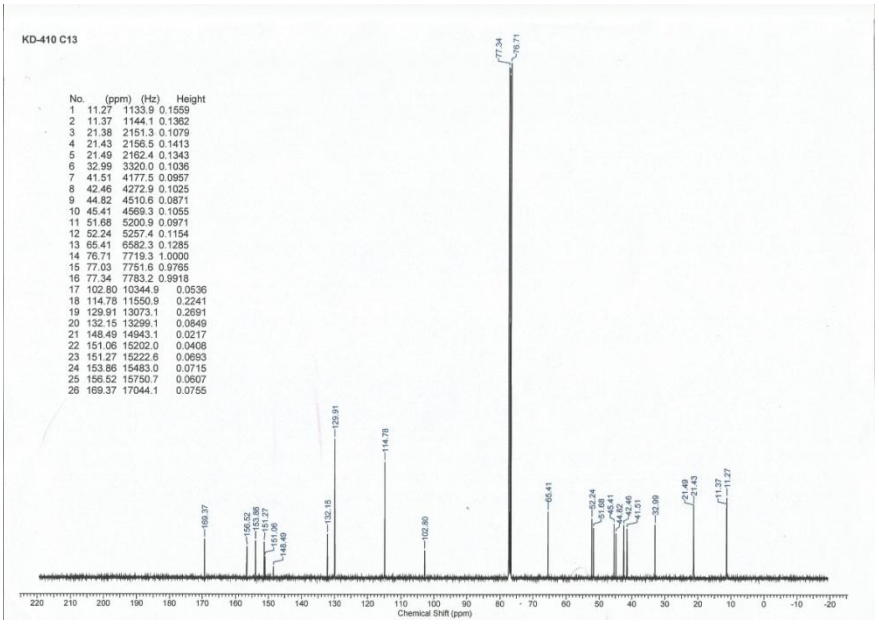
Methyl 2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (10)



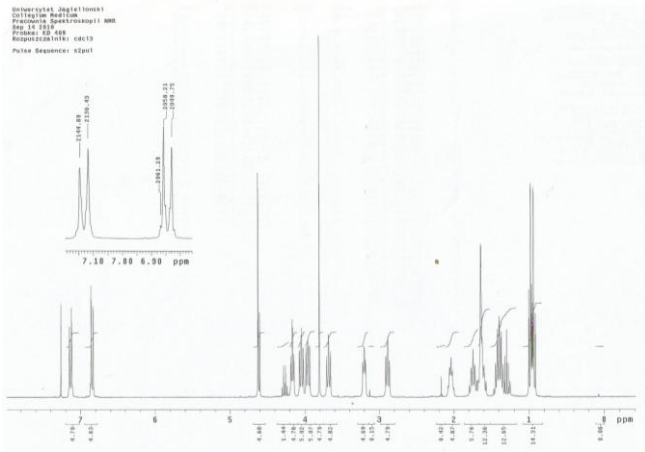


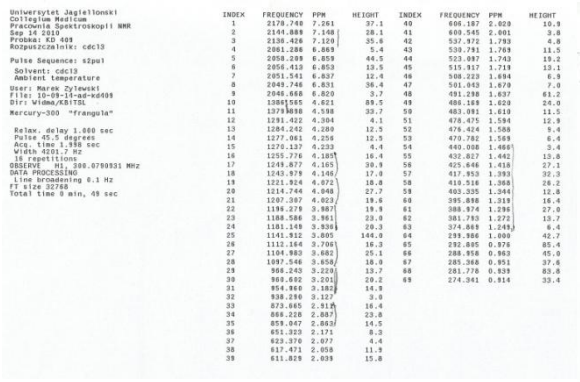
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2178.740	7.261	24.2	40	695.931	2.319	8.9
2	2167.710	7.157	3.3	41	686.833	2.886	3.2
3	2144.632	7.147	26.7	42	546.178	1.820	8.1
4	2136.169	7.119	32.6	43	538.741	1.795	14.5
5	2133.368	7.109	3.7	44	531.560	1.771	14.8
6	2061.030	6.868	4.3	45	524.123	1.747	8.6
7	2057.852	6.858	35.4	46	517.189	1.724	3.2
8	2056.157	6.852	10.3	47	510.531	1.701	8.9
9	2051.284	6.836	9.7	48	503.894	1.677	14.0
10	2049.089	6.830	28.7	49	495.401	1.651	18.0
11	2046.668	6.820	2.7	50	491.554	1.638	110.7
12	1386.053	4.619	91.7	51	488.220	1.627	11.1
13	1255.776	4.185	13.7	52	374.869	1.249	3.0
14	1249.621	4.164	25.5	53	298.447	0.995	38.5
15	1243.723	4.145	14.1	54	290.754	0.969	82.3
16	1219.666	4.065	15.2	55	283.060	0.943	78.9
17	1206.486	4.014	19.1	56	275.023	0.919	25.0
18	1197.049	3.989	15.8				
19	1186.278	3.953	15.6				
20	1180.379	3.934	19.6				
21	1178.584	3.928	17.6				
22	1176.789	3.922	19.0				
23	1171.147	3.903	18.4				
24	1141.655	3.805	144.0				
25	1112.933	3.708	19.4				
26	1105.752	3.685	20.8				
27	1098.315	3.660	14.9				
28	964.961	3.216	19.1				
29	959.576	3.198	17.5				
30	953.677	3.178	13.7				
31	937.008	3.123	2.8				
32	873.152	2.910	13.5				
33	865.715	2.885	19.7				
34	858.791	2.862	11.9				
35	851.579	2.171	17.9				
36	851.068	2.170	17.9				
37	823.370	2.077	3.7				
38	817.471	2.058	9.7				
39	811.829	2.039	13.0				



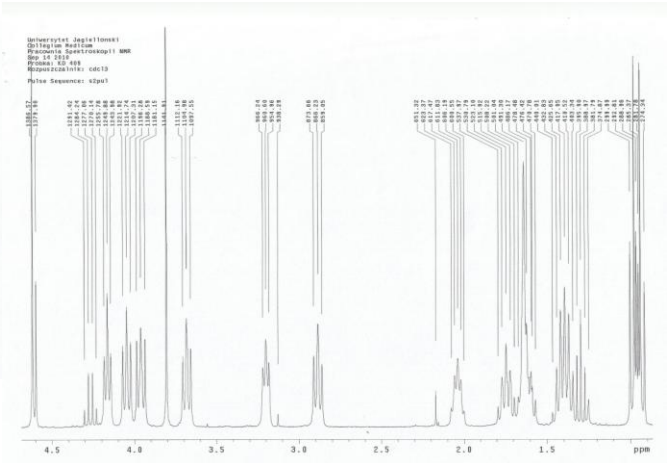


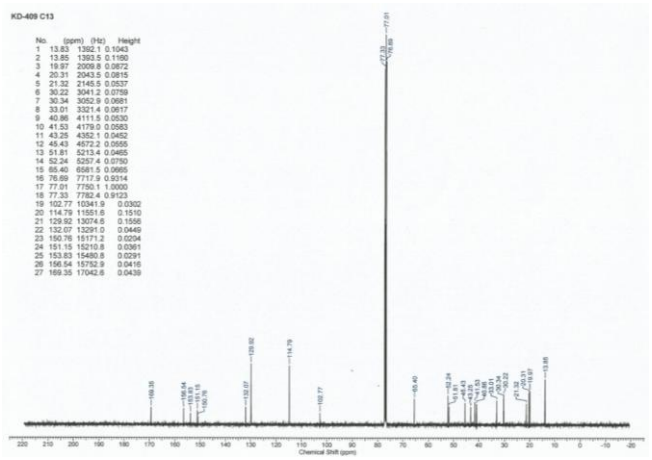
Methyl 2-(4-(2-(2,4-dioxo-1,3-dibutyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetate (11)



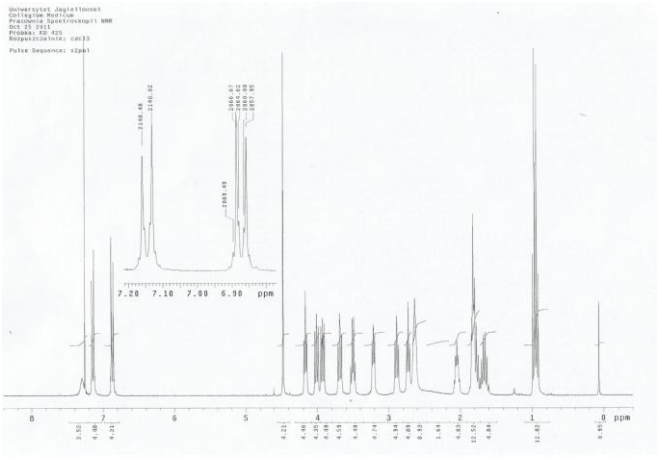


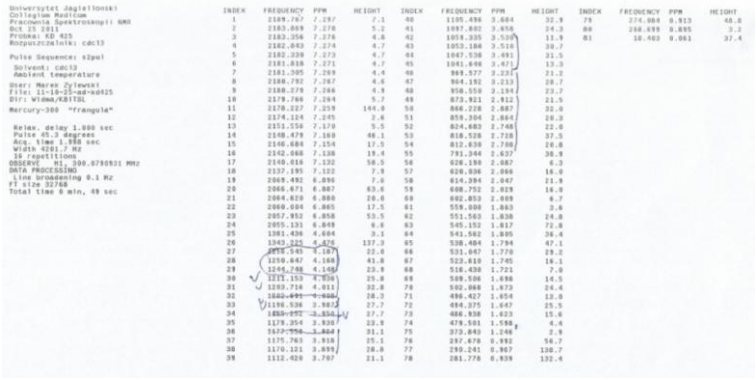
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2178.748	7.261	37.1	40	606.187	2.020	10.9
2	2144.889	7.148	28.1	41	603.545	2.001	3.8
3	2138.426	7.129	35.6	42	537.972	1.793	4.8
4	2061.286	6.869	5.4	43	530.791	1.769	11.5
5	2058.288	6.859	44.5	44	523.097	1.743	19.2
6	2056.413	6.853	13.5	45	515.917	1.719	13.1
7	2051.541	6.837	12.4	46	508.223	1.694	6.9
8	2049.746	6.831	36.4	47	501.043	1.670	7.0
9	2046.668	6.820	3.7	48	491.298	1.637	61.2
10	1384.565	4.621	89.5	49	488.168	1.628	26.0
11	1379.988	4.598	33.7	50	483.081	1.610	11.5
12	1291.422	4.304	4.1	51	478.475	1.594	12.9
13	1284.242	4.280	12.5	52	476.424	1.588	9.4
14	1277.061	4.256	12.5	53	470.782	1.569	6.4
15	1270.137	4.233	4.4	54	460.098	1.460	3.4
16	1255.776	4.185	16.4	55	432.827	1.442	13.8
17	1249.877	4.165	30.9	56	425.646	1.418	27.1
18	1243.979	4.146	17.8	57	417.953	1.393	32.3
19	1221.924	4.072	18.8	58	410.516	1.368	28.2
20	1214.744	4.048	27.7	59	403.335	1.344	12.8
21	1207.397	4.023	19.6	60	395.888	1.319	16.4
22	1196.279	3.987	19.9	61	388.974	1.296	27.0
23	1188.586	3.961	23.9	62	381.793	1.272	13.7
24	1181.149	3.936	20.3	63	374.865	1.249	6.4
25	1141.912	3.805	146.0	64	293.986	1.000	42.7
26	1112.164	3.706	16.3	65	292.805	0.976	85.4
27	1104.983	3.682	25.1	66	288.958	0.963	45.0
28	1097.546	3.658	18.9	67	285.368	0.951	37.6
29	966.243	3.220	13.7	68	281.776	0.939	83.6
30	960.692	3.201	20.2	69	274.341	0.914	33.4
31	954.860	3.182	14.9				
32	938.256	3.127	3.8				
33	873.665	2.911	16.4				
34	866.226	2.887	23.8				
35	859.047	2.863	14.5				
36	651.323	2.171	8.3				
37	623.376	2.077	4.4				
38	617.471	2.058	11.9				
39	611.829	2.039	15.8				

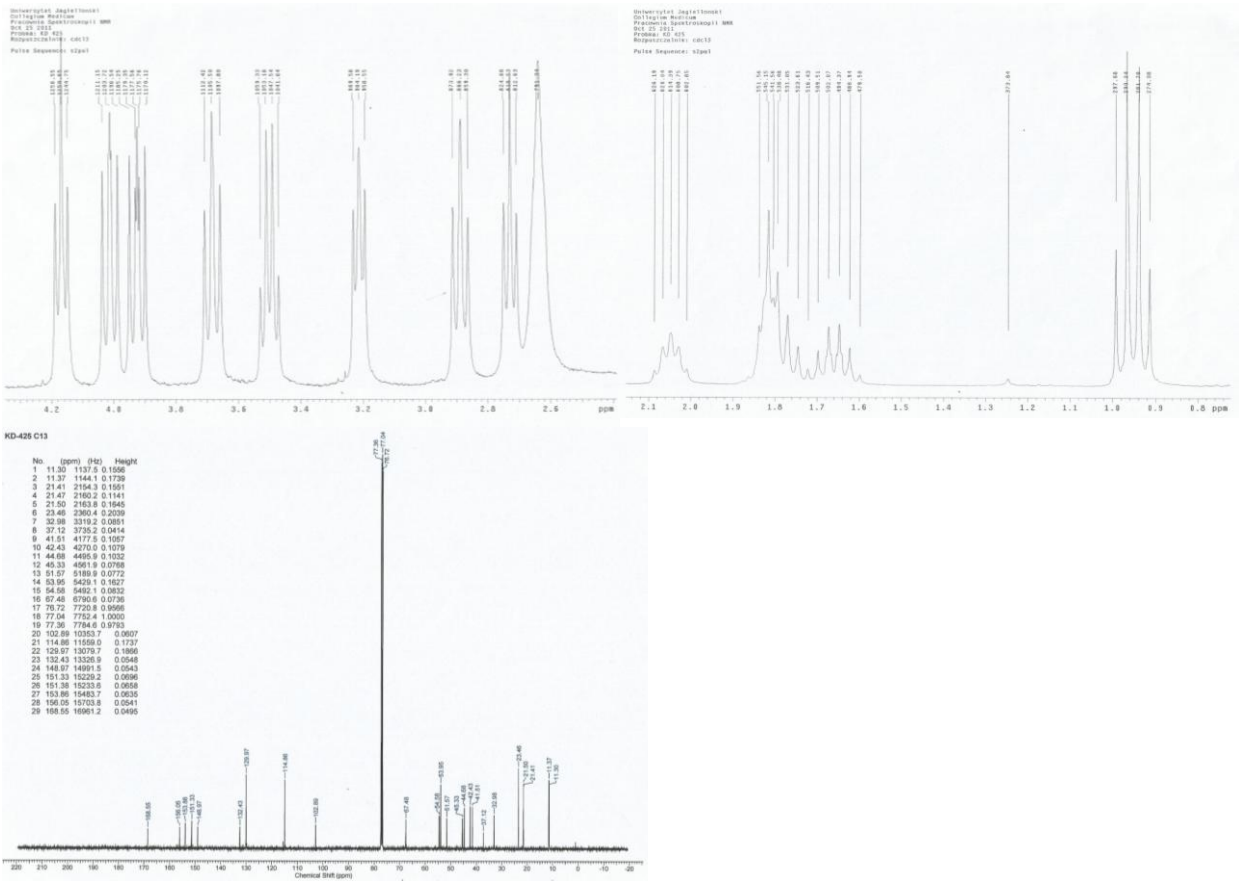




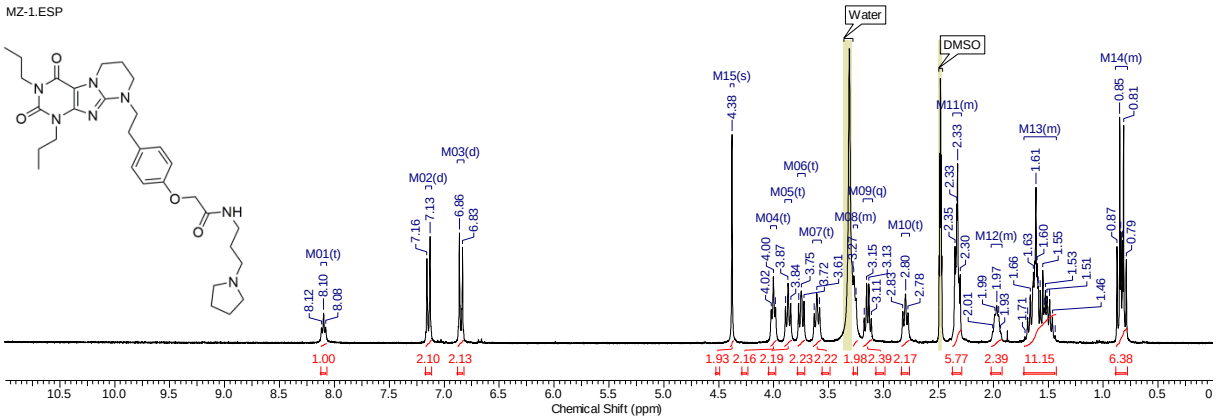
2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(pyrrolidin-1-yl)ethyl)acetamide (12)







2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-ylo)ethyl)phenoxy)-N-(3-(pyrrolidin-1-yl)propyl)acetamide (13)



No.	(ppm)	(Hz)
1	0.79	236.7
2	0.81	244.4
3	0.82	247.2
4	0.84	251.8
5	0.85	254.9
6	0.87	262.3
7	1.44	431.3
8	1.46	438.8
9	1.49	446.5
10	1.51	453.7
11	1.53	458.0

No.	(ppm)	(Hz)
12	1.54	460.8
13	1.55	464.9
14	1.57	471.9
15	1.59	477.2
16	1.60	480.1
17	1.61	483.7
18	1.63	490.3
19	1.66	499.0
20	1.69	506.2
21	1.71	513.7
22	1.93	580.1

No.	(ppm)	(Hz)
23	1.95	585.2
24	1.97	590.9
25	1.99	595.7
26	2.01	602.1
27	2.30	690.9
28	2.33	697.8
29	2.33	699.9
30	2.35	705.0
31	2.78	833.0
32	2.80	839.9
33	2.83	847.8

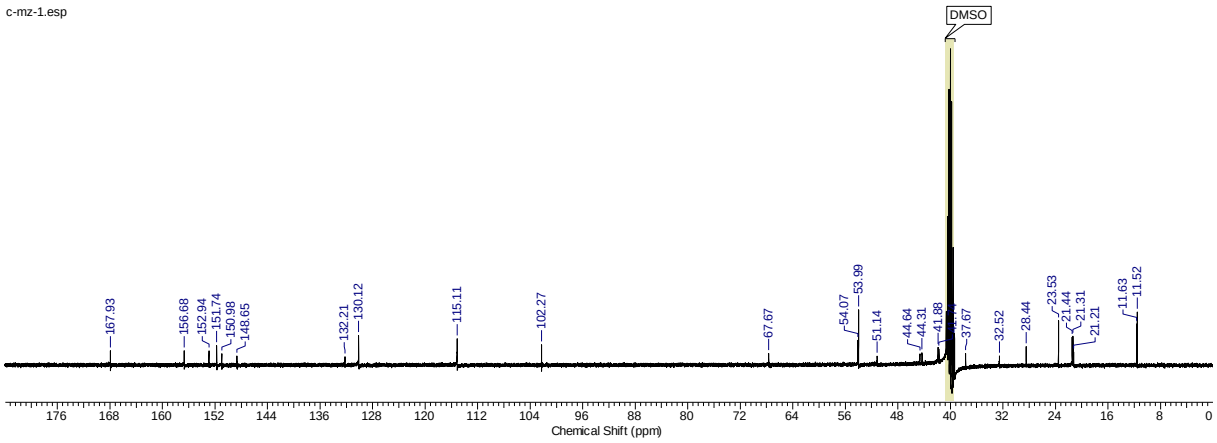
No.	(ppm)	(Hz)
34	3.11	933.8
35	3.13	940.4
36	3.15	946.3
37	3.18	953.0
38	3.25	975.0
39	3.27	981.2
40	3.58	1074.8
41	3.61	1082.3
42	3.63	1089.7
43	3.72	1117.6
44	3.75	1124.8

No.	(ppm)	(Hz)
45	3.77	1132.3
46	3.84	1153.8
47	3.87	1161.2
48	3.89	1167.9
49	3.98	1195.6
50	4.00	1201.3
51	4.02	1206.9
52	4.38	1314.4
53	6.83	2050.7
54	6.86	2059.4
55	7.13	2139.4

No.	(ppm)	(Hz)
56	7.16	2148.1
57	8.08	2424.6
58	8.10	2430.0
59	8.12	2435.6

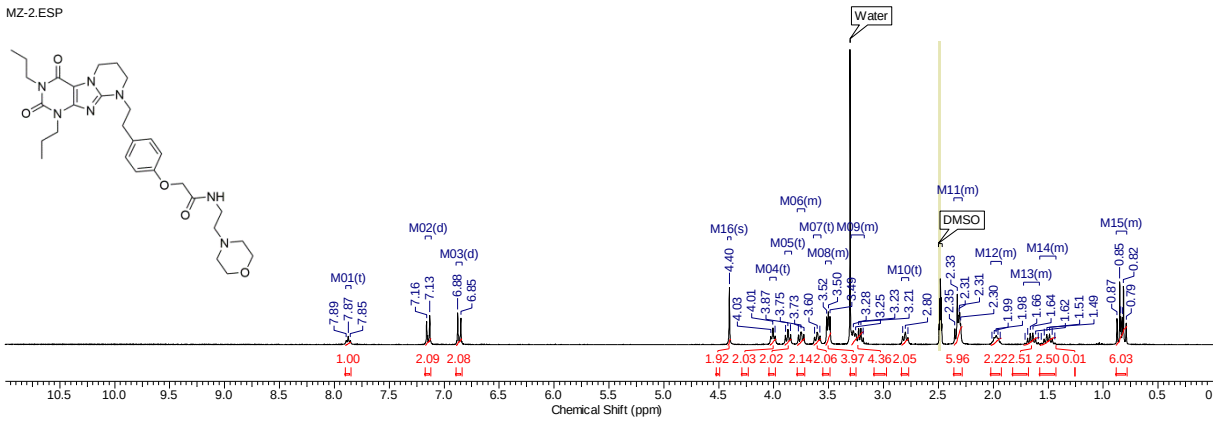
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M14	[0.78 .. 0.89]
2	1.57	10	m	-	M13	[1.43 .. 1.72]
3	1.97	2	m	-	M12	[1.92 .. 2.02]
4	2.33	6	m	-	M11	[2.29 .. 2.37]
5	2.80	2	t	7.44	M10	[2.76 .. 2.84]
6	3.14	2	q	6.67	M09	[3.10 .. 3.19]
7	3.26	2	m	-	M08	[3.24 .. 3.28]
8	3.61	2	t	7.44	M07	[3.57 .. 3.64]
9	3.75	2	t	7.40	M06	[3.71 .. 3.78]
10	3.87	2	t	7.05	M05	[3.84 .. 3.90]
11	4.00	2	t	5.64	M04	[3.97 .. 4.03]
12	4.38	2	s	-	M15	[4.36 .. 4.40]
13	6.85	2	d	8.72	M03	[6.82 .. 6.88]
14	7.14	2	d	8.72	M02	[7.12 .. 7.17]
15	8.10	1	t	5.51	M01	[8.07 .. 8.12]

^{1}H NMR (300 MHz, DMSO-d_6) ppm 0.78 - 0.89 (m, 6 H) 1.43 - 1.72 (m, 10 H) 1.92 - 2.02 (m, 2 H) 2.29 - 2.37 (m, 6 H) 2.80 (t, *J*=7.44 Hz, 2 H) 3.14 (q, *J*=6.67 Hz, 2 H) 3.24 - 3.28 (m, 2 H) 3.61 (t, *J*=7.44 Hz, 2 H) 3.75 (t, *J*=7.40 Hz, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.00 (t, *J*=5.64 Hz, 2 H) 4.38 (s, 2 H) 6.85 (d, *J*=8.72 Hz, 2 H) 7.14 (d, *J*=8.72 Hz, 2 H) 8.10 (t, *J*=5.51 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	11.52	1159.5	5	21.44	2157.2	9	37.67	3790.9	13	44.64	4492.3	17	67.67	6809.7	21	132.21	13304.9	25	152.94	15390.5
2	11.63	1170.5	6	23.53	2367.8	10	41.74	4200.3	14	51.14	5146.6	18	102.27	10291.3	22	148.65	14959.2	26	156.68	15767.6
3	21.21	2134.5	7	28.44	2862.2	11	41.88	4215.0	15	53.99	5433.5	19	115.11	11583.9	23	150.98	15193.2	27	167.93	16898.8
4	21.31	2144.7	8	32.52	3273.0	12	44.31	4459.2	16	54.07	5441.5	20	130.12	13094.4	24	151.74	15270.2			

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-ylo)ethyl)phenoxy)-N-(2-morpholinoethyl)acetamide (14)



No.	(ppm)	(Hz)
1	0.79	236.9
2	0.82	244.6
3	0.82	247.2
4	0.84	251.8
5	0.85	254.9
6	0.87	262.1
7	1.44	431.9
8	1.46	439.3
9	1.49	446.7
10	1.51	453.9
11	1.54	461.3

No.	(ppm)	(Hz)
12	1.56	469.0
13	1.59	477.8
14	1.62	484.9
15	1.64	492.1
16	1.66	499.3
17	1.69	506.5
18	1.71	513.4
19	1.94	581.4
20	1.96	587.5
21	1.98	592.9
22	1.99	597.8

No.	(ppm)	(Hz)
23	2.01	603.7
24	2.30	689.6
25	2.31	692.2
26	2.31	694.0
27	2.33	698.8
28	2.35	705.5
29	2.78	833.7
30	2.80	840.4
31	2.83	848.1
32	3.18	955.6
33	3.21	962.2

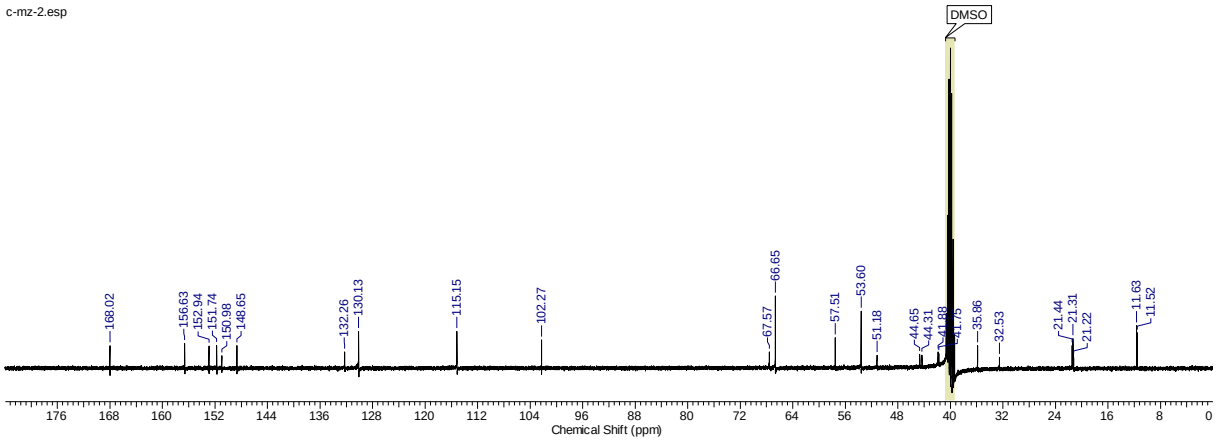
No.	(ppm)	(Hz)
34	3.23	968.1
35	3.25	976.6
36	3.28	983.0
37	3.49	1046.3
38	3.50	1051.0
39	3.52	1055.6
40	3.58	1073.8
41	3.60	1081.5
42	3.63	1088.4
43	3.73	1117.9
44	3.75	1125.3

No.	(ppm)	(Hz)
45	3.77	1132.8
46	3.85	1154.1
47	3.87	1161.5
48	3.89	1168.2
49	3.99	1196.4
50	4.01	1202.5
51	4.03	1208.2
52	4.40	1321.3
53	6.85	2055.3
54	6.88	2063.7
55	7.13	2140.2

No.	(ppm)	(Hz)
56	7.16	2148.9
57	7.85	2357.1
58	7.87	2362.8
59	7.89	2368.2

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M15	[0.78 .. 0.88]
2	1.50	2	m	-	M14	[1.43 .. 1.58]
3	1.65	2	m	-	M13	[1.58 .. 1.72]
4	1.97	2	m	-	M12	[1.93 .. 2.02]
5	2.32	6	m	-	M11	[2.29 .. 2.36]
6	2.80	2	t	7.18	M10	[2.77 .. 2.84]
7	3.23	4	m	-	M09	[3.17 .. 3.30]
8	3.50	4	m	-	M08	[3.48 .. 3.53]
9	3.60	2	t	7.31	M07	[3.57 .. 3.64]
10	3.75	2	m	-	M06	[3.72 .. 3.78]
11	3.87	2	t	7.05	M05	[3.84 .. 3.90]
12	4.01	2	t	5.90	M04	[3.98 .. 4.04]
13	4.40	2	s	-	M16	[4.39 .. 4.42]
14	6.86	2	d	8.46	M03	[6.84 .. 6.89]
15	7.15	2	d	8.72	M02	[7.12 .. 7.17]
16	7.87	1	t	5.51	M01	[7.85 .. 7.90]

^{1}H NMR (300 MHz, DMSO-d_6) ? ppm 0.78 - 0.88 (m, 6 H) 1.43 - 1.58 (m, 2 H) 1.58 - 1.72 (m, 2 H) 1.93 - 2.02 (m, 2 H) 2.29 - 2.36 (m, 6 H) 2.80 (t, *J*=7.18 Hz, 2 H) 3.17 - 3.30 (m, 4 H) 3.48 - 3.53 (m, 4 H) 3.60 (t, *J*=7.31 Hz, 2 H) 3.72 - 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.40 (s, 2 H) 6.86 (d, *J*=8.46 Hz, 2 H) 7.15 (d, *J*=8.72 Hz, 2 H) 7.87 (t, *J*=5.51 Hz, 1 H)



No.	(ppm)	(Hz)
1	11.52	1159.5
2	11.63	1170.5
3	21.22	2135.2
4	21.31	2144.7

No.	(ppm)	(Hz)
5	21.44	2157.2
6	32.53	3273.7
7	35.86	3608.3
8	41.75	4201.0

No.	(ppm)	(Hz)
9	41.88	4215.0
10	44.31	4459.2
11	44.65	4493.7
12	51.18	5150.3

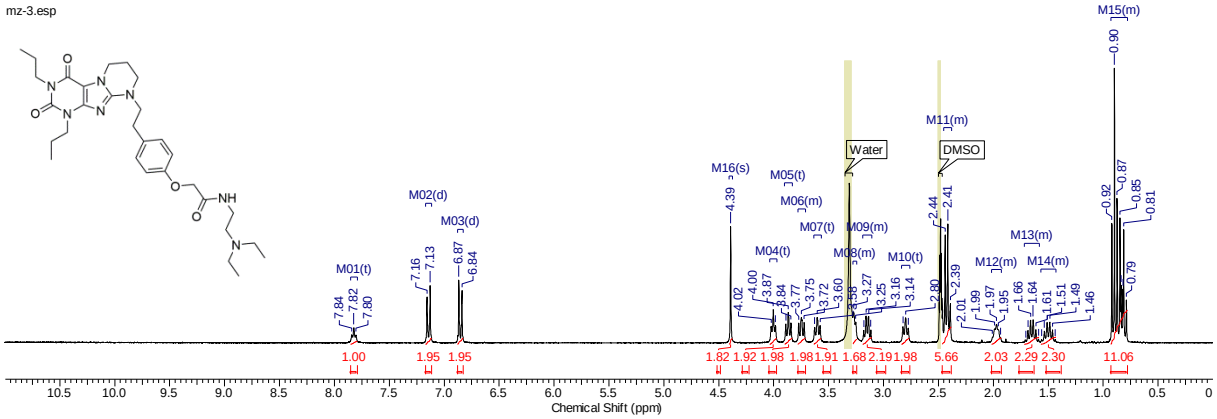
No.	(ppm)	(Hz)
13	53.60	5393.8
14	57.51	5787.8
15	66.65	6707.0
16	67.57	6800.1

No.	(ppm)	(Hz)
17	102.27	10292.1
18	115.15	11587.6
19	130.13	13095.1
20	132.26	13309.3

No.	(ppm)	(Hz)
21	148.65	14959.2
22	150.98	15193.2
23	151.74	15270.2
24	152.94	15390.5

No.	(ppm)	(Hz)
25	156.63	15761.7
26	168.02	16908.4

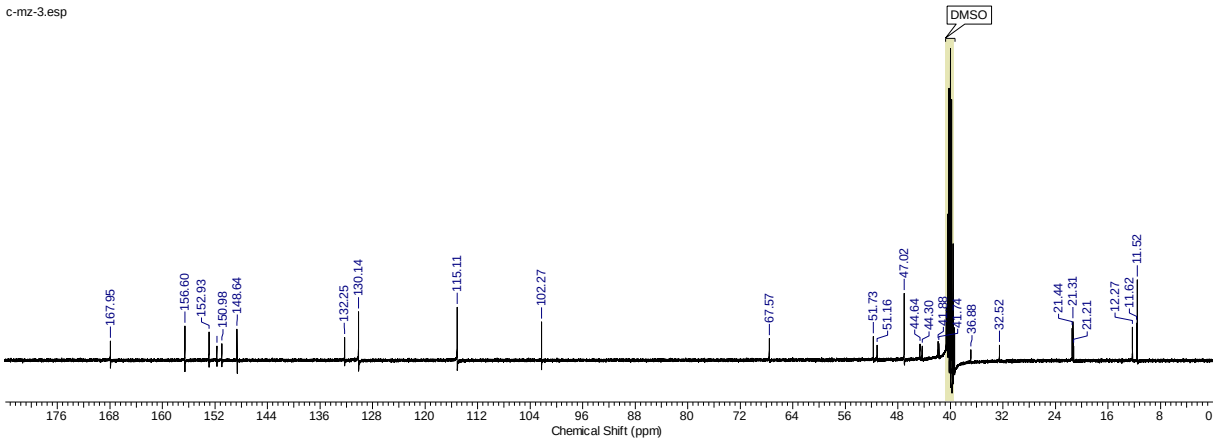
N-(2-(diethylamino)ethyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (15)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	0.79	236.4	11	1.49	446.0	21	1.93	580.3	31	2.82	847.1	41	3.72	1117.1	51	6.84	2051.9
2	0.81	243.9	12	1.51	453.1	22	1.95	586.2	32	3.12	935.0	42	3.75	1124.6	52	6.87	2060.7
3	0.82	246.4	13	1.53	460.6	23	1.97	591.4	33	3.14	940.9	43	3.77	1131.7	53	7.13	2139.1
4	0.84	251.3	14	1.56	468.0	24	1.99	596.8	34	3.16	948.1	44	3.84	1153.0	54	7.16	2147.6
5	0.85	254.1	15	1.59	476.7	25	2.01	602.7	35	3.18	954.3	45	3.87	1160.7	55	7.80	2341.8
6	0.87	262.1	16	1.61	483.9	26	2.39	717.6	36	3.25	976.1	46	3.89	1167.1	56	7.82	2347.7
7	0.90	269.3	17	1.64	491.4	27	2.41	724.5	37	3.27	981.7	47	3.98	1195.6	57	7.84	2353.0
8	0.92	276.4	18	1.66	498.3	28	2.44	731.7	38	3.58	1073.5	48	4.00	1201.5			
9	1.44	431.3	19	1.68	505.5	29	2.77	832.5	39	3.60	1081.5	49	4.02	1207.4			
10	1.46	438.5	20	1.70	511.6	30	2.80	839.6	40	3.63	1088.2	50	4.39	1317.9			

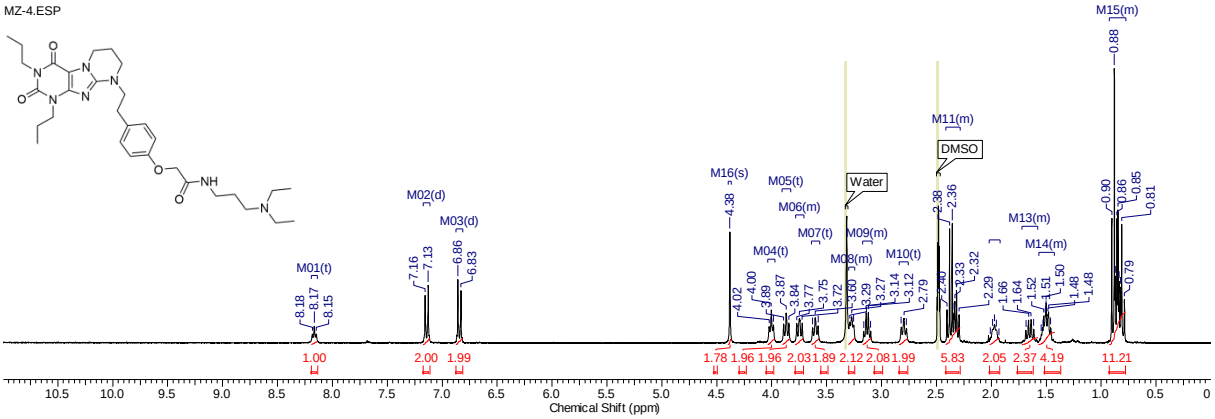
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.85	12	m	-	M15	[0.78 .. 0.93]
2	1.50	2	m	-	M14	[1.43 .. 1.57]
3	1.65	2	m	-	M13	[1.58 .. 1.72]
4	1.97	2	m	-	M12	[1.93 .. 2.01]
5	2.41	6	m	-	M11	[2.38 .. 2.45]
6	2.80	2	t	7.31	M10	[2.76 .. 2.84]
7	3.15	2	m	-	M09	[3.11 .. 3.19]
8	3.26	2	m	-	M08	[3.24 .. 3.28]
9	3.60	2	t	7.31	M07	[3.57 .. 3.63]
10	3.75	2	m	-	M06	[3.71 .. 3.78]
11	3.87	2	t	7.05	M05	[3.83 .. 3.90]
12	4.00	2	t	5.90	M04	[3.97 .. 4.04]
13	4.39	2	s	-	M16	[4.38 .. 4.41]
14	6.85	2	d	8.72	M03	[6.83 .. 6.88]
15	7.14	2	d	8.46	M02	[7.11 .. 7.17]
16	7.82	1	t	5.64	M01	[7.79 .. 7.85]

^{1}H NMR (300 MHz, DMSO-d_6) ? ppm 0.78 - 0.93 (m, 12 H) 1.43 - 1.57 (m, 2 H) 1.58 - 1.72 (m, 2 H) 1.93 - 2.01 (m, 2 H) 2.38 - 2.45 (m, 6 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.11 - 3.19 (m, 2 H) 3.24 - 3.28 (m, 2 H) 3.60 (t, *J*=7.31 Hz, 2 H) 3.71 - 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.00 (t, *J*=5.90 Hz, 2 H) 4.39 (s, 2 H) 6.85 (d, *J*=8.72 Hz, 2 H) 7.14 (d, *J*=8.46 Hz, 2 H) 7.82 (t, *J*=5.64 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	11.52	1158.8	5	21.31	2144.7	9	41.74	4200.3	13	47.02	4732.1	17	102.27	10291.3	21	148.64	14958.5	25	156.60	15758.8
2	11.62	1169.8	6	21.44	2157.2	10	41.88	4214.2	14	51.16	5148.1	18	115.11	11583.9	22	150.98	15193.2	26	167.95	16901.0
3	12.27	1234.4	7	32.52	3273.0	11	44.30	4457.8	15	51.73	5205.3	19	130.14	13095.9	23	151.73	15269.5			
4	21.21	2134.5	8	36.88	3711.0	12	44.64	4492.3	16	67.57	6800.1	20	132.25	13308.6	24	152.93	15389.8			

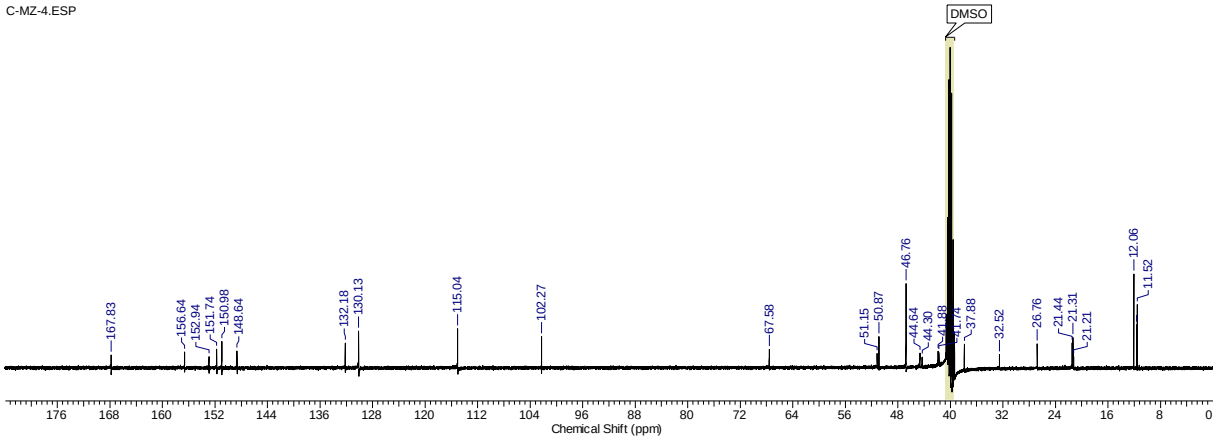
N-(3-(diethylamino)propyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (16)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	0.79	236.4	12	1.48	445.4	23	1.96	587.0	34	2.77	831.9	45	3.60	1081.5	56	4.38	1314.6
2	0.81	243.9	13	1.50	450.3	24	1.97	591.6	35	2.79	838.6	46	3.63	1088.2	57	6.83	2049.4
3	0.82	246.7	14	1.51	452.6	25	1.99	597.0	36	2.82	846.6	47	3.72	1117.1	58	6.86	2057.8
4	0.84	251.3	15	1.52	457.0	26	2.01	602.9	37	3.10	929.9	48	3.75	1124.6	59	7.13	2138.9
5	0.85	254.1	16	1.53	459.3	27	2.29	688.3	38	3.12	936.6	49	3.77	1131.7	60	7.16	2147.6
6	0.86	256.9	17	1.55	463.7	28	2.32	695.2	39	3.14	942.2	50	3.84	1153.3	61	8.15	2444.9
7	0.87	261.6	18	1.61	484.2	29	2.33	699.9	40	3.16	948.9	51	3.87	1160.7	62	8.17	2450.2
8	0.88	264.1	19	1.64	491.6	30	2.34	701.9	41	3.25	976.1	52	3.89	1167.4	63	8.18	2455.4
9	0.90	271.1	20	1.66	498.3	31	2.36	707.0	42	3.27	982.0	53	3.98	1195.6			
10	1.46	438.0	21	1.69	505.7	32	2.38	714.2	43	3.29	986.8	54	4.00	1201.5			
11	1.48	443.7	22	1.93	579.3	33	2.40	721.4	44	3.58	1073.5	55	4.02	1207.2			

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.85	12	m	-	M15	[0.78 .. 0.93]
2	1.50	4	m	-	M14	[1.43 .. 1.57]
3	1.65	2	m	-	M13	[1.58 .. 1.72]
4	1.97	2	m	-	M12	[1.92 .. 2.02]
5	2.35	6	m	-	M11	[2.28 .. 2.41]
6	2.80	2	t	7.31	M10	[2.76 .. 2.84]
7	3.13	2	m	-	M09	[3.09 .. 3.17]
8	3.27	2	m	-	M08	[3.25 .. 3.30]
9	3.60	2	t	7.31	M07	[3.56 .. 3.64]
10	3.75	2	m	-	M06	[3.71 .. 3.78]
11	3.87	2	t	7.05	M05	[3.83 .. 3.91]
12	4.00	2	t	5.77	M04	[3.97 .. 4.03]
13	4.38	2	s	-	M16	[4.37 .. 4.39]
14	6.84	2	d	8.46	M03	[6.81 .. 6.87]
15	7.14	2	d	8.72	M02	[7.11 .. 7.17]
16	8.16	1	t	5.26	M01	[8.14 .. 8.19]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.78 - 0.93 (m, 12 H) 1.43 - 1.57 (m, 4 H) 1.58 - 1.72 (m, 2 H) 1.92 - 2.02 (m, 2 H) 2.28 - 2.41 (m, 6 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.09 - 3.17 (m, 2 H) 3.25 - 3.30 (m, 2 H) 3.60 (t, *J*=7.31 Hz, 2 H) 3.71 - 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.00 (t, *J*=5.77 Hz, 2 H) 4.38 (s, 2 H) 6.84 (d, *J*=8.46 Hz, 2 H) 7.14 (d, *J*=8.72 Hz, 2 H) 8.16 (t, *J*=5.26 Hz, 1 H)



No.	(ppm)	(Hz)
1	11.52	1158.8
2	11.63	1170.5
3	12.06	1213.8
4	21.21	2134.5

No.	(ppm)	(Hz)
5	21.31	2144.7
6	21.44	2157.2
7	26.76	2692.7
8	32.52	3273.0

No.	(ppm)	(Hz)
9	37.88	3812.2
10	41.74	4200.3
11	41.88	4214.2
12	44.30	4458.5

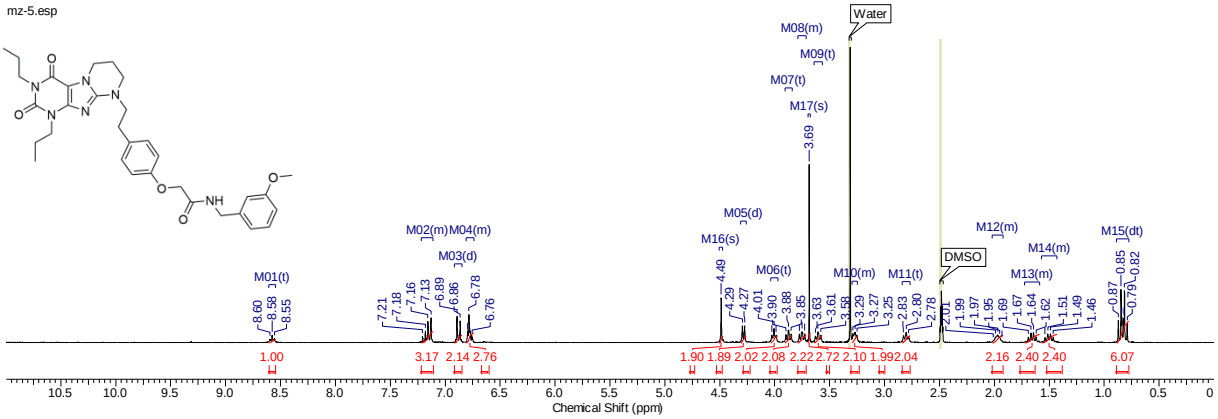
No.	(ppm)	(Hz)
13	44.64	4492.3
14	46.76	4705.7
15	50.87	5119.5
16	51.15	5147.4

No.	(ppm)	(Hz)
17	67.58	6800.9
18	102.27	10291.3
19	115.04	11576.6
20	130.13	13095.1

No.	(ppm)	(Hz)
21	132.18	13301.3
22	148.64	14958.5
23	150.98	15193.2
24	151.74	15270.2

No.	(ppm)	(Hz)
25	152.94	15390.5
26	156.64	15763.2
27	167.83	16889.3

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(3-methoxybenzyl)acetamide (17)



No.	(ppm)	(Hz)
1	0.79	236.9
2	0.82	244.6
3	0.82	246.4
4	0.84	251.8
5	0.85	254.1
6	0.87	261.3
7	1.46	439.3
8	1.49	446.7
9	1.51	453.9
10	1.54	461.6

No.	(ppm)	(Hz)
11	1.62	485.7
12	1.64	493.1
13	1.67	500.1
14	1.69	507.3
15	1.93	579.3
16	1.95	585.7
17	1.97	591.1
18	1.99	596.5
19	2.01	602.7
20	2.78	834.0

No.	(ppm)	(Hz)
21	2.80	840.7
22	2.83	848.6
23	3.25	975.8
24	3.27	980.7
25	3.29	986.6
26	3.58	1074.0
27	3.61	1082.0
28	3.63	1088.9
29	3.69	1106.1
30	3.73	1118.2

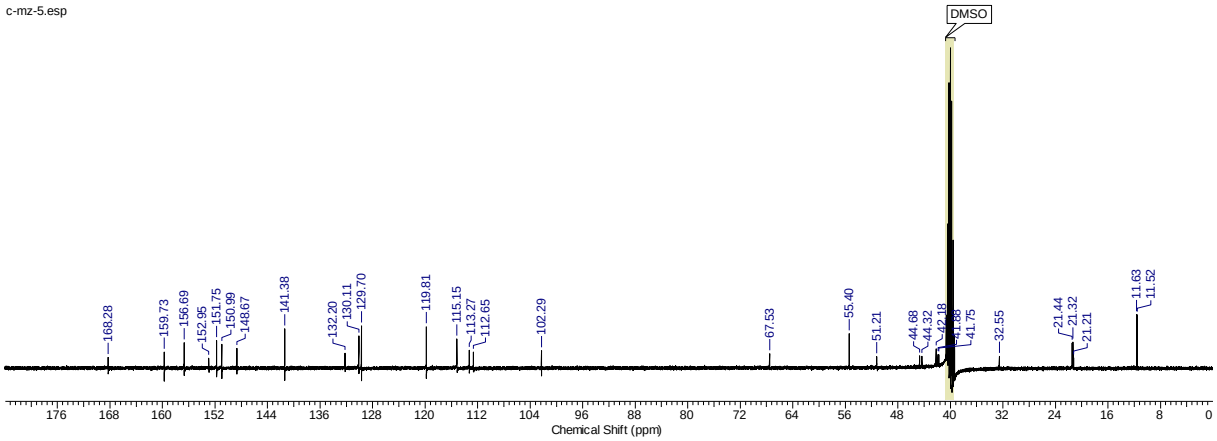
No.	(ppm)	(Hz)
31	3.75	1125.6
32	3.78	1133.0
33	3.85	1155.3
34	3.88	1163.0
35	3.90	1169.5
36	3.99	1196.4
37	4.01	1202.3
38	4.03	1208.2
39	4.27	1282.6
40	4.29	1288.7

No.	(ppm)	(Hz)
41	4.49	1346.4
42	6.76	2027.3
43	6.78	2036.0
44	6.80	2039.4
45	6.86	2059.6
46	6.89	2068.4
47	7.13	2139.4
48	7.16	2148.1
49	7.18	2154.8
50	7.21	2162.7

No.	(ppm)	(Hz)
51	8.55	2567.2
52	8.58	2573.6
53	8.60	2579.8

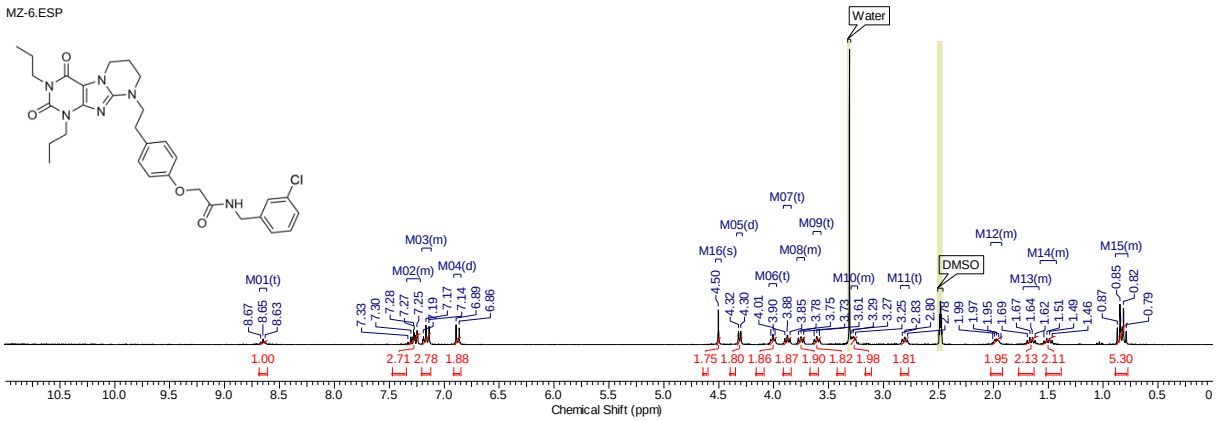
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	dt	9.49, 7.44	M15	[0.77 .. 0.89]
2	1.50	2	m	-	M14	[1.43 .. 1.57]
3	1.65	2	m	-	M13	[1.59 .. 1.73]
4	1.97	2	m	-	M12	[1.92 .. 2.02]
5	2.80	2	t	7.31	M11	[2.77 .. 2.84]
6	3.27	2	m	-	M10	[3.25 .. 3.30]
7	3.60	2	t	7.44	M09	[3.57 .. 3.64]
8	3.69	3	s	-	M17	[3.68 .. 3.70]
9	3.75	2	m	-	M08	[3.71 .. 3.79]
10	3.87	2	t	7.05	M07	[3.84 .. 3.91]
11	4.01	2	t	5.90	M06	[3.97 .. 4.03]
12	4.28	2	d	6.16	M05	[4.26 .. 4.31]
13	4.49	2	s	-	M16	[4.47 .. 4.51]
14	6.78	3	m	-	M04	[6.74 .. 6.81]
15	6.88	2	d	8.72	M03	[6.85 .. 6.92]
16	7.17	3	m	-	M02	[7.11 .. 7.22]
17	8.58	1	t	6.28	M01	[8.55 .. 8.60]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.83 (dt, *J*=9.49, 7.44 Hz, 6 H) 1.43 - 1.57 (m, 2 H) 1.59 - 1.73 (m, 2 H) 1.92 - 2.02 (m, 2 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.25 - 3.30 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.69 (s, 3 H) 3.71 - 3.79 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.28 (d, *J*=6.16 Hz, 2 H) 4.49 (s, 2 H) 6.74 - 6.81 (m, 3 H) 6.88 (d, *J*=8.72 Hz, 2 H) 7.11 - 7.22 (m, 3 H) 8.58 (t, *J*=6.28 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	11.52	1159.5	6	32.55	3275.2	11	44.68	4496.7	16	112.65	11336.0	21	130.11	13092.9	26	151.75	15271.0
2	11.63	1170.5	7	41.75	4201.0	12	51.21	5153.2	17	113.27	11398.3	22	132.20	13303.5	27	152.95	15392.0
3	21.21	2134.5	8	41.88	4215.0	13	55.40	5575.0	18	115.15	11588.3	23	141.38	14227.1	28	156.69	15768.4
4	21.32	2145.5	9	42.18	4245.0	14	67.53	6795.7	19	119.81	12057.1	24	148.67	14960.7	29	159.73	16074.3
5	21.44	2158.0	10	44.32	4460.0	15	102.29	10293.5	20	129.70	13051.8	25	150.99	15194.7	30	168.28	16934.0

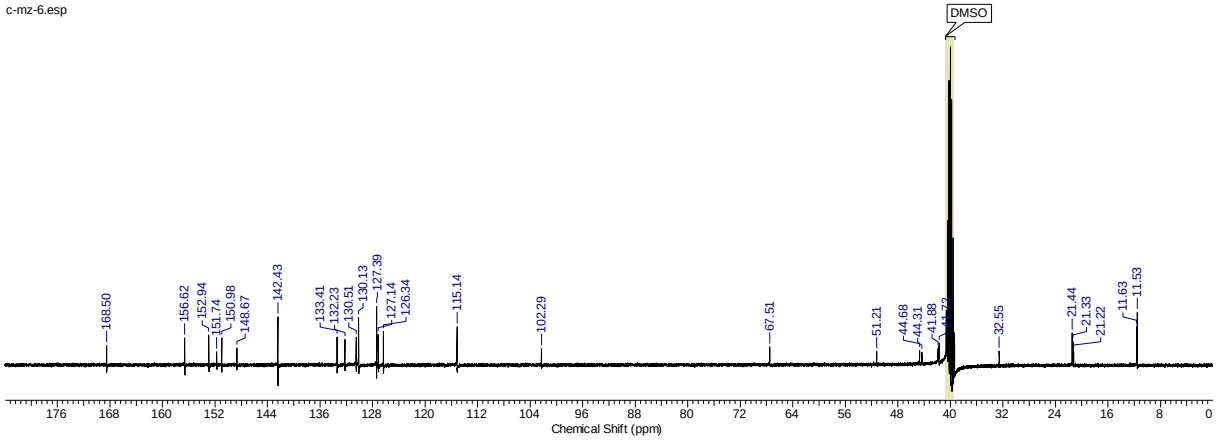
N-(3-chlorobenzyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (18)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	0.79	236.9	10	1.62	486.0	19	2.78	834.8	28	3.73	1118.4	37	4.30	1290.2	46	7.27	2182.2
2	0.82	244.6	11	1.64	493.4	20	2.80	841.7	29	3.75	1125.9	38	4.32	1296.4	47	7.28	2184.3
3	0.84	252.1	12	1.67	500.3	21	2.83	849.4	30	3.78	1133.0	39	4.50	1351.5	48	7.30	2191.5
4	0.85	254.1	13	1.69	507.5	22	3.25	976.6	31	3.85	1155.9	40	6.86	2059.6	49	7.33	2199.9
5	0.87	261.6	14	1.93	579.6	23	3.27	982.2	32	3.88	1163.3	41	6.89	2068.4	50	8.63	2589.5
6	1.46	439.5	15	1.95	585.7	24	3.29	987.1	33	3.90	1170.0	42	7.14	2142.0	51	8.65	2595.7
7	1.49	447.0	16	1.97	591.4	25	3.58	1074.8	34	3.99	1196.6	43	7.17	2150.7	52	8.67	2602.1
8	1.51	454.2	17	1.99	596.5	26	3.61	1082.5	35	4.01	1202.3	44	7.19	2157.4			
9	1.54	461.6	18	2.01	602.1	27	3.63	1089.4	36	4.03	1208.2	45	7.25	2174.8			

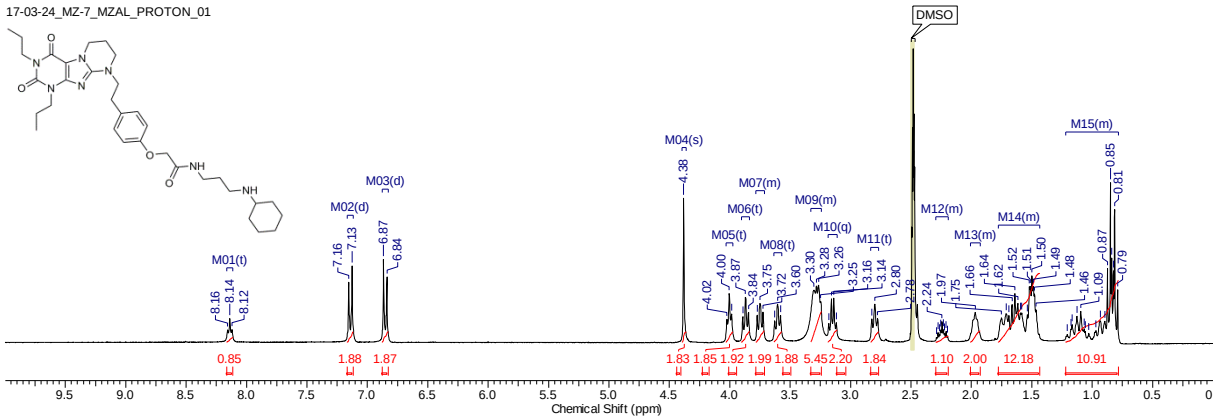
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M15	[0.78 .. 0.89]
2	1.50	2	m	-	M14	[1.43 .. 1.57]
3	1.66	2	m	-	M13	[1.59 .. 1.73]
4	1.97	2	m	-	M12	[1.92 .. 2.02]
5	2.81	2	t	7.31	M11	[2.77 .. 2.85]
6	3.27	2	m	-	M10	[3.24 .. 3.30]
7	3.61	2	t	7.31	M09	[3.57 .. 3.64]
8	3.75	2	m	-	M08	[3.72 .. 3.79]
9	3.88	2	t	7.05	M07	[3.84 .. 3.91]
10	4.01	2	t	5.77	M06	[3.98 .. 4.04]
11	4.31	2	d	6.16	M05	[4.29 .. 4.34]
12	4.50	2	s	-	M16	[4.48 .. 4.53]
13	6.88	2	d	8.72	M04	[6.85 .. 6.91]
14	7.16	3	m	-	M03	[7.12 .. 7.20]
15	7.29	3	m	-	M02	[7.22 .. 7.34]
16	8.65	1	t	6.28	M01	[8.62 .. 8.68]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.78 - 0.89 (m, 6 H) 1.43 - 1.57 (m, 2 H) 1.59 - 1.73 (m, 2 H) 1.92 - 2.02 (m, 2 H) 2.81 (t, *J*=7.31 Hz, 2 H) 3.24 - 3.30 (m, 2 H) 3.61 (t, *J*=7.31 Hz, 2 H) 3.72 - 3.79 (m, 2 H) 3.88 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.31 (d, *J*=6.16 Hz, 2 H) 4.50 (s, 2 H) 6.88 (d, *J*=8.72 Hz, 2 H) 7.12 - 7.20 (m, 3 H) 7.22 - 7.34 (m, 3 H) 8.65 (t, *J*=6.28 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	11.53	1160.3	5	21.44	2158.0	9	44.31	4459.2	13	102.29	10293.5	17	127.39	12819.3	21	133.41	13425.2	25	151.74	15270.2
2	11.63	1170.5	6	32.55	3276.0	10	44.68	4496.7	14	115.14	11586.9	18	130.13	13095.1	22	142.43	14333.4	26	152.94	15391.3
3	21.22	2135.2	7	41.72	4198.1	11	51.21	5153.2	15	126.34	12714.4	19	130.51	13134.0	23	148.67	14960.7	27	156.62	15761.0
4	21.33	2146.2	8	41.88	4215.0	12	67.51	6793.5	16	127.14	12794.4	20	132.23	13307.1	24	150.98	15193.9	28	168.50	16956.8

N-(3-(cyclohexylamino)propyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (19)



No.	(ppm)	(Hz)
1	0.79	237.1
2	0.81	244.1
3	0.82	247.0
4	0.84	251.7
5	0.85	254.6
6	0.87	262.3
7	0.90	268.7
8	0.93	279.8
9	0.97	291.0
10	1.03	308.6
11	1.06	317.3
12	1.07	320.3
13	1.09	328.5

No.	(ppm)	(Hz)
14	1.13	337.9
15	1.17	350.2
16	1.18	353.1
17	1.21	361.9
18	1.46	439.3
19	1.48	443.4
20	1.49	446.3
21	1.50	449.8
22	1.51	453.9
23	1.52	456.3
24	1.54	460.9
25	1.58	475.0
26	1.59	477.9

No.	(ppm)	(Hz)
27	1.62	485.0
28	1.64	492.0
29	1.66	499.0
30	1.69	506.7
31	1.71	513.7
32	1.75	525.4
33	1.97	590.5
34	2.20	659.0
35	2.21	663.1
36	2.22	666.7
37	2.23	669.6
38	2.24	673.1
39	2.25	676.6

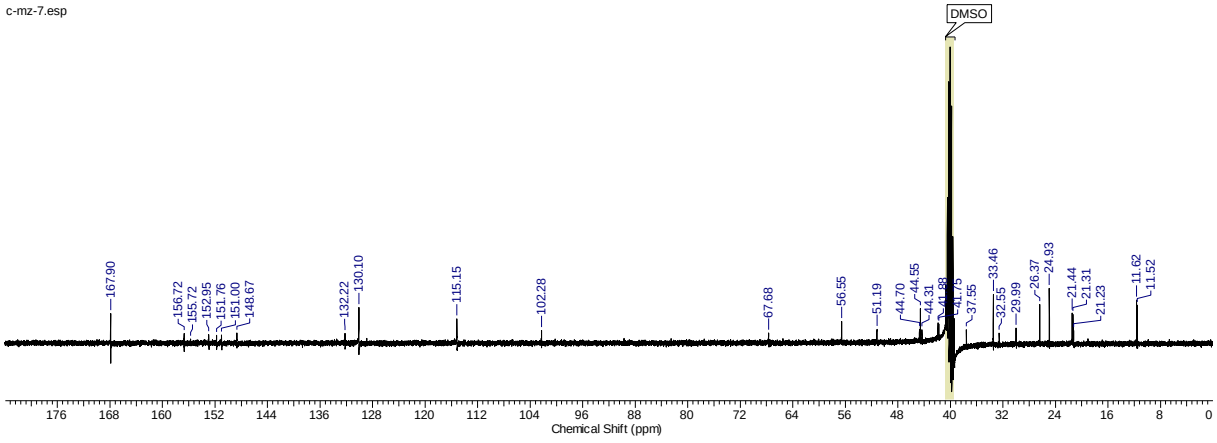
No.	(ppm)	(Hz)
40	2.26	679.6
41	2.28	683.1
42	2.29	686.6
43	2.78	833.1
44	2.80	839.6
45	2.82	847.2
46	3.12	935.7
47	3.14	942.1
48	3.16	948.0
49	3.18	954.4
50	3.25	974.4
51	3.26	979.6
52	3.28	984.9

No.	(ppm)	(Hz)
53	3.30	991.4
54	3.58	1074.0
55	3.60	1081.6
56	3.63	1088.7
57	3.72	1117.4
58	3.75	1125.0
59	3.77	1132.0
60	3.84	1153.7
61	3.87	1161.3
62	3.89	1167.8
63	3.99	1195.9
64	4.00	1201.8
65	4.02	1207.6

No.	(ppm)	(Hz)
66	4.38	1314.9
67	6.84	2051.6
68	6.87	2060.4
69	7.13	2138.4
70	7.16	2147.2
71	8.12	2436.7
72	8.14	2442.6
73	8.16	2447.8

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.98	10	m	-	M15	[0.78 .. 1.22]
2	1.58	12	m	-	M14	[1.43 .. 1.78]
3	1.97	2	m	-	M13	[1.93 .. 2.01]
4	2.24	1	m	-	M12	[2.19 .. 2.29]
5	2.80	2	t	7.03	M11	[2.77 .. 2.83]
6	3.15	2	q	6.45	M10	[3.11 .. 3.19]
7	3.27	5	m	-	M09	[3.24 .. 3.33]
8	3.60	2	t	7.33	M08	[3.57 .. 3.64]
9	3.75	2	m	-	M07	[3.71 .. 3.78]
10	3.87	2	t	7.03	M06	[3.84 .. 3.90]
11	4.00	2	t	5.86	M05	[3.98 .. 4.03]
12	4.38	2	s	-	M04	[4.36 .. 4.39]
13	6.85	2	d	8.79	M03	[6.83 .. 6.88]
14	7.14	2	d	8.79	M02	[7.12 .. 7.17]
15	8.14	1	t	5.57	M01	[8.11 .. 8.17]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.78 - 1.22 (m, 10 H) 1.43 - 1.78 (m, 12 H) 1.93 - 2.01 (m, 2 H) 2.19 - 2.29 (m, 1 H) 2.80 (t, *J*=7.03 Hz, 2 H) 3.15 (q, *J*=6.45 Hz, 2 H) 3.24 - 3.33 (m, 5 H) 3.60 (t, *J*=7.33 Hz, 2 H) 3.71 - 3.78 (m, 2 H) 3.87 (t, *J*=7.03 Hz, 2 H) 4.00 (t, *J*=5.86 Hz, 2 H) 4.38 (s, 2 H) 6.85 (d, *J*=8.79 Hz, 2 H) 7.14 (d, *J*=8.79 Hz, 2 H) 8.14 (t, *J*=5.57 Hz, 1 H)



No.	(ppm)	(Hz)
1	11.52	1158.8
2	11.62	1169.8
3	21.23	2135.9
4	21.31	2144.7
5	21.44	2157.2

No.	(ppm)	(Hz)
6	24.93	2508.6
7	26.37	2653.9
8	29.99	3018.5
9	32.55	3276.0
10	33.46	3367.7

No.	(ppm)	(Hz)
11	37.55	3778.5
12	41.75	4201.0
13	41.88	4215.0
14	44.31	4459.2
15	44.55	4482.7

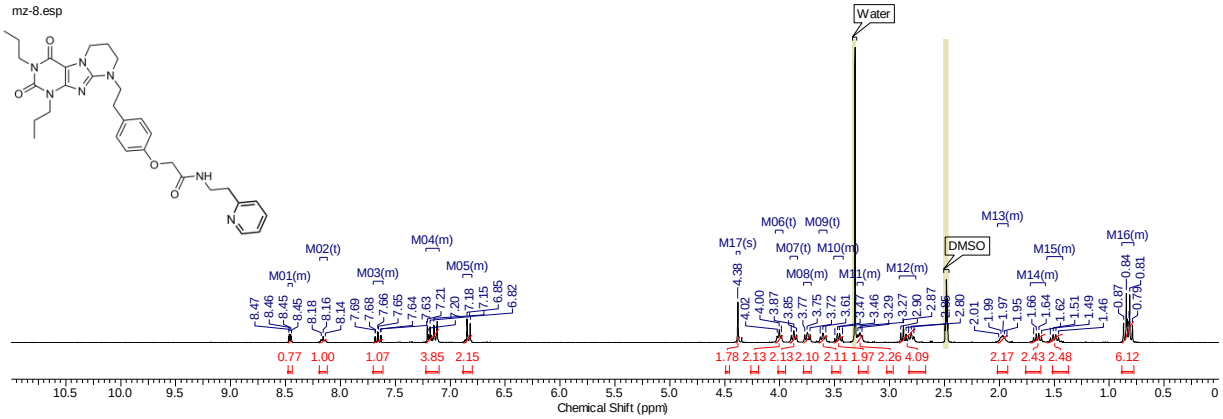
No.	(ppm)	(Hz)
16	44.70	4498.1
17	51.19	5151.0
18	56.55	5690.9
19	67.68	6811.1
20	102.28	10292.8

No.	(ppm)	(Hz)
21	115.15	11587.6
22	130.10	13092.2
23	132.22	13305.7
24	148.67	14960.7
25	151.00	15195.4

No.	(ppm)	(Hz)
26	151.76	15271.7
27	152.95	15392.0
28	155.72	15670.8
29	156.71	15769.8
30	156.72	15771.3

No.	(ppm)	(Hz)
31	167.90	16896.6

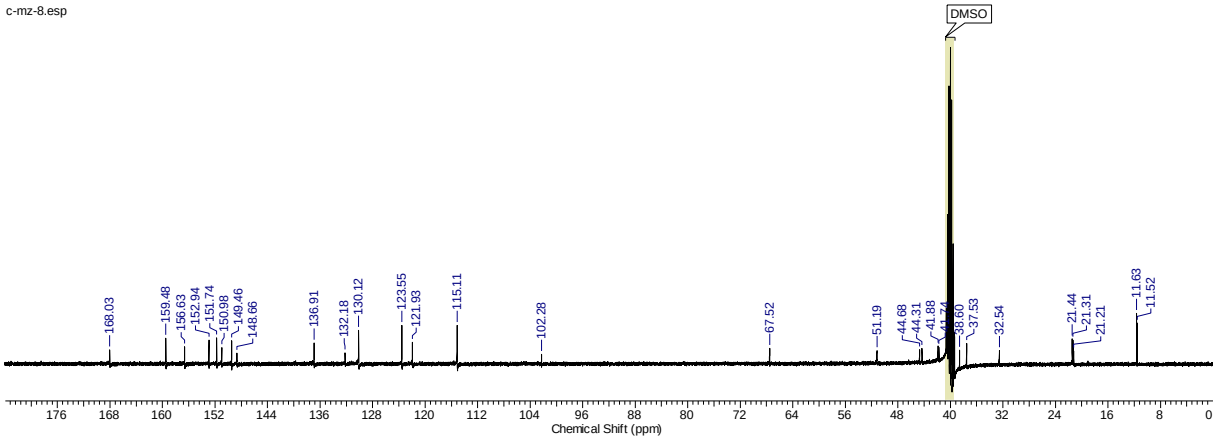
2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(pyridin-2-yl)ethyl)acetamide (20)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	0.79	236.4	12	1.66	499.0	23	2.87	862.2	34	3.63	1089.2	45	6.82	2046.1	56	7.69	2306.4
2	0.81	243.9	13	1.69	506.5	24	2.90	869.6	35	3.72	1117.1	46	6.85	2054.8	57	8.14	2442.0
3	0.82	245.9	14	1.93	579.3	25	3.25	975.3	36	3.75	1125.6	47	7.15	2145.0	58	8.16	2447.7
4	0.84	253.4	15	1.95	586.2	26	3.27	980.7	37	3.77	1131.7	48	7.18	2155.6	59	8.18	2453.3
5	0.87	260.8	16	1.97	590.6	27	3.29	986.3	38	3.85	1154.6	49	7.20	2159.2	60	8.45	2534.4
6	1.46	438.3	17	1.99	596.2	28	3.43	1029.4	39	3.87	1162.0	50	7.21	2163.3	61	8.45	2536.2
7	1.49	445.7	18	2.01	602.1	29	3.46	1036.9	40	3.89	1168.7	51	7.63	2289.2	62	8.46	2540.0
8	1.51	453.1	19	2.78	833.5	30	3.47	1042.8	41	3.98	1195.6	52	7.64	2291.2	63	8.47	2541.8
9	1.53	460.6	20	2.80	840.4	31	3.50	1049.7	42	4.00	1201.5	53	7.65	2296.9			
10	1.62	484.7	21	2.83	848.1	32	3.58	1074.6	43	4.02	1207.4	54	7.66	2298.7			
11	1.64	492.1	22	2.85	855.0	33	3.61	1082.3	44	4.38	1314.6	55	7.68	2304.6			

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M16	[0.78 .. 0.88]
2	1.50	2	m	-	M15	[1.42 .. 1.57]
3	1.65	2	m	-	M14	[1.58 .. 1.72]
4	1.97	2	m	-	M13	[1.92 .. 2.02]
5	2.84	4	m	-	M12	[2.76 .. 2.91]
6	3.27	2	m	-	M11	[3.24 .. 3.29]
7	3.46	2	m	-	M10	[3.42 .. 3.51]
8	3.61	2	t	7.31	M09	[3.57 .. 3.64]
9	3.75	2	m	-	M08	[3.71 .. 3.78]
10	3.87	2	t	7.05	M07	[3.84 .. 3.91]
11	4.00	2	t	5.90	M06	[3.97 .. 4.04]
12	4.38	2	s	-	M17	[4.36 .. 4.40]
13	6.83	2	m	-	M05	[6.80 .. 6.89]
14	7.18	4	m	-	M04	[7.10 .. 7.22]
15	7.66	1	m	-	M03	[7.61 .. 7.70]
16	8.16	1	t	5.64	M02	[8.12 .. 8.19]
17	8.46	1	m	-	M01	[8.44 .. 8.48]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.78 - 0.88 (m, 6 H) 1.42 - 1.57 (m, 2 H) 1.58 - 1.72 (m, 2 H) 1.92 - 2.02 (m, 2 H) 2.76 - 2.91 (m, 4 H) 3.24 - 3.29 (m, 2 H) 3.42 - 3.51 (m, 2 H) 3.61 (t, *J*=7.31 Hz, 2 H) 3.71 - 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.00 (t, *J*=5.90 Hz, 2 H) 4.38 (s, 2 H) 6.80 - 6.89 (m, 2 H) 7.10 - 7.22 (m, 4 H) 7.61 - 7.70 (m, 1 H) 8.16 (t, *J*=5.64 Hz, 1 H) 8.44 - 8.48 (m, 1 H)



No.	(ppm)	(Hz)
1	11.52	1159.5
2	11.63	1170.5
3	21.21	2134.5
4	21.31	2144.7
5	21.44	2157.2

No.	(ppm)	(Hz)
6	32.54	3274.5
7	37.53	3776.3
8	38.60	3884.8
9	41.74	4200.3
10	41.88	4215.0

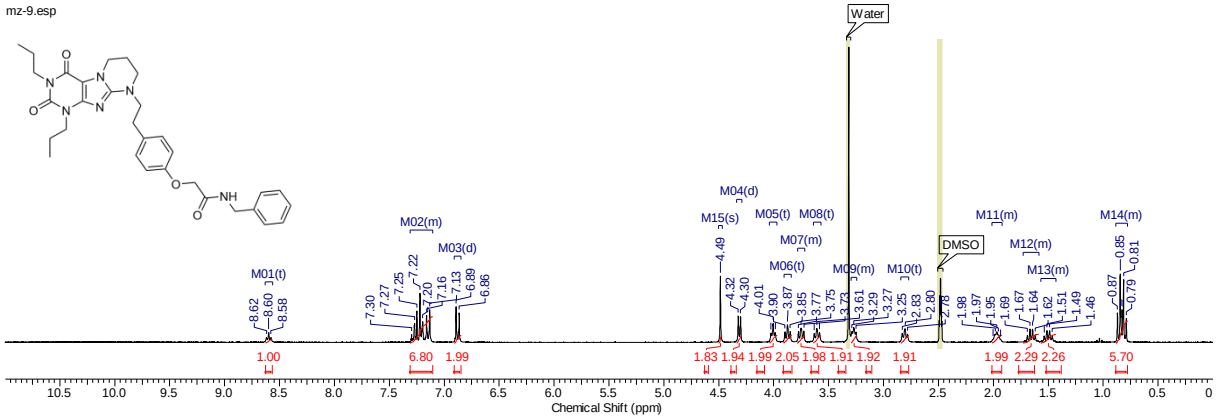
No.	(ppm)	(Hz)
11	44.31	4459.2
12	44.68	4495.9
13	51.19	5151.0
14	67.52	6795.0
15	102.28	10292.8

No.	(ppm)	(Hz)
16	115.11	11583.9
17	121.93	12270.6
18	123.55	12433.4
19	130.12	13094.4
20	132.18	13302.0

No.	(ppm)	(Hz)
21	136.91	13777.4
22	148.66	14959.9
23	149.46	15040.6
24	150.98	15193.9
25	151.74	15270.2

No.	(ppm)	(Hz)
26	152.94	15390.5
27	156.63	15762.5
28	159.48	16049.3
29	168.03	16909.1

N-benzyl-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (21)



No.	(ppm)	(Hz)
1	0.79	236.7
2	0.81	244.4
3	0.82	246.2
4	0.84	251.6
5	0.85	253.6
6	0.87	261.0
7	1.46	439.0
8	1.49	446.5
9	1.51	453.7

No.	(ppm)	(Hz)
10	1.54	461.3
11	1.62	485.5
12	1.64	492.9
13	1.67	499.8
14	1.69	507.0
15	1.93	579.8
16	1.95	586.2
17	1.97	590.6
18	1.98	595.0

No.	(ppm)	(Hz)
19	2.00	601.4
20	2.78	834.5
21	2.80	841.2
22	2.83	849.1
23	3.25	975.6
24	3.27	981.5
25	3.29	986.6
26	3.58	1074.8
27	3.61	1082.5

No.	(ppm)	(Hz)
28	3.63	1089.4
29	3.73	1117.9
30	3.75	1125.6
31	3.77	1132.8
32	3.85	1155.3
33	3.87	1162.8
34	3.90	1169.5
35	3.99	1196.1
36	4.01	1202.0

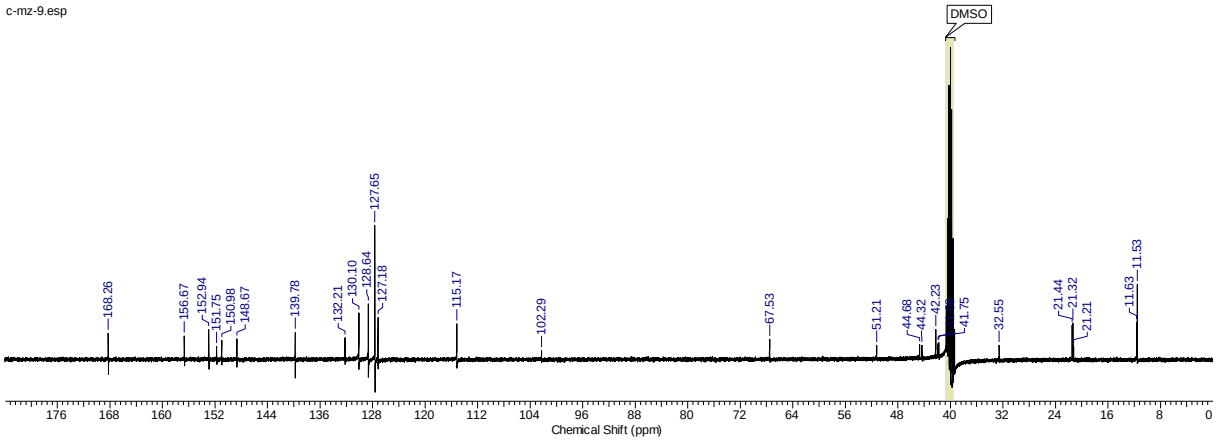
No.	(ppm)	(Hz)
37	4.02	1207.7
38	4.30	1291.0
39	4.32	1297.2
40	4.49	1345.9
41	6.86	2059.6
42	6.89	2068.4
43	7.13	2140.2
44	7.16	2148.9
45	7.20	2159.4

No.	(ppm)	(Hz)
46	7.22	2166.8
47	7.25	2175.6
48	7.27	2181.5
49	7.30	2189.7
50	8.58	2574.1
51	8.60	2580.3
52	8.62	2586.2

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M14	[0.78 .. 0.88]
2	1.50	2	m	-	M13	[1.43 .. 1.57]
3	1.65	2	m	-	M12	[1.59 .. 1.73]
4	1.97	2	m	-	M11	[1.92 .. 2.01]
5	2.80	2	t	7.31	M10	[2.77 .. 2.84]
6	3.27	2	m	-	M09	[3.24 .. 3.29]
7	3.61	2	t	7.31	M08	[3.57 .. 3.64]
8	3.75	2	m	-	M07	[3.72 .. 3.78]
9	3.87	2	t	7.05	M06	[3.84 .. 3.91]
10	4.01	2	t	5.77	M05	[3.97 .. 4.04]
11	4.31	2	d	6.16	M04	[4.29 .. 4.34]
12	4.49	2	s	-	M15	[4.47 .. 4.50]
13	6.88	2	d	8.72	M03	[6.85 .. 6.91]
14	7.22	7	m	-	M02	[7.11 .. 7.31]
15	8.60	1	t	6.03	M01	[8.56 .. 8.63]

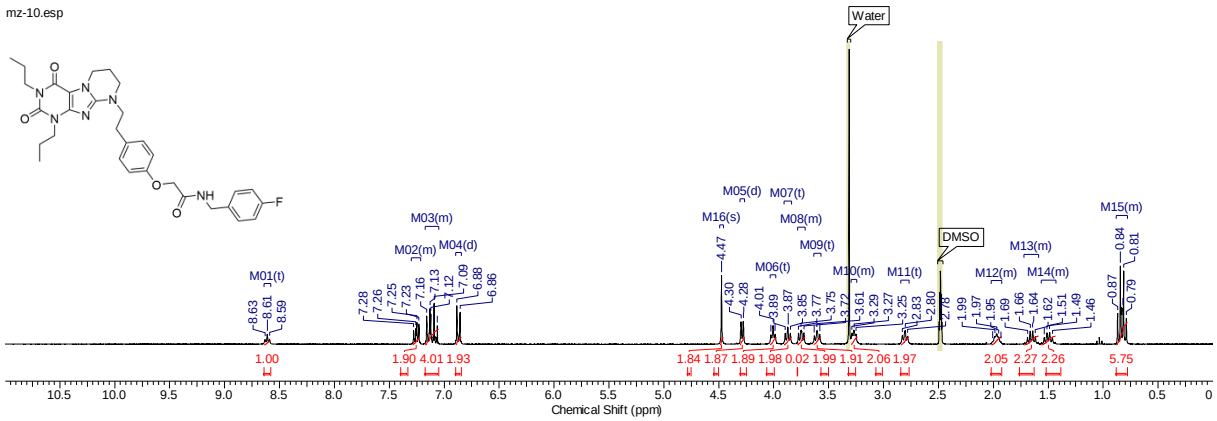
^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.78 - 0.88 (m, 6 H) 1.43 - 1.57 (m, 2 H) 1.59 - 1.73 (m, 2 H) 1.92 - 2.01 (m, 2 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.24 - 3.29 (m, 2 H) 3.61 (t, *J*=7.31 Hz, 2 H) 3.72

- 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.31 (d, *J*=6.16 Hz, 2 H) 4.49 (s, 2 H) 6.88 (d, *J*=8.72 Hz, 2 H) 7.11 - 7.31 (m, 7 H) 8.60 (t, *J*=6.03 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	11.53	1160.3	5	21.44	2158.0	9	42.23	4249.4	13	67.53	6795.7	17	127.65	12845.7	21	139.78	14066.4	25	152.94	15391.3
2	11.63	1170.5	6	32.55	3276.0	10	44.32	4460.0	14	102.29	10293.5	18	128.64	12945.5	22	148.67	14960.7	26	156.67	15766.1
3	21.21	2134.5	7	41.75	4201.0	11	44.68	4495.9	15	115.17	11589.8	19	130.10	13092.2	23	150.98	15193.9	27	168.26	16932.6
4	21.32	2145.5	8	41.89	4215.7	12	51.21	5153.2	16	127.18	12798.8	20	132.21	13304.2	24	151.75	15271.0			

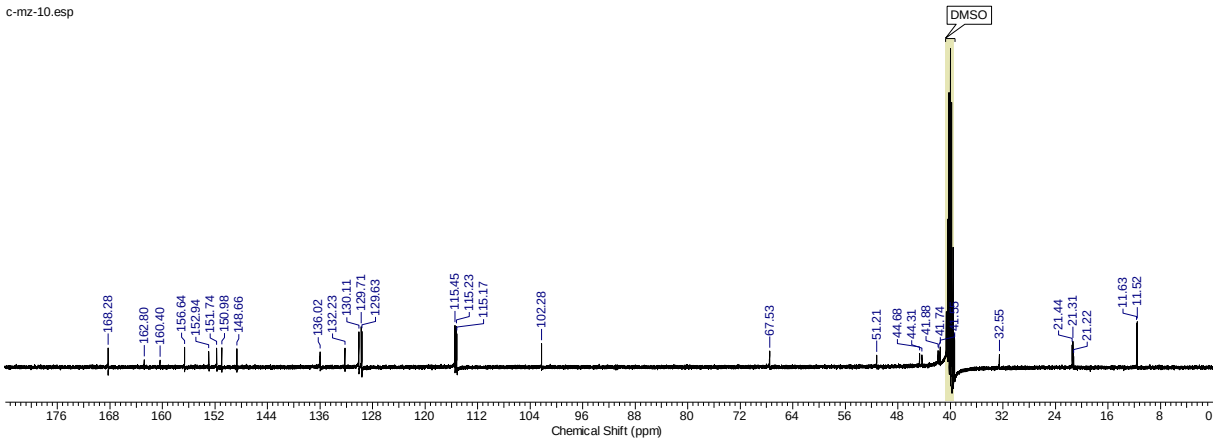
2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-fluorobenzyl)acetamide (22)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	0.79	236.7	11	1.64	492.4	21	2.83	848.6	31	3.85	1154.6	41	6.88	2066.1	51	8.59	2578.0
2	0.81	244.1	12	1.66	499.3	22	3.25	975.6	32	3.87	1161.0	42	7.06	2119.7	52	8.61	2584.1
3	0.82	245.7	13	1.69	506.7	23	3.27	980.4	33	3.89	1168.7	43	7.09	2128.4	53	8.63	2590.3
4	0.84	253.4	14	1.93	579.6	24	3.29	986.3	34	3.99	1196.4	44	7.12	2137.4			
5	0.87	260.5	15	1.95	586.0	25	3.58	1074.3	35	4.01	1202.3	45	7.13	2139.7			
6	1.46	438.8	16	1.97	590.6	26	3.61	1082.3	36	4.03	1208.2	46	7.16	2148.4			
7	1.49	446.2	17	1.99	596.0	27	3.63	1089.2	37	4.28	1283.6	47	7.23	2169.7			
8	1.51	453.7	18	2.01	602.1	28	3.72	1117.6	38	4.30	1289.7	48	7.25	2175.3			
9	1.54	461.1	19	2.78	834.2	29	3.75	1125.3	39	4.47	1342.8	49	7.26	2178.4			
10	1.62	485.2	20	2.80	840.9	30	3.77	1132.5	40	6.86	2057.3	50	7.28	2184.0			

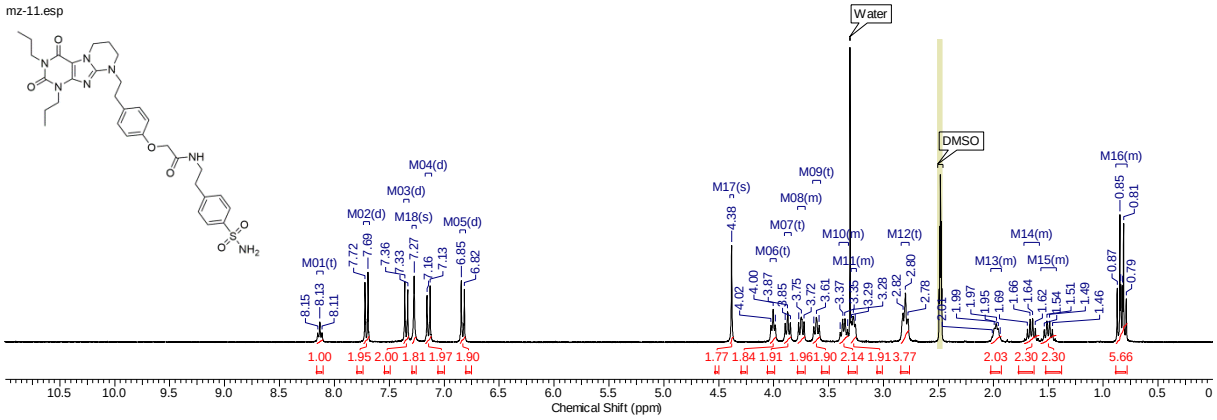
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M15	[0.78 .. 0.88]
2	1.50	2	m	-	M14	[1.43 .. 1.56]
3	1.65	2	m	-	M13	[1.59 .. 1.72]
4	1.97	2	m	-	M12	[1.92 .. 2.02]
5	2.80	2	t	7.18	M11	[2.77 .. 2.84]
6	3.27	2	m	-	M10	[3.24 .. 3.29]
7	3.61	2	t	7.44	M09	[3.57 .. 3.63]
8	3.75	2	m	-	M08	[3.72 .. 3.78]
9	3.87	2	t	7.05	M07	[3.84 .. 3.90]
10	4.01	2	t	5.90	M06	[3.98 .. 4.03]
11	4.29	2	d	6.16	M05	[4.27 .. 4.31]
12	4.47	2	s	-	M16	[4.46 .. 4.49]
13	6.87	2	d	8.72	M04	[6.84 .. 6.89]
14	7.11	4	m	-	M03	[7.05 .. 7.17]
15	7.25	2	m	-	M02	[7.22 .. 7.30]
16	8.61	1	t	6.16	M01	[8.58 .. 8.64]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.78 - 0.88 (m, 6 H) 1.43 - 1.56 (m, 2 H) 1.59 - 1.72 (m, 2 H) 1.92 - 2.02 (m, 2 H) 2.80 (t, *J*=7.18 Hz, 2 H) 3.24 - 3.29 (m, 2 H) 3.61 (t, *J*=7.44 Hz, 2 H) 3.72 - 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.29 (d, *J*=6.16 Hz, 2 H) 4.47 (s, 2 H) 6.87 (d, *J*=8.72 Hz, 2 H) 7.05 - 7.17 (m, 4 H) 7.22 - 7.30 (m, 2 H) 8.61 (t, *J*=6.16 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	11.52	1159.5	6	32.55	3275.2	11	44.68	4495.9	16	115.23	11596.4	21	132.23	13306.4	26	152.94	15391.3
2	11.63	1170.5	7	41.55	4181.2	12	51.21	5153.2	17	115.45	11617.7	22	136.02	13687.9	27	156.64	15763.2
3	21.22	2135.2	8	41.74	4200.3	13	67.53	6795.7	18	129.63	13045.2	23	148.66	14959.9	28	160.40	16141.0
4	21.31	2144.7	9	41.88	4215.0	14	102.28	10292.8	19	129.71	13053.3	24	150.98	15193.9	29	162.80	16383.1
5	21.44	2157.2	10	44.31	4459.2	15	115.17	11589.8	20	130.11	13092.9	25	151.74	15270.2	30	168.28	16934.8

2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-sulfamoylphenethyl)acetamide (23)



No.	(ppm)	(Hz)
1	0.79	236.9
2	0.81	244.4
3	0.82	246.9
4	0.84	251.8
5	0.85	254.4
6	0.87	261.8
7	1.46	438.8
8	1.49	446.2
9	1.51	453.7
10	1.54	461.1

No.	(ppm)	(Hz)
11	1.62	485.2
12	1.64	492.6
13	1.66	499.6
14	1.69	507.0
15	1.94	581.1
16	1.95	586.5
17	1.97	592.1
18	1.99	597.5
19	2.01	603.2
20	2.78	833.0

No.	(ppm)	(Hz)
21	2.80	840.4
22	2.82	847.1
23	3.26	977.1
24	3.28	983.0
25	3.29	988.1
26	3.33	998.4
27	3.35	1005.8
28	3.37	1011.7
29	3.39	1018.6
30	3.59	1076.1

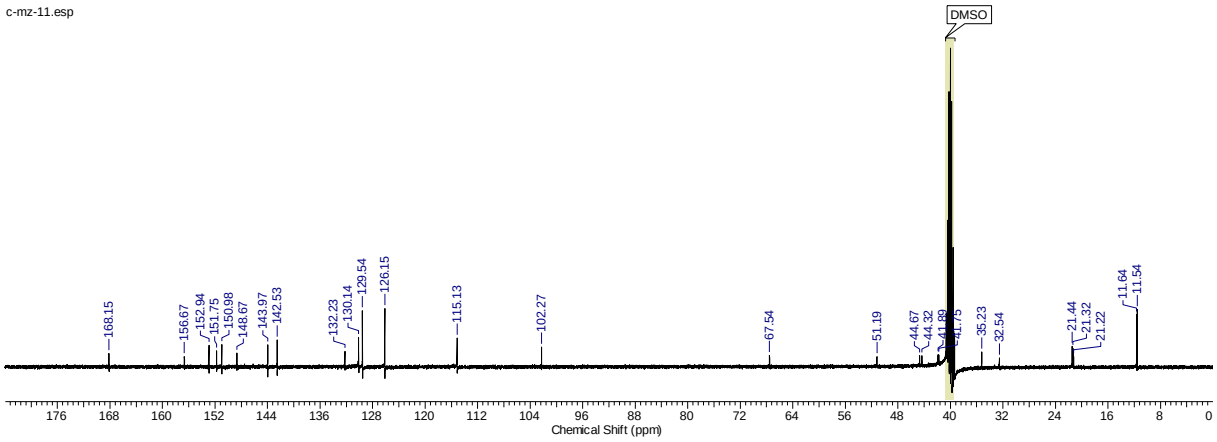
No.	(ppm)	(Hz)
31	3.61	1083.8
32	3.63	1090.7
33	3.72	1117.4
34	3.75	1124.8
35	3.77	1132.0
36	3.85	1154.8
37	3.87	1162.3
38	3.90	1168.9
39	3.99	1196.1
40	4.00	1201.8

No.	(ppm)	(Hz)
41	4.02	1207.7
42	4.38	1315.4
43	6.82	2045.5
44	6.85	2054.3
45	7.13	2139.1
46	7.16	2147.9
47	7.27	2182.7
48	7.33	2200.2
49	7.36	2208.6
50	7.69	2308.9

No.	(ppm)	(Hz)
51	7.72	2317.1
52	8.11	2434.3
53	8.13	2440.2
54	8.15	2446.1

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M16	[0.78 .. 0.88]
2	1.50	2	m	-	M15	[1.43 .. 1.57]
3	1.65	2	m	-	M14	[1.58 .. 1.72]
4	1.97	2	m	-	M13	[1.93 .. 2.02]
5	2.80	4	t	7.05	M12	[2.77 .. 2.84]
6	3.27	2	m	-	M11	[3.25 .. 3.30]
7	3.36	2	m	-	M10	[3.32 .. 3.40]
8	3.61	2	t	7.31	M09	[3.57 .. 3.64]
9	3.75	2	m	-	M08	[3.72 .. 3.78]
10	3.87	2	t	7.05	M07	[3.84 .. 3.90]
11	4.01	2	t	5.77	M06	[3.98 .. 4.03]
12	4.38	2	s	-	M17	[4.37 .. 4.40]
13	6.83	2	d	8.72	M05	[6.80 .. 6.86]
14	7.14	2	d	8.72	M04	[7.11 .. 7.17]
15	7.27	2	s	-	M18	[7.26 .. 7.29]
16	7.35	2	d	8.46	M03	[7.32 .. 7.37]
17	7.71	2	d	8.21	M02	[7.68 .. 7.73]
18	8.13	1	t	5.90	M01	[8.10 .. 8.16]

^{1}H NMR (300 MHz, DMSO-d_6) ? ppm 0.78 - 0.88 (m, 6 H) 1.43 - 1.57 (m, 2 H) 1.58 - 1.72 (m, 2 H) 1.93 - 2.02 (m, 2 H) 2.80 (t, *J*=7.05 Hz, 4 H) 3.25 - 3.30 (m, 2 H) 3.32 - 3.40 (m, 2 H) 3.61 (t, *J*=7.31 Hz, 2 H) 3.72 - 3.78 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.38 (s, 2 H) 6.83 (d, *J*=8.72 Hz, 2 H) 7.14 (d, *J*=8.72 Hz, 2 H) 7.27 (s, 2 H) 7.35 (d, *J*=8.46 Hz, 2 H) 7.71 (d, *J*=8.21 Hz, 2 H) 8.13 (t, *J*=5.90 Hz, 1 H)



No.	(ppm)	(Hz)
1	11.54	1161.0
2	11.64	1171.3
3	21.22	2135.2
4	21.32	2145.5

No.	(ppm)	(Hz)
5	21.44	2158.0
6	32.54	3274.5
7	35.23	3545.2
8	41.75	4201.0

No.	(ppm)	(Hz)
9	41.89	4215.7
10	44.32	4460.0
11	44.67	4495.2
12	51.19	5151.0

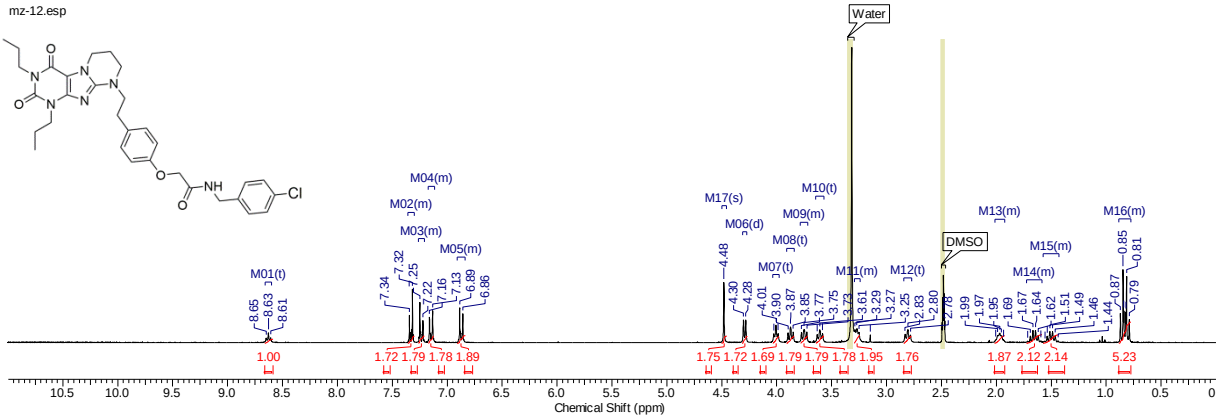
No.	(ppm)	(Hz)
13	67.54	6797.2
14	102.27	10292.1
15	115.13	11585.4
16	126.15	12695.3

No.	(ppm)	(Hz)
17	129.54	13036.4
18	130.14	13095.9
19	132.23	13306.4
20	142.53	14343.0

No.	(ppm)	(Hz)
21	143.97	14488.2
22	148.67	14960.7
23	150.98	15193.9
24	151.75	15271.0

No.	(ppm)	(Hz)
25	152.94	15390.5
26	156.67	15766.1
27	168.15	16921.6

N-(4-chlorobenzyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (24)



No.	(ppm)	(Hz)
1	0.79	236.7
2	0.81	244.4
3	0.82	246.4
4	0.84	251.8
5	0.85	253.9
6	0.87	261.3
7	1.44	431.6
8	1.46	439.3
9	1.49	446.5
10	1.51	453.9

No.	(ppm)	(Hz)
11	1.54	461.3
12	1.56	467.2
13	1.59	478.5
14	1.62	485.7
15	1.64	493.1
16	1.67	500.1
17	1.69	507.5
18	1.72	514.9
19	1.93	580.1
20	1.95	586.2

No.	(ppm)	(Hz)
21	1.97	591.1
22	1.99	596.5
23	2.01	602.1
24	2.78	834.8
25	2.80	841.7
26	2.83	849.6
27	3.15	944.8
28	3.25	975.6
29	3.27	981.2
30	3.29	986.3

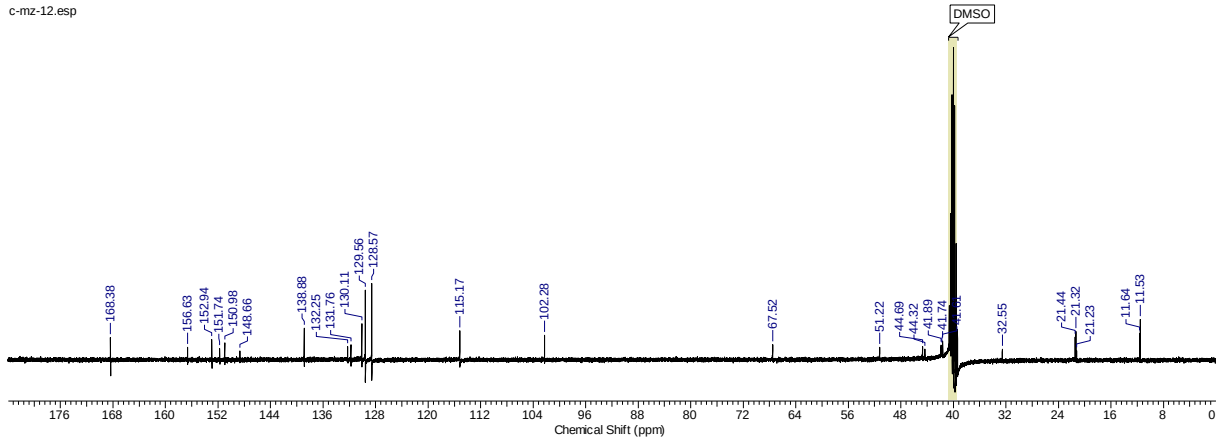
No.	(ppm)	(Hz)
31	3.58	1074.8
32	3.61	1082.8
33	3.63	1089.4
34	3.73	1117.9
35	3.75	1125.3
36	3.77	1132.8
37	3.85	1155.1
38	3.87	1162.8
39	3.90	1169.2
40	3.99	1196.4

No.	(ppm)	(Hz)
41	4.01	1202.3
42	4.03	1208.2
43	4.28	1284.9
44	4.30	1291.0
45	4.48	1344.4
46	6.86	2057.8
47	6.89	2066.6
48	7.13	2140.4
49	7.16	2149.1
50	7.22	2166.8

No.	(ppm)	(Hz)
51	7.25	2175.3
52	7.32	2195.6
53	7.34	2204.0
54	8.61	2583.1
55	8.63	2589.2
56	8.65	2595.4

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M16	[0.77 .. 0.88]
2	1.50	2	m	-	M15	[1.43 .. 1.57]
3	1.66	2	m	-	M14	[1.58 .. 1.72]
4	1.97	2	m	-	M13	[1.92 .. 2.01]
5	2.81	2	t	7.44	M12	[2.77 .. 2.84]
6	3.27	2	m	-	M11	[3.24 .. 3.29]
7	3.61	2	t	7.31	M10	[3.57 .. 3.64]
8	3.75	2	m	-	M09	[3.72 .. 3.79]
9	3.87	2	t	7.05	M08	[3.84 .. 3.91]
10	4.01	2	t	5.90	M07	[3.98 .. 4.03]
11	4.29	2	d	6.16	M06	[4.27 .. 4.31]
12	4.48	2	s	-	M17	[4.46 .. 4.50]
13	6.87	2	m	-	M05	[6.84 .. 6.91]
14	7.15	2	m	-	M04	[7.11 .. 7.17]
15	7.23	2	m	-	M03	[7.21 .. 7.26]
16	7.33	2	m	-	M02	[7.30 .. 7.36]
17	8.63	1	t	6.16	M01	[8.60 .. 8.66]

^{1}H NMR (300 MHz, DMSO-d_6) ppm 0.77 - 0.88 (m, 6 H) 1.43 - 1.57 (m, 2 H) 1.58 - 1.72 (m, 2 H) 1.92 - 2.01 (m, 2 H) 2.81 (t, *J*=7.44 Hz, 2 H) 3.24 - 3.29 (m, 2 H) 3.61 (t, *J*=7.31 Hz, 2 H) 3.72 - 3.79 (m, 2 H) 3.87 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.29 (d, *J*=6.16 Hz, 2 H) 4.48 (s, 2 H) 6.84 - 6.91 (m, 2 H) 7.11 - 7.17 (m, 2 H) 7.21 - 7.26 (m, 2 H) 7.30 - 7.36 (m, 2 H) 8.63 (t, *J*=6.16 Hz, 1 H)



No.	(ppm)	(Hz)
1	11.53	1160.3
2	11.64	1171.3
3	21.23	2135.9
4	21.32	2145.5

No.	(ppm)	(Hz)
5	21.44	2158.0
6	32.55	3275.2
7	41.61	4187.8
8	41.74	4200.3

No.	(ppm)	(Hz)
9	41.89	4215.7
10	44.32	4460.0
11	44.69	4497.4
12	51.22	5154.7

No.	(ppm)	(Hz)
13	67.52	6795.0
14	102.28	10292.8
15	115.17	11589.8
16	128.57	12938.9

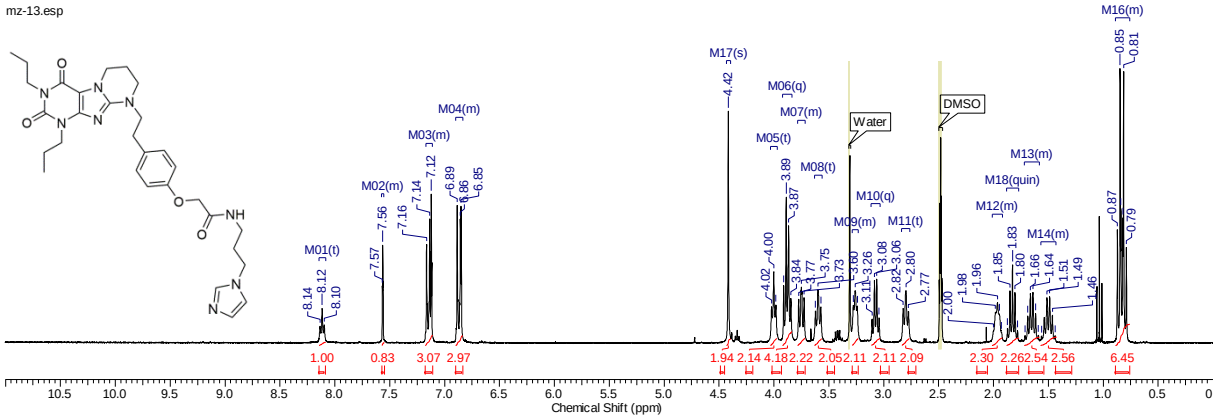
No.	(ppm)	(Hz)
17	129.56	13037.9
18	130.11	13093.7
19	131.76	13259.5
20	132.25	13308.6

No.	(ppm)	(Hz)
21	138.88	13975.4
22	148.66	14959.9
23	150.98	15193.9
24	151.74	15270.2

No.	(ppm)	(Hz)
25	152.94	15391.3
26	156.63	15761.7
27	168.38	16944.3

N-(3-(1H-imidazol-1-yl)propyl)-2-(4-(2-(2,4-dioxo-1,3-dipropyl-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (25)

mz-13.esp



No.	(ppm)	(Hz)
1	0.79	236.7
2	0.81	244.4
3	0.82	246.2
4	0.84	251.8
5	0.85	253.9
6	0.87	261.0
7	1.44	431.9
8	1.46	439.0
9	1.49	446.5
10	1.51	453.9
11	1.56	468.8

No.	(ppm)	(Hz)
12	1.59	477.5
13	1.62	484.7
14	1.64	492.1
15	1.66	499.0
16	1.69	506.2
17	1.71	513.9
18	1.78	534.2
19	1.80	541.1
20	1.83	548.0
21	1.85	555.0
22	1.87	561.6

No.	(ppm)	(Hz)
23	1.93	578.3
24	1.95	584.2
25	1.96	589.1
26	1.98	594.7
27	2.00	600.1
28	2.77	832.5
29	2.80	839.4
30	2.82	846.8
31	3.04	912.7
32	3.06	919.1
33	3.08	925.3

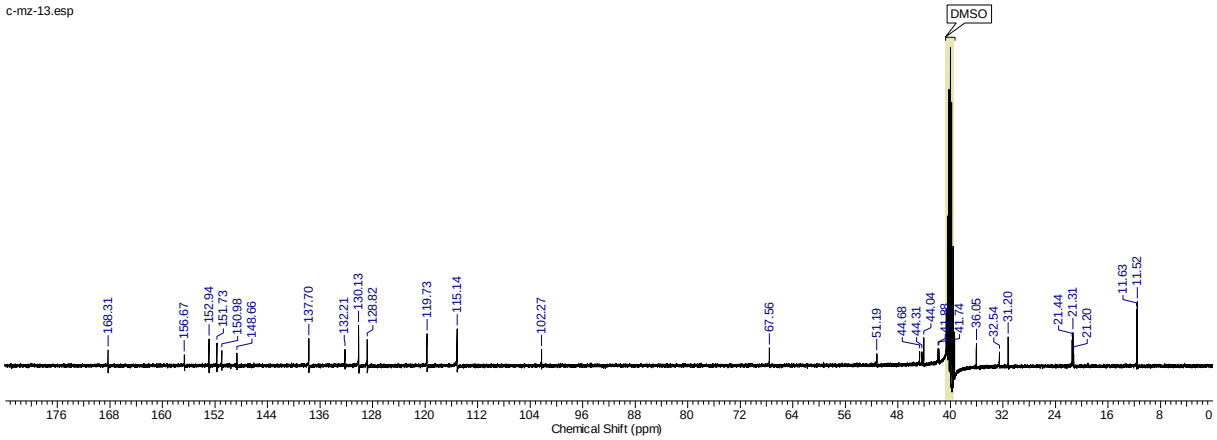
No.	(ppm)	(Hz)
34	3.11	932.0
35	3.24	972.2
36	3.26	978.1
37	3.28	983.3
38	3.57	1072.0
39	3.60	1079.7
40	3.62	1086.6
41	3.73	1117.9
42	3.75	1125.3
43	3.77	1132.5
44	3.84	1153.8

No.	(ppm)	(Hz)
45	3.87	1160.0
46	3.89	1166.9
47	3.91	1173.6
48	3.98	1194.8
49	4.00	1200.7
50	4.02	1206.6
51	4.42	1325.1
52	6.85	2055.5
53	6.86	2057.6
54	6.89	2066.3
55	7.12	2136.8

No.	(ppm)	(Hz)
56	7.14	2141.2
57	7.16	2149.9
58	7.56	2269.7
59	7.57	2271.0
60	8.10	2429.7
61	8.12	2435.4
62	8.14	2441.3

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.83	6	m	-	M16	[0.76 .. 0.89]
2	1.49	2	m	-	M14	[1.43 .. 1.57]
3	1.65	2	m	-	M13	[1.58 .. 1.72]
4	1.83	2	quin	6.86	M18	[1.77 .. 1.88]
5	1.96	2	m	-	M12	[1.92 .. 2.01]
6	2.80	2	t	7.18	M11	[2.76 .. 2.84]
7	3.07	2	q	6.50	M10	[3.03 .. 3.11]
8	3.26	2	m	-	M09	[3.23 .. 3.29]
9	3.60	2	t	7.31	M08	[3.56 .. 3.63]
10	3.75	2	m	-	M07	[3.71 .. 3.78]
11	3.88	4	q	6.33	M06	[3.83 .. 3.92]
12	4.00	2	t	5.90	M05	[3.97 .. 4.03]
13	4.42	2	s	-	M17	[4.40 .. 4.43]
14	6.86	3	m	-	M04	[6.83 .. 6.90]
15	7.14	3	m	-	M03	[7.11 .. 7.17]
16	7.57	1	m	-	M02	[7.55 .. 7.57]
17	8.12	1	t	5.77	M01	[8.08 .. 8.14]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.76 - 0.89 (m, 6 H) 1.43 - 1.57 (m, 2 H) 1.58 - 1.72 (m, 2 H) 1.83 (quin, *J*=6.86 Hz, 2 H) 1.92 - 2.01 (m, 2 H) 2.80 (t, *J*=7.18 Hz, 2 H) 3.07 (q, *J*=6.50 Hz, 2 H) 3.23 - 3.29 (m, 2 H) 3.60 (t, *J*=7.31 Hz, 2 H) 3.71 - 3.78 (m, 2 H) 3.88 (q, *J*=6.33 Hz, 4 H) 4.00 (t, *J*=5.90 Hz, 2 H) 4.42 (s, 2 H) 6.83 - 6.90 (m, 3 H) 7.11 - 7.17 (m, 3 H) 7.55 - 7.57 (m, 1 H) 8.12 (t, *J*=5.77 Hz, 1 H)



No.	(ppm)	(Hz)
1	11.52	1159.5
2	11.63	1170.5
3	21.20	2133.7
4	21.31	2144.7

No.	(ppm)	(Hz)
5	21.44	2157.2
6	31.20	3139.5
7	32.54	3274.5
8	36.05	3627.3

No.	(ppm)	(Hz)
9	41.74	4200.3
10	41.88	4215.0
11	44.04	4432.1
12	44.31	4459.2

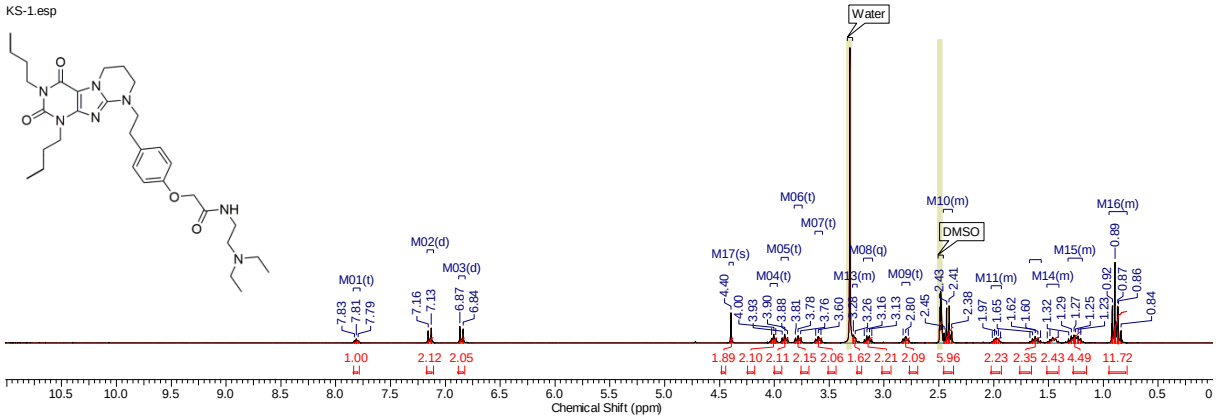
No.	(ppm)	(Hz)
13	44.68	4496.7
14	51.19	5151.8
15	67.56	6798.7
16	102.27	10292.1

No.	(ppm)	(Hz)
17	115.14	11586.9
18	119.73	12048.3
19	128.82	12963.1
20	130.13	13095.1

No.	(ppm)	(Hz)
21	132.21	13304.9
22	137.70	13857.3
23	148.66	14959.9
24	150.98	15193.9

No.	(ppm)	(Hz)
25	151.73	15269.5
26	152.94	15390.5
27	156.67	15766.1
28	168.31	16937.7

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(diethylamino)ethyl)acetamide (26)



No.	(ppm)	(Hz)
1	0.84	251.6
2	0.86	259.0
3	0.87	261.0
4	0.89	268.2
5	0.92	275.4
6	1.21	362.1
7	1.23	369.0
8	1.25	376.5
9	1.27	380.3
10	1.29	387.7

No.	(ppm)	(Hz)
11	1.32	395.2
12	1.41	423.9
13	1.49	446.5
14	1.51	453.1
15	1.57	471.9
16	1.60	479.6
17	1.62	486.7
18	1.65	493.7
19	1.67	500.6
20	1.94	581.4

No.	(ppm)	(Hz)
21	1.96	587.3
22	1.97	592.4
23	1.99	597.5
24	2.01	603.4
25	2.38	714.7
26	2.41	721.9
27	2.43	728.8
28	2.45	736.0
29	2.78	833.5
30	2.80	840.7

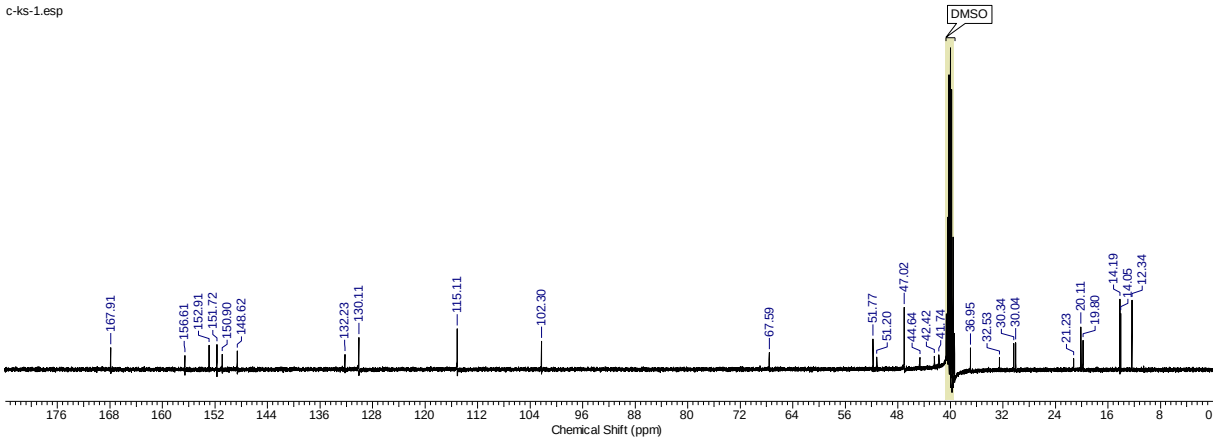
No.	(ppm)	(Hz)
31	2.83	848.1
32	3.11	934.0
33	3.13	940.2
34	3.16	947.4
35	3.18	953.8
36	3.26	978.6
37	3.28	984.5
38	3.57	1072.5
39	3.60	1080.2
40	3.62	1087.4

No.	(ppm)	(Hz)
41	3.76	1128.2
42	3.78	1135.6
43	3.81	1142.5
44	3.88	1164.8
45	3.90	1171.8
46	3.93	1178.9
47	3.99	1196.1
48	4.00	1201.8
49	4.02	1207.7
50	4.40	1319.0

No.	(ppm)	(Hz)
51	6.84	2052.2
52	6.87	2060.9
53	7.13	2139.1
54	7.16	2147.9
55	7.79	2338.9
56	7.81	2344.3
57	7.83	2349.7

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	12	m	-	M16	[0.78 .. 0.95]
2	1.26	4	m	-	M15	[1.19 .. 1.32]
3	1.46	2	m	-	M14	[1.41 .. 1.51]
4	1.62	2	m	-	M12	[1.57 .. 1.67]
5	1.97	2	m	-	M11	[1.93 .. 2.02]
6	2.42	6	m	-	M10	[2.37 .. 2.46]
7	2.80	2	t	7.31	M09	[2.76 .. 2.84]
8	3.15	2	q	7.20	M08	[3.10 .. 3.19]
9	3.27	2	m	-	M13	[3.25 .. 3.28]
10	3.60	2	t	7.44	M07	[3.56 .. 3.63]
11	3.78	2	t	7.40	M06	[3.75 .. 3.82]
12	3.91	2	t	7.05	M05	[3.87 .. 3.94]
13	4.01	2	t	5.77	M04	[3.97 .. 4.04]
14	4.40	2	s	-	M17	[4.37 .. 4.41]
15	6.85	2	d	8.72	M03	[6.82 .. 6.88]
16	7.14	2	d	8.72	M02	[7.11 .. 7.17]
17	7.81	1	t	5.39	M01	[7.78 .. 7.84]

^{1}H NMR (300 MHz, DMSO-d_6) ppm 0.78 - 0.95 (m, 12 H) 1.19 - 1.32 (m, 4 H) 1.41 - 1.51 (m, 2 H) 1.57 - 1.67 (m, 2 H) 1.93 - 2.02 (m, 2 H) 2.37 - 2.46 (m, 6 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.15 (q, *J*=7.20 Hz, 2 H) 3.25 - 3.28 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.78 (t, *J*=7.40 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.40 (s, 2 H) 6.85 (d, *J*=8.72 Hz, 2 H) 7.14 (d, *J*=8.72 Hz, 2 H) 7.81 (t, *J*=5.39 Hz, 1 H)



No.	(ppm)	(Hz)
1	12.34	1241.7
2	14.05	1414.1
3	14.19	1428.0
4	19.80	1992.9

No.	(ppm)	(Hz)
5	20.11	2023.7
6	21.23	2135.9
7	30.04	3022.9
8	30.34	3052.9

No.	(ppm)	(Hz)
9	32.53	3273.7
10	36.95	3718.3
11	41.74	4200.3
12	42.42	4269.2

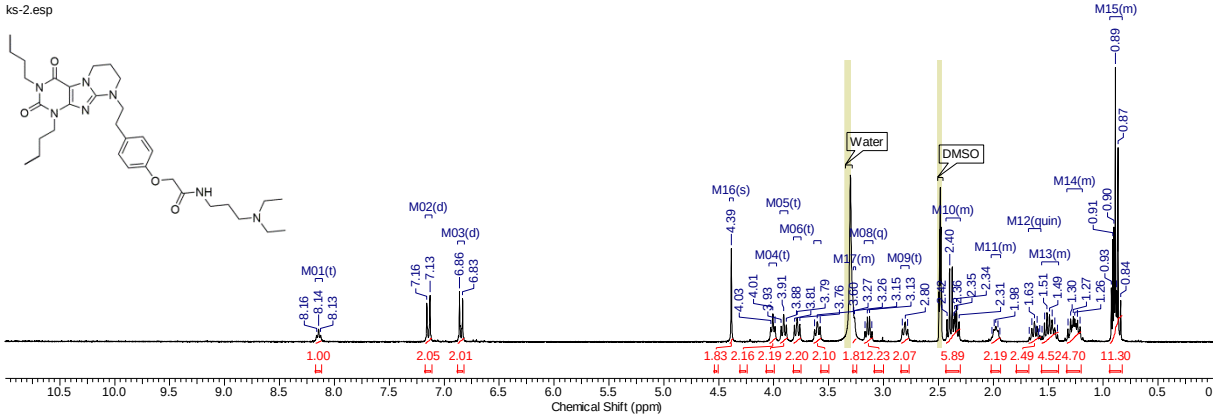
No.	(ppm)	(Hz)
13	44.64	4492.3
14	47.02	4731.4
15	51.20	5152.5
16	51.77	5209.7

No.	(ppm)	(Hz)
17	67.59	6801.6
18	102.30	10294.3
19	115.11	11583.9
20	130.11	13093.7

No.	(ppm)	(Hz)
21	132.23	13307.1
22	148.62	14956.3
23	150.90	15185.1
24	151.72	15268.0

No.	(ppm)	(Hz)
25	152.91	15387.6
26	156.61	15760.3
27	167.91	16897.4

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(3-(diethylamino)propyl)acetamide (27)



No.	(ppm)	(Hz)
1	0.84	252.3
2	0.87	259.8
3	0.88	263.1
4	0.89	266.7
5	0.90	270.5
6	0.91	273.9
7	0.93	277.7
8	1.21	363.1
9	1.23	370.0
10	1.26	377.5
11	1.27	381.3
12	1.30	388.8

No.	(ppm)	(Hz)
13	1.32	396.5
14	1.42	424.9
15	1.44	432.6
16	1.46	439.5
17	1.49	446.7
18	1.51	453.4
19	1.53	460.3
20	1.56	467.0
21	1.58	473.4
22	1.59	476.5
23	1.60	480.6
24	1.61	483.9

No.	(ppm)	(Hz)
25	1.63	487.8
26	1.65	494.9
27	1.67	501.9
28	1.94	582.4
29	1.96	587.5
30	1.98	593.7
31	1.99	598.3
32	2.01	604.2
33	2.31	694.0
34	2.34	700.9
35	2.35	705.5
36	2.36	707.6

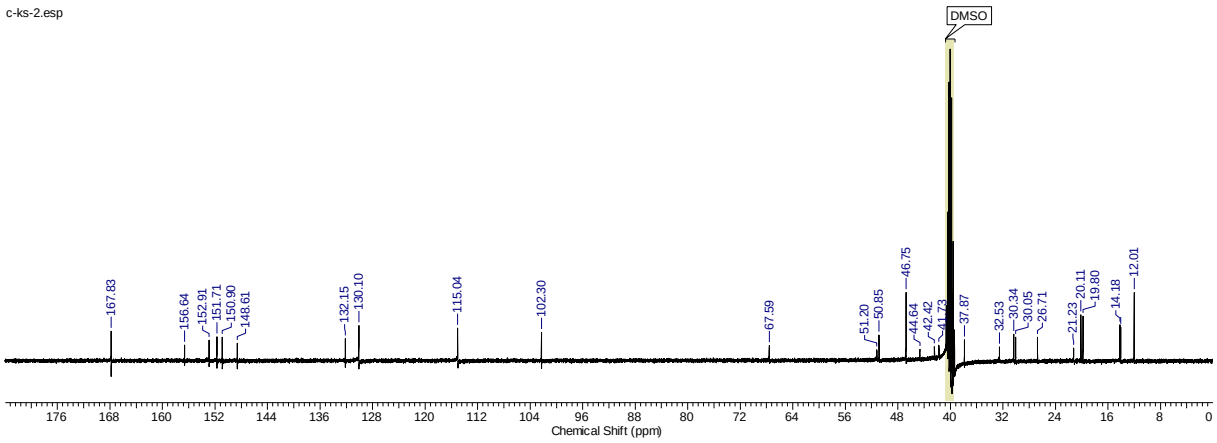
No.	(ppm)	(Hz)
37	2.40	719.6
38	2.42	726.8
39	2.78	834.2
40	2.80	840.9
41	2.83	848.9
42	3.11	932.0
43	3.13	938.4
44	3.15	944.3
45	3.17	950.9
46	3.26	979.4
47	3.27	980.2
48	3.58	1073.5

No.	(ppm)	(Hz)
49	3.60	1081.0
50	3.63	1088.7
51	3.76	1128.9
52	3.79	1136.4
53	3.81	1143.5
54	3.88	1165.6
55	3.91	1172.8
56	3.93	1179.7
57	3.99	1196.6
58	4.01	1202.5
59	4.03	1208.4
60	4.39	1316.1

No.	(ppm)	(Hz)
61	6.83	2050.4
62	6.86	2058.9
63	7.13	2139.4
64	7.16	2148.1
65	8.13	2438.4
66	8.14	2443.8
67	8.16	2449.2

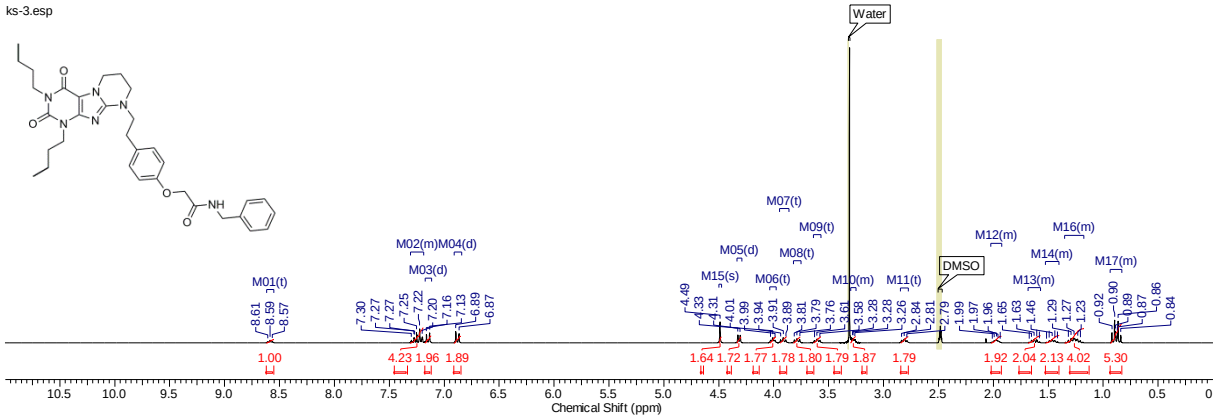
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.89	12	m	-	M15	[0.83 .. 0.94]
2	1.26	4	m	-	M14	[1.19 .. 1.33]
3	1.49	4	m	-	M13	[1.41 .. 1.56]
4	1.63	2	quin	7.10	M12	[1.57 .. 1.68]
5	1.98	2	m	-	M11	[1.93 .. 2.02]
6	2.36	6	m	-	M10	[2.30 .. 2.43]
7	2.80	2	t	7.31	M09	[2.77 .. 2.84]
8	3.14	2	q	6.50	M08	[3.10 .. 3.18]
9	3.27	2	m	-	M17	[3.25 .. 3.27]
10	3.60	2	t	7.57	M07	[3.57 .. 3.63]
11	3.79	2	t	7.40	M06	[3.75 .. 3.82]
12	3.91	2	t	7.05	M05	[3.87 .. 3.94]
13	4.01	2	t	5.90	M04	[3.97 .. 4.04]
14	4.39	2	s	-	M16	[4.37 .. 4.40]
15	6.85	2	d	8.46	M03	[6.82 .. 6.88]
16	7.14	2	d	8.72	M02	[7.11 .. 7.17]
17	8.14	1	t	5.39	M01	[8.11 .. 8.17]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.83 - 0.94 (m, 12 H) 1.19 - 1.33 (m, 4 H) 1.41 - 1.56 (m, 4 H) 1.63 (quin, *J*=7.10 Hz, 2 H) 1.93 - 2.02 (m, 2 H) 2.30 - 2.43 (m, 6 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.14 (q, *J*=6.50 Hz, 2 H) 3.25 - 3.27 (m, 2 H) 3.60 (t, *J*=7.57 Hz, 2 H) 3.79 (t, *J*=7.40 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.39 (s, 2 H) 6.85 (d, *J*=8.46 Hz, 2 H) 7.14 (d, *J*=8.72 Hz, 2 H) 8.14 (t, *J*=5.39 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	12.01	1208.7	5	20.11	2023.7	9	30.34	3052.9	13	42.42	4269.2	17	51.20	5152.5	21	130.10	13092.2	25	151.71	15267.3
2	14.05	1414.1	6	21.23	2135.9	10	32.53	3273.7	14	44.64	4492.3	18	67.59	6801.6	22	132.15	13299.1	26	152.91	15387.6
3	14.18	1427.3	7	26.71	2687.6	11	37.87	3810.7	15	46.75	4705.0	19	102.30	10294.3	23	148.61	14955.5	27	156.64	15763.2
4	19.80	1992.9	8	30.05	3023.6	12	41.73	4199.5	16	50.85	5117.3	20	115.04	11576.6	24	150.90	15185.1	28	167.83	16889.3

N-benzyl-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (28)



No.	(ppm)	(Hz)
1	0.84	252.1
2	0.86	259.5
3	0.87	261.6
4	0.89	266.7
5	0.90	269.0
6	0.92	276.2
7	1.21	362.6
8	1.23	369.8
9	1.27	380.0
10	1.29	387.5
11	1.32	395.2

No.	(ppm)	(Hz)
12	1.42	424.9
13	1.44	432.6
14	1.46	439.5
15	1.49	447.5
16	1.51	454.4
17	1.58	473.9
18	1.60	481.4
19	1.63	488.3
20	1.65	495.7
21	1.68	502.6
22	1.94	581.4

No.	(ppm)	(Hz)
23	1.96	587.3
24	1.97	592.1
25	1.99	597.5
26	2.01	603.2
27	2.79	836.0
28	2.81	844.0
29	2.84	850.9
30	3.26	978.1
31	3.28	984.0
32	3.28	985.1
33	3.58	1074.0

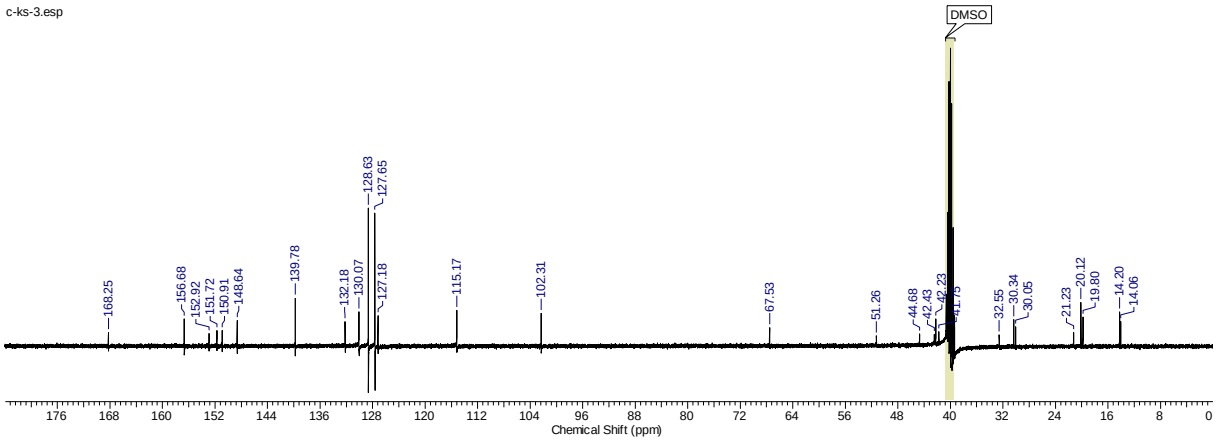
No.	(ppm)	(Hz)
34	3.61	1082.0
35	3.63	1088.9
36	3.76	1129.2
37	3.79	1136.6
38	3.81	1143.8
39	3.89	1167.1
40	3.91	1174.3
41	3.94	1181.2
42	3.99	1196.9
43	4.01	1202.8
44	4.03	1208.7

No.	(ppm)	(Hz)
45	4.31	1292.0
46	4.33	1298.2
47	4.49	1346.9
48	6.87	2060.2
49	6.89	2068.9
50	7.13	2140.4
51	7.16	2149.1
52	7.20	2160.7
53	7.22	2167.6
54	7.25	2176.1
55	7.27	2181.7

No.	(ppm)	(Hz)
56	7.27	2183.0
57	7.30	2190.2
58	8.57	2570.8
59	8.59	2576.7
60	8.61	2582.8

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M17	[0.83 .. 0.93]
2	1.26	4	m	-	M16	[1.18 .. 1.35]
3	1.47	2	m	-	M14	[1.40 .. 1.53]
4	1.63	2	m	-	M13	[1.57 .. 1.68]
5	1.97	2	m	-	M12	[1.93 .. 2.02]
6	2.81	2	t	7.44	M11	[2.77 .. 2.84]
7	3.27	2	m	-	M10	[3.25 .. 3.30]
8	3.60	2	t	7.44	M09	[3.57 .. 3.64]
9	3.79	2	t	7.20	M08	[3.75 .. 3.82]
10	3.91	2	t	7.05	M07	[3.86 .. 3.95]
11	4.01	2	t	5.90	M06	[3.98 .. 4.04]
12	4.32	2	d	6.16	M05	[4.29 .. 4.34]
13	4.49	2	s	-	M15	[4.48 .. 4.50]
14	6.88	2	d	8.72	M04	[6.84 .. 6.91]
15	7.15	2	d	8.72	M03	[7.12 .. 7.17]
16	7.25	5	m	-	M02	[7.19 .. 7.31]
17	8.59	1	t	6.03	M01	[8.55 .. 8.62]

^{1}H NMR (300 MHz, DMSO-d_6) ppm 0.83 - 0.93 (m, 6 H) 1.18 - 1.35 (m, 4 H) 1.40 - 1.53 (m, 2 H) 1.57 - 1.68 (m, 2 H) 1.93 - 2.02 (m, 2 H) 2.81 (t, *J*=7.44 Hz, 2 H) 3.25 - 3.30 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.79 (t, *J*=7.20 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.32 (d, *J*=6.16 Hz, 2 H) 4.49 (s, 2 H) 6.88 (d, *J*=8.72 Hz, 2 H) 7.15 (d, *J*=8.72 Hz, 2 H) 7.19 - 7.31 (m, 5 H) 8.59 (t, *J*=6.03 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.06	1414.8
2	14.20	1428.8
3	19.80	1992.9
4	20.12	2024.4

No.	(ppm)	(Hz)
5	21.23	2135.9
6	30.05	3023.6
7	30.34	3052.9
8	32.55	3276.0

No.	(ppm)	(Hz)
9	41.75	4201.0
10	42.23	4249.4
11	42.43	4270.0
12	44.68	4496.7

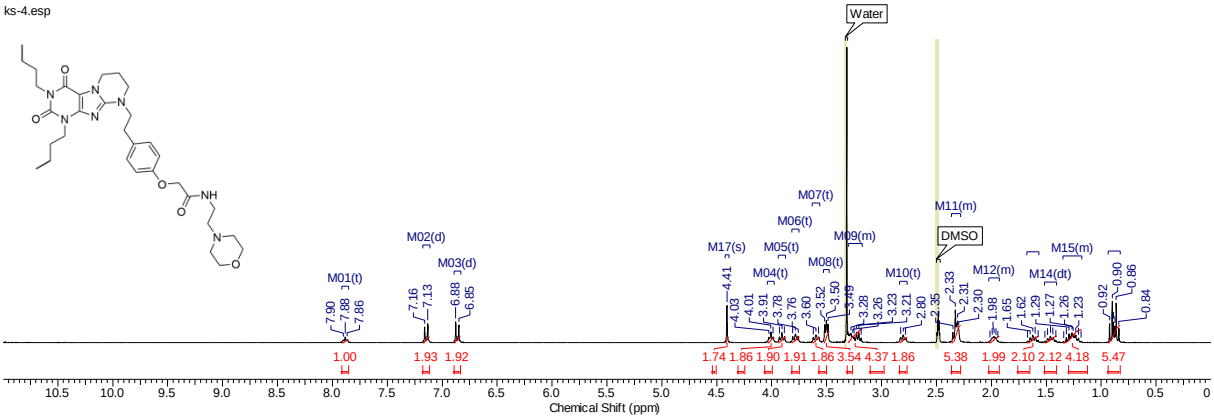
No.	(ppm)	(Hz)
13	51.26	5158.4
14	67.53	6795.7
15	102.31	10295.7
16	115.17	11589.8

No.	(ppm)	(Hz)
17	127.18	12798.0
18	127.65	12845.7
19	128.63	12944.7
20	130.07	13089.3

No.	(ppm)	(Hz)
21	132.18	13302.0
22	139.78	14066.4
23	148.64	14957.7
24	150.91	15186.6

No.	(ppm)	(Hz)
25	151.72	15268.0
26	152.92	15389.1
27	156.68	15766.9
28	168.25	16931.1

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-morpholinoethyl)acetamide (29)



No.	(ppm)	(Hz)
1	0.84	251.8
2	0.86	259.3
3	0.87	262.3
4	0.89	266.4
5	0.90	269.8
6	0.92	277.2
7	1.18	354.9
8	1.21	362.1
9	1.23	369.3
10	1.26	376.7
11	1.27	380.0
12	1.29	387.7

No.	(ppm)	(Hz)
13	1.32	395.2
14	1.34	402.6
15	1.41	423.9
16	1.44	431.9
17	1.46	438.8
18	1.49	446.5
19	1.51	453.4
20	1.57	472.1
21	1.60	480.1
22	1.62	487.0
23	1.65	494.2
24	1.67	501.1

No.	(ppm)	(Hz)
25	1.94	582.1
26	1.96	587.3
27	1.98	592.9
28	1.99	598.3
29	2.01	603.7
30	2.30	689.6
31	2.31	692.2
32	2.33	698.6
33	2.35	705.2
34	2.78	834.0
35	2.80	840.7
36	2.83	848.4

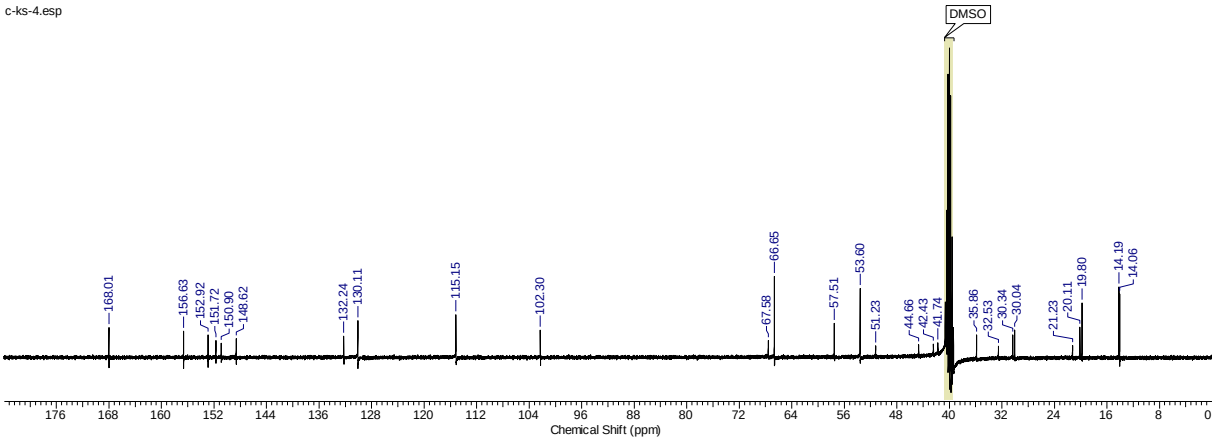
No.	(ppm)	(Hz)
37	3.19	955.8
38	3.21	962.2
39	3.23	968.4
40	3.25	975.0
41	3.26	978.6
42	3.28	983.8
43	3.49	1046.3
44	3.50	1051.0
45	3.52	1055.6
46	3.57	1072.0
47	3.60	1079.2
48	3.62	1086.6

No.	(ppm)	(Hz)
49	3.76	1128.2
50	3.78	1135.6
51	3.81	1142.8
52	3.88	1165.3
53	3.91	1172.3
54	3.93	1179.2
55	3.99	1196.6
56	4.01	1202.5
57	4.03	1208.2
58	4.41	1322.6
59	6.85	2055.0
60	6.88	2063.7

No.	(ppm)	(Hz)
61	7.13	2139.9
62	7.16	2148.6
63	7.86	2360.0
64	7.88	2365.6
65	7.90	2371.0

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M16	[0.83 .. 0.93]
2	1.26	4	m	-	M15	[1.18 .. 1.35]
3	1.46	2	dt	14.68, 7.41	M14	[1.41 .. 1.52]
4	1.62	2	quin	7.25	M13	[1.57 .. 1.68]
5	1.98	2	m	-	M12	[1.93 .. 2.02]
6	2.32	6	m	-	M11	[2.28 .. 2.36]
7	2.80	2	t	7.18	M10	[2.77 .. 2.84]
8	3.23	4	m	-	M09	[3.17 .. 3.30]
9	3.50	4	t	4.60	M08	[3.48 .. 3.53]
10	3.60	2	t	7.31	M07	[3.56 .. 3.63]
11	3.78	2	t	7.20	M06	[3.75 .. 3.82]
12	3.91	2	t	6.92	M05	[3.87 .. 3.94]
13	4.01	2	t	5.77	M04	[3.98 .. 4.04]
14	4.41	2	s	-	M17	[4.39 .. 4.42]
15	6.86	2	d	8.72	M03	[6.83 .. 6.89]
16	7.15	2	d	8.72	M02	[7.11 .. 7.18]
17	7.88	1	t	5.51	M01	[7.85 .. 7.91]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.83 - 0.93 (m, 6 H) 1.18 - 1.35 (m, 4 H) 1.46 (dt, *J*=14.68, 7.41 Hz, 2 H) 1.62 (quin, *J*=7.25 Hz, 2 H) 1.93 - 2.02 (m, 2 H) 2.28 - 2.36 (m, 6 H) 2.80 (t, *J*=7.18 Hz, 2 H) 3.17 - 3.30 (m, 4 H) 3.50 (t, *J*=4.60 Hz, 4 H) 3.60 (t, *J*=7.31 Hz, 2 H) 3.78 (t, *J*=7.20 Hz, 2 H) 3.91 (t, *J*=6.92 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.41 (s, 2 H) 6.86 (d, *J*=8.72 Hz, 2 H) 7.15 (d, *J*=8.72 Hz, 2 H) 7.88 (t, *J*=5.51 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.06	1414.8
2	14.19	1428.0
3	19.80	1992.2
4	20.11	2023.7

No.	(ppm)	(Hz)
5	21.23	2135.9
6	30.04	3022.9
7	30.34	3052.9
8	32.53	3273.7

No.	(ppm)	(Hz)
9	35.86	3608.3
10	41.74	4200.3
11	42.43	4270.0
12	44.66	4494.5

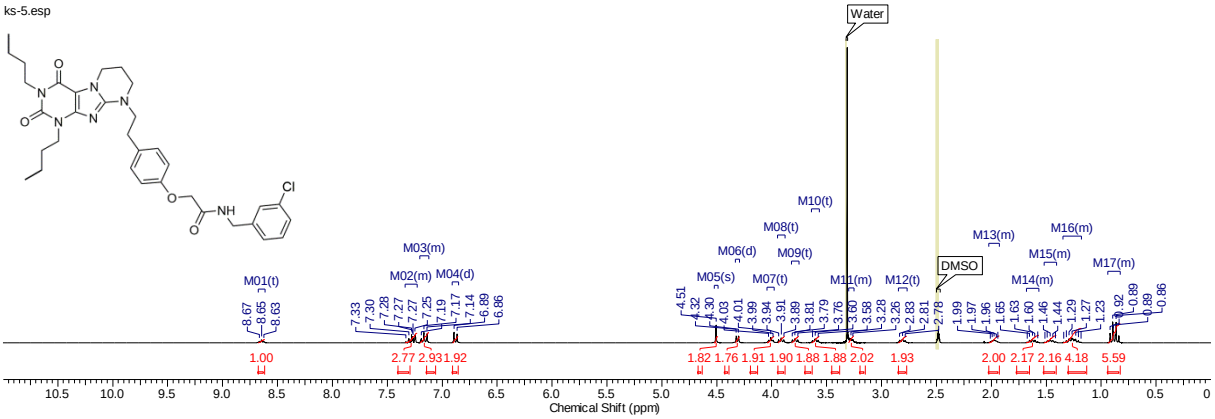
No.	(ppm)	(Hz)
13	51.23	5155.4
14	53.60	5393.8
15	57.51	5787.8
16	66.65	6707.0

No.	(ppm)	(Hz)
17	67.58	6800.9
18	102.30	10295.0
19	115.15	11587.6
20	130.11	13092.9

No.	(ppm)	(Hz)
21	132.24	13307.9
22	148.62	14956.3
23	150.90	15185.9
24	151.72	15268.0

No.	(ppm)	(Hz)
25	152.92	15388.3
26	156.63	15762.5
27	168.01	16907.6

N-(3-chlorobenzyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (30)



No.	(ppm)	(Hz)
1	0.86	259.3
2	0.89	266.4
3	0.89	268.5
4	0.92	275.7
5	1.18	355.4
6	1.21	362.6
7	1.23	369.5
8	1.27	379.8
9	1.29	387.5
10	1.32	394.9
11	1.34	402.6

No.	(ppm)	(Hz)
12	1.42	424.9
13	1.44	432.6
14	1.46	439.5
15	1.49	447.2
16	1.51	454.2
17	1.58	473.7
18	1.60	481.1
19	1.63	488.0
20	1.65	495.5
21	1.67	502.4
22	1.94	582.1

No.	(ppm)	(Hz)
23	1.96	587.0
24	1.97	592.4
25	1.99	597.8
26	2.01	603.4
27	2.78	835.5
28	2.81	842.5
29	2.83	850.7
30	3.26	978.6
31	3.28	983.8
32	3.58	1073.5
33	3.60	1081.5

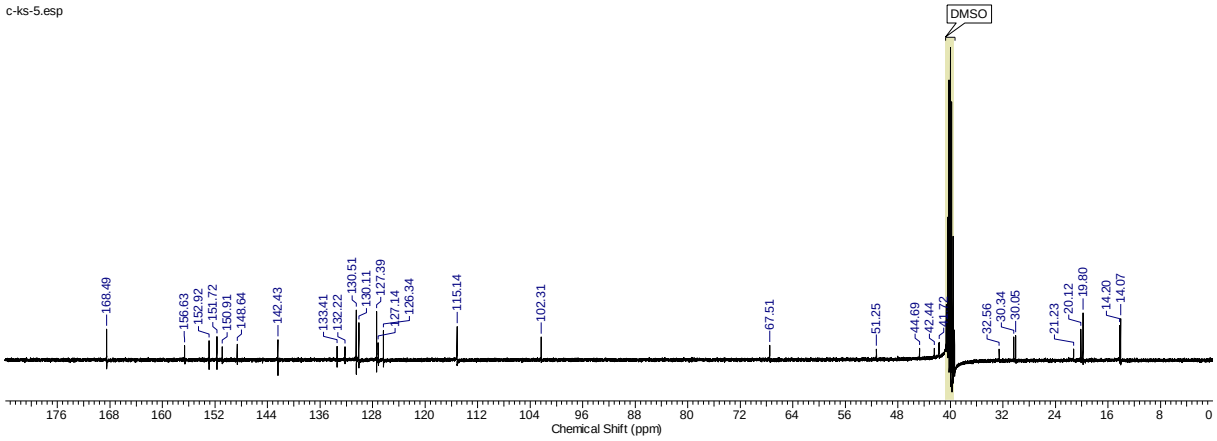
No.	(ppm)	(Hz)
34	3.63	1088.4
35	3.76	1129.2
36	3.79	1136.6
37	3.81	1143.8
38	3.89	1167.1
39	3.91	1174.3
40	3.94	1181.2
41	3.99	1196.9
42	4.01	1202.8
43	4.03	1208.7
44	4.30	1291.0

No.	(ppm)	(Hz)
45	4.32	1297.2
46	4.51	1352.6
47	6.86	2059.9
48	6.89	2068.6
49	7.14	2142.0
50	7.17	2150.7
51	7.19	2157.9
52	7.25	2174.8
53	7.27	2180.4
54	7.27	2182.2
55	7.28	2184.3

No.	(ppm)	(Hz)
56	7.30	2191.5
57	7.33	2199.9
58	8.63	2588.2
59	8.65	2594.4
60	8.67	2600.5

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.89	6	m	-	M17	[0.83 .. 0.94]
2	1.26	4	m	-	M16	[1.18 .. 1.35]
3	1.47	2	m	-	M15	[1.41 .. 1.52]
4	1.63	2	m	-	M14	[1.57 .. 1.68]
5	1.97	2	m	-	M13	[1.93 .. 2.02]
6	2.81	2	t	7.57	M12	[2.77 .. 2.85]
7	3.27	2	m	-	M11	[3.25 .. 3.30]
8	3.60	2	t	7.44	M10	[3.57 .. 3.64]
9	3.79	2	t	7.20	M09	[3.75 .. 3.82]
10	3.91	2	t	7.05	M08	[3.88 .. 3.95]
11	4.01	2	t	5.90	M07	[3.98 .. 4.04]
12	4.31	2	d	6.16	M06	[4.29 .. 4.33]
13	4.51	2	s	-	M05	[4.49 .. 4.52]
14	6.88	2	d	8.72	M04	[6.85 .. 6.91]
15	7.17	3	m	-	M03	[7.12 .. 7.21]
16	7.28	3	m	-	M02	[7.23 .. 7.34]
17	8.65	1	t	6.16	M01	[8.61 .. 8.68]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.83 - 0.94 (m, 6 H) 1.18 - 1.35 (m, 4 H) 1.41 - 1.52 (m, 2 H) 1.57 - 1.68 (m, 2 H) 1.93 - 2.02 (m, 2 H) 2.81 (t, *J*=7.57 Hz, 2 H) 3.25 - 3.30 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.79 (t, *J*=7.20 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.31 (d, *J*=6.16 Hz, 2 H) 4.51 (s, 2 H) 6.88 (d, *J*=8.72 Hz, 2 H) 7.12 - 7.21 (m, 3 H) 7.23 - 7.34 (m, 3 H) 8.65 (t, *J*=6.16 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.07	1415.6
2	14.20	1428.8
3	19.80	1992.9
4	20.12	2024.4
5	21.23	2135.9

No.	(ppm)	(Hz)
6	30.05	3023.6
7	30.34	3052.9
8	32.56	3276.7
9	41.72	4198.1
10	42.44	4270.7

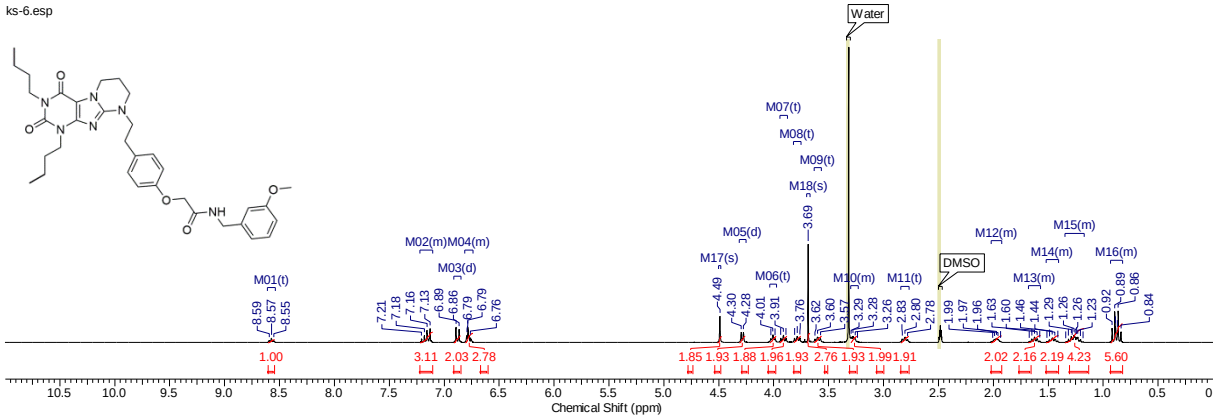
No.	(ppm)	(Hz)
11	44.69	4497.4
12	51.25	5157.6
13	67.51	6793.5
14	102.31	10295.7
15	115.14	11586.9

No.	(ppm)	(Hz)
16	126.34	12713.7
17	127.14	12794.4
18	127.39	12819.3
19	130.11	13092.9
20	130.51	13133.3

No.	(ppm)	(Hz)
21	132.22	13305.7
22	133.41	13425.2
23	142.43	14333.4
24	148.64	14957.7
25	150.91	15186.6

No.	(ppm)	(Hz)
26	151.72	15268.0
27	152.92	15389.1
28	156.63	15761.7
29	168.49	16956.0

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(3-methoxybenzyl)acetamide (31)



No.	(ppm)	(Hz)
1	0.84	251.6
2	0.86	259.0
3	0.87	261.0
4	0.89	266.2
5	0.89	268.5
6	0.92	275.7
7	1.18	354.9
8	1.21	362.1
9	1.23	369.3
10	1.24	372.4
11	1.26	377.0
12	1.26	379.5

No.	(ppm)	(Hz)
13	1.28	384.4
14	1.29	387.0
15	1.32	394.7
16	1.34	402.1
17	1.41	424.4
18	1.44	432.1
19	1.46	439.0
20	1.49	446.7
21	1.51	453.9
22	1.58	473.1
23	1.60	480.8
24	1.63	487.8

No.	(ppm)	(Hz)
25	1.65	494.9
26	1.67	502.1
27	1.93	580.6
28	1.96	587.3
29	1.97	592.1
30	1.99	597.3
31	2.01	602.1
32	2.78	834.5
33	2.80	841.4
34	2.83	849.1
35	3.24	971.2
36	3.26	977.6

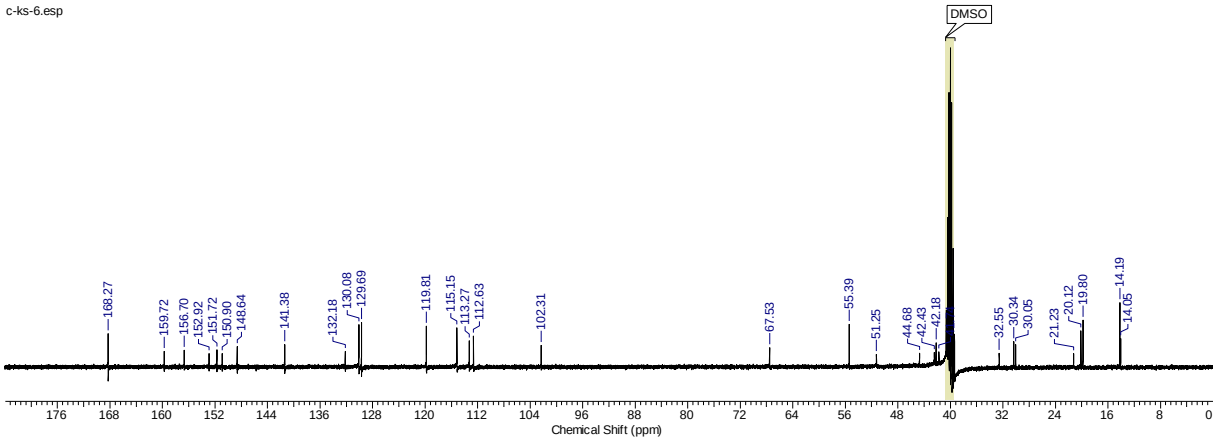
No.	(ppm)	(Hz)
37	3.28	983.5
38	3.29	988.6
39	3.57	1072.5
40	3.60	1080.5
41	3.62	1087.4
42	3.69	1106.4
43	3.76	1128.7
44	3.79	1136.1
45	3.81	1143.3
46	3.89	1166.6
47	3.91	1173.6
48	3.93	1180.7

No.	(ppm)	(Hz)
49	3.99	1196.6
50	4.01	1202.5
51	4.03	1208.2
52	4.28	1283.1
53	4.30	1289.2
54	4.49	1347.2
55	6.76	2028.6
56	6.79	2036.3
57	6.79	2038.9
58	6.86	2059.9
59	6.89	2068.6
60	7.13	2139.4

No.	(ppm)	(Hz)
61	7.16	2147.9
62	7.18	2154.8
63	7.21	2162.7
64	8.55	2566.7
65	8.57	2572.8
66	8.59	2579.0

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M16	[0.82 .. 0.93]
2	1.26	4	m	-	M15	[1.17 .. 1.35]
3	1.46	2	m	-	M14	[1.40 .. 1.52]
4	1.63	2	m	-	M13	[1.57 .. 1.68]
5	1.97	2	m	-	M12	[1.92 .. 2.02]
6	2.80	2	t	7.31	M11	[2.77 .. 2.84]
7	3.27	2	m	-	M10	[3.23 .. 3.30]
8	3.60	2	t	7.44	M09	[3.57 .. 3.63]
9	3.69	3	s	-	M18	[3.67 .. 3.70]
10	3.79	2	t	7.40	M08	[3.75 .. 3.82]
11	3.91	2	t	7.05	M07	[3.87 .. 3.94]
12	4.01	2	t	5.77	M06	[3.97 .. 4.03]
13	4.29	2	d	6.16	M05	[4.25 .. 4.31]
14	4.49	2	s	-	M17	[4.48 .. 4.50]
15	6.78	3	m	-	M04	[6.74 .. 6.81]
16	6.88	2	d	8.72	M03	[6.85 .. 6.91]
17	7.17	3	m	-	M02	[7.11 .. 7.22]
18	8.57	1	t	6.16	M01	[8.54 .. 8.61]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.82 - 0.93 (m, 6 H) 1.17 - 1.35 (m, 4 H) 1.40 - 1.52 (m, 2 H) 1.57 - 1.68 (m, 2 H) 1.92 - 2.02 (m, 2 H) 2.80 (t, *J*=7.31 Hz, 2 H) 3.23 - 3.30 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.69 (s, 3 H) 3.79 (t, *J*=7.40 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.29 (d, *J*=6.16 Hz, 2 H) 4.49 (s, 2 H) 6.74 - 6.81 (m, 3 H) 6.88 (d, *J*=8.72 Hz, 2 H) 7.11 - 7.22 (m, 3 H) 8.57 (t, *J*=6.16 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.05	1414.1
2	14.19	1428.0
3	19.80	1992.2
4	20.12	2024.4
5	21.23	2135.9

No.	(ppm)	(Hz)
6	30.05	3023.6
7	30.34	3052.9
8	32.55	3276.0
9	41.74	4200.3
10	42.18	4245.0

No.	(ppm)	(Hz)
11	42.43	4270.0
12	44.68	4496.7
13	51.25	5157.6
14	55.39	5574.3
15	67.53	6795.7

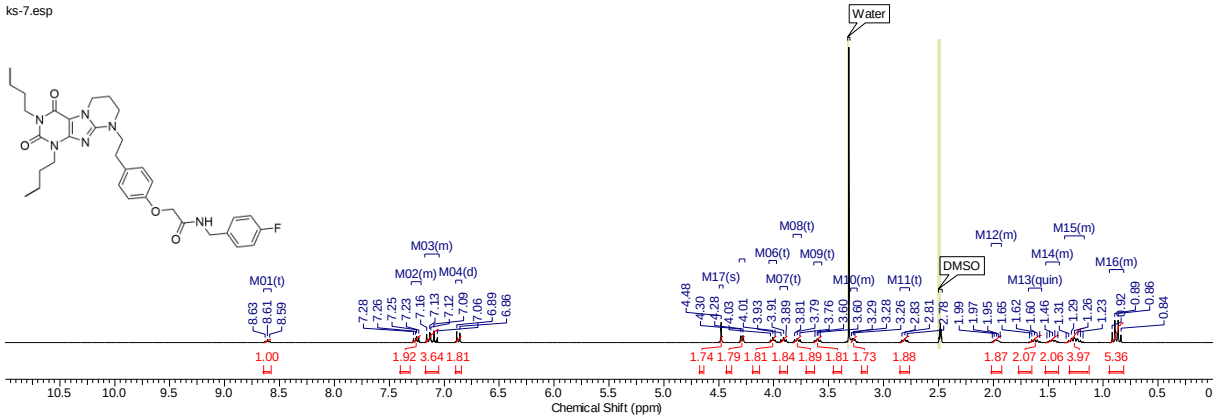
No.	(ppm)	(Hz)
16	102.31	10295.7
17	112.63	11334.5
18	113.27	11398.3
19	115.15	11587.6
20	119.81	12056.4

No.	(ppm)	(Hz)
21	129.69	13051.1
22	130.08	13090.0
23	132.18	13301.3
24	141.38	14227.1
25	148.64	14957.7

No.	(ppm)	(Hz)
26	150.90	15185.9
27	151.72	15268.0
28	152.92	15389.1
29	156.70	15769.1
30	159.72	16073.5

No.	(ppm)	(Hz)
31	168.27	16933.3

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-fluorobenzyl)acetamide (32)



No.	(ppm)	(Hz)
1	0.84	251.6
2	0.86	259.0
3	0.89	268.2
4	0.92	275.4
5	1.18	354.9
6	1.21	362.1
7	1.23	369.3
8	1.26	379.0
9	1.29	386.7
10	1.31	394.2
11	1.34	401.6

No.	(ppm)	(Hz)
12	1.41	424.2
13	1.44	432.1
14	1.46	438.8
15	1.49	446.7
16	1.51	453.9
17	1.58	472.9
18	1.60	480.6
19	1.62	487.5
20	1.65	494.7
21	1.67	501.6
22	1.94	581.6

No.	(ppm)	(Hz)
23	1.95	586.5
24	1.97	591.9
25	1.99	597.5
26	2.01	602.7
27	2.78	835.3
28	2.81	841.9
29	2.83	849.9
30	3.26	978.1
31	3.28	983.0
32	3.29	988.1
33	3.58	1073.0

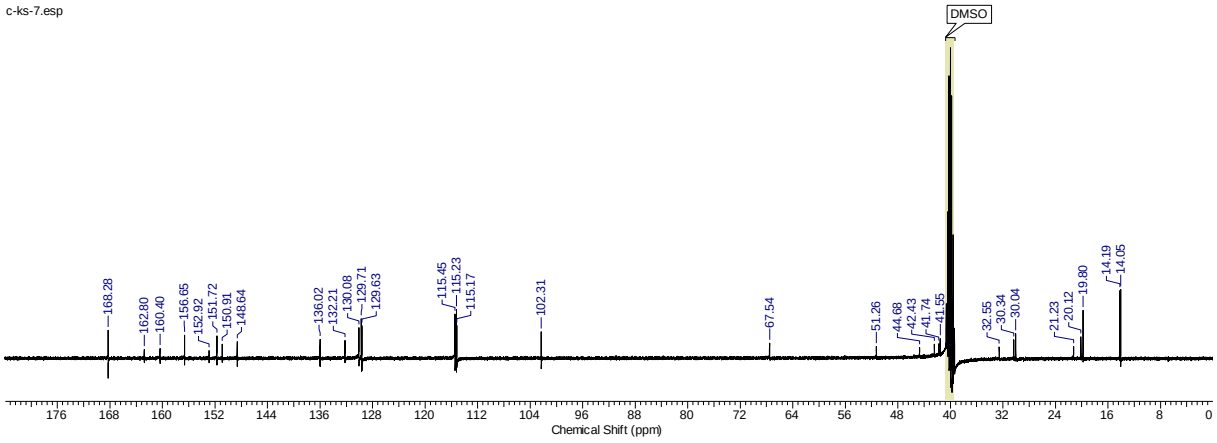
No.	(ppm)	(Hz)
34	3.60	1079.4
35	3.60	1081.0
36	3.63	1087.9
37	3.76	1128.7
38	3.79	1136.1
39	3.81	1143.3
40	3.89	1166.4
41	3.91	1173.3
42	3.93	1180.2
43	3.99	1196.6
44	4.01	1202.8

No.	(ppm)	(Hz)
45	4.03	1208.7
46	4.28	1284.1
47	4.30	1290.2
48	4.48	1343.8
49	6.86	2057.8
50	6.89	2066.6
51	7.06	2119.9
52	7.09	2128.6
53	7.12	2137.6
54	7.13	2139.9
55	7.16	2148.6

No.	(ppm)	(Hz)
56	7.23	2170.2
57	7.25	2175.8
58	7.26	2178.9
59	7.28	2184.5
60	8.59	2577.4
61	8.61	2583.6
62	8.63	2589.8

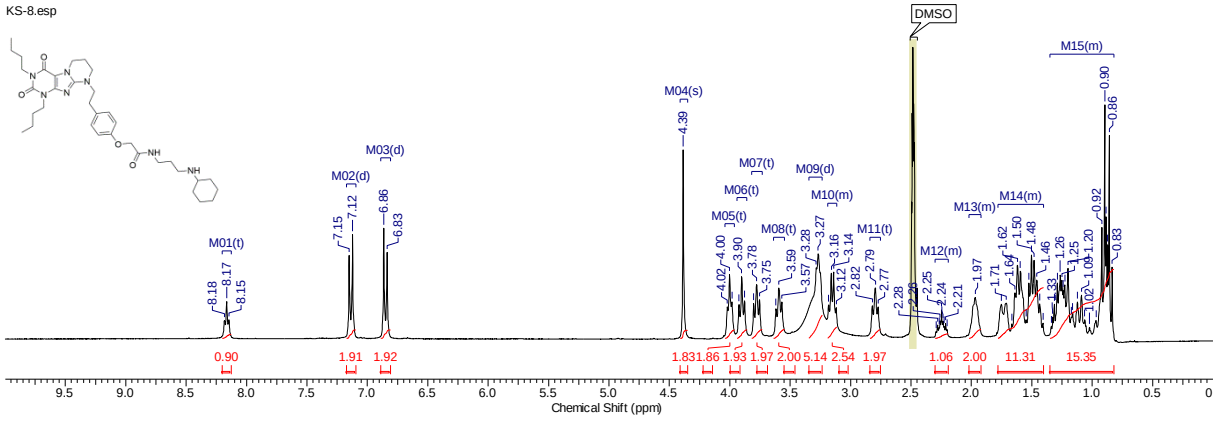
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M16	[0.81 .. 0.94]
2	1.26	4	m	-	M15	[1.17 .. 1.35]
3	1.46	2	m	-	M14	[1.40 .. 1.52]
4	1.62	2	quin	7.18	M13	[1.56 .. 1.68]
5	1.97	2	m	-	M12	[1.93 .. 2.02]
6	2.81	2	t	7.31	M11	[2.76 .. 2.85]
7	3.28	2	m	-	M10	[3.24 .. 3.30]
8	3.60	2	t	7.44	M09	[3.56 .. 3.64]
9	3.79	2	t	7.40	M08	[3.75 .. 3.82]
10	3.91	2	t	6.92	M07	[3.88 .. 3.94]
11	4.01	2	t	6.03	M06	[3.97 .. 4.04]
12	4.29	2	d	6.16	M05	[4.26 .. 4.31]
13	4.48	2	s	-	M17	[4.46 .. 4.49]
14	6.87	2	d	8.72	M04	[6.84 .. 6.90]
15	7.11	4	m	-	M03	[7.05 .. 7.18]
16	7.26	2	m	-	M02	[7.21 .. 7.30]
17	8.61	1	t	6.16	M01	[8.58 .. 8.65]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.81 - 0.94 (m, 6 H) 1.17 - 1.35 (m, 4 H) 1.40 - 1.52 (m, 2 H) 1.62 (quin, *J*=7.18 Hz, 2 H) 1.93 - 2.02 (m, 2 H) 2.81 (t, *J*=7.31 Hz, 2 H) 3.24 - 3.30 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.79 (t, *J*=7.40 Hz, 2 H) 3.91 (t, *J*=6.92 Hz, 2 H) 4.01 (t, *J*=6.03 Hz, 2 H) 4.29 (d, *J*=6.16 Hz, 2 H) 4.48 (s, 2 H) 6.87 (d, *J*=8.72 Hz, 2 H) 7.05 - 7.18 (m, 4 H) 7.21 - 7.30 (m, 2 H) 8.61 (t, *J*=6.16 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	14.05	1414.1	6	30.04	3022.9	11	42.43	4270.0	16	115.17	11589.8	21	130.08	13090.7	26	151.72	15268.0	31	168.28	16934.8
2	14.19	1428.0	7	30.34	3052.9	12	44.68	4496.7	17	115.23	11596.4	22	132.21	13304.9	27	152.92	15389.1						
3	19.80	1992.2	8	32.55	3276.0	13	51.26	5158.4	18	115.45	11617.7	23	136.02	13687.9	28	156.65	15763.9						
4	20.12	2024.4	9	41.55	4181.2	14	67.54	6796.5	19	129.63	13045.2	24	148.64	14957.7	29	160.40	16141.0						
5	21.23	2135.9	10	41.74	4200.3	15	102.31	10295.7	20	129.71	13053.3	25	150.91	15186.6	30	162.80	16383.1						

N-(3-(cyclohexylamino)propyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (33)



No.	(ppm)	(Hz)
1	0.83	250.5
2	0.86	257.6
3	0.87	261.7
4	0.88	265.2
5	0.90	268.7
6	0.92	276.3
7	0.97	290.4
8	1.02	306.8
9	1.06	318.5
10	1.09	326.7
11	1.12	336.7
12	1.16	349.0
13	1.17	351.9

No.	(ppm)	(Hz)
14	1.20	360.1
15	1.23	367.8
16	1.24	371.9
17	1.25	375.4
18	1.26	379.5
19	1.29	386.5
20	1.31	394.1
21	1.33	398.2
22	1.34	401.8
23	1.41	422.3
24	1.43	430.5
25	1.46	437.5
26	1.48	444.5

No.	(ppm)	(Hz)
27	1.50	451.0
28	1.52	457.4
29	1.55	463.9
30	1.59	478.5
31	1.62	485.6
32	1.64	492.0
33	1.66	499.6
34	1.71	513.7
35	1.75	525.4
36	1.97	590.5
37	2.20	660.8
38	2.21	663.7
39	2.23	667.8

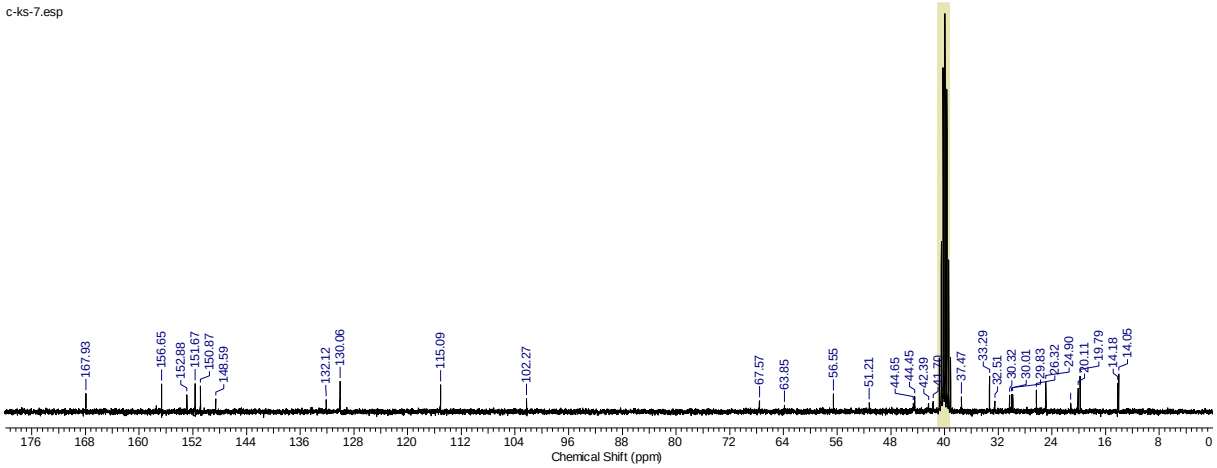
No.	(ppm)	(Hz)
40	2.24	670.8
41	2.25	674.3
42	2.26	677.8
43	2.27	680.2
44	2.28	684.3
45	2.29	687.8
46	2.77	832.0
47	2.79	838.4
48	2.82	846.0
49	3.12	935.7
50	3.14	942.1
51	3.16	948.0
52	3.18	955.0

No.	(ppm)	(Hz)
53	3.27	980.8
54	3.28	985.5
55	3.57	1071.1
56	3.59	1078.7
57	3.62	1085.7
58	3.75	1126.2
59	3.78	1133.8
60	3.80	1140.8
61	3.88	1163.7
62	3.90	1170.7
63	3.92	1177.8
64	3.98	1194.8
65	4.00	1200.6

No.	(ppm)	(Hz)
66	4.02	1206.5
67	4.39	1316.1
68	6.83	2051.0
69	6.86	2059.8
70	7.12	2137.2
71	7.15	2146.0
72	8.15	2444.3
73	8.17	2450.2
74	8.18	2455.5

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	1.11	16	m	-	M15	[0.82 .. 1.35]
2	1.56	10	m	-	M14	[1.40 .. 1.78]
3	1.97	2	m	-	M13	[1.92 .. 2.02]
4	2.25	1	m	-	M12	[2.19 .. 2.30]
5	2.80	2	t	7.03	M11	[2.75 .. 2.84]
6	3.15	2	m	-	M10	[3.11 .. 3.19]
7	3.28	5	d	4.69	M09	[3.23 .. 3.34]
8	3.59	2	t	7.33	M08	[3.55 .. 3.64]
9	3.78	2	t	7.33	M07	[3.73 .. 3.82]
10	3.90	2	t	7.03	M06	[3.86 .. 3.94]
11	4.00	2	t	5.86	M05	[3.96 .. 4.04]
12	4.39	2	s	-	M04	[4.35 .. 4.41]
13	6.85	2	d	8.79	M03	[6.81 .. 6.89]
14	7.14	2	d	8.79	M02	[7.10 .. 7.17]
15	8.16	1	t	5.57	M01	[8.13 .. 8.20]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.82 - 1.35 (m, 16 H) 1.40 - 1.78 (m, 10 H) 1.92 - 2.02 (m, 2 H) 2.19 - 2.30 (m, 1 H) 2.80 (t, *J*=7.03 Hz, 2 H) 3.11 - 3.19 (m, 2 H) 3.28 (d, *J*=4.69 Hz, 5 H) 3.59 (t, *J*=7.33 Hz, 2 H) 3.78 (t, *J*=7.33 Hz, 2 H) 3.90 (t, *J*=7.03 Hz, 2 H) 4.00 (t, *J*=5.86 Hz, 2 H) 4.39 (s, 2 H) 6.85 (d, *J*=8.79 Hz, 2 H) 7.14 (d, *J*=8.79 Hz, 2 H) 8.16 (t, *J*=5.57 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.05	1060.1
2	14.18	1070.4
3	19.79	1493.1
4	20.11	1517.3
5	21.19	1599.1

No.	(ppm)	(Hz)
6	24.90	1878.9
7	26.32	1986.0
8	29.83	2250.9
9	30.01	2264.7
10	30.32	2287.8

No.	(ppm)	(Hz)
11	32.51	2453.6
12	33.29	2512.3
13	37.47	2827.9
14	41.70	3146.9
15	42.39	3198.7

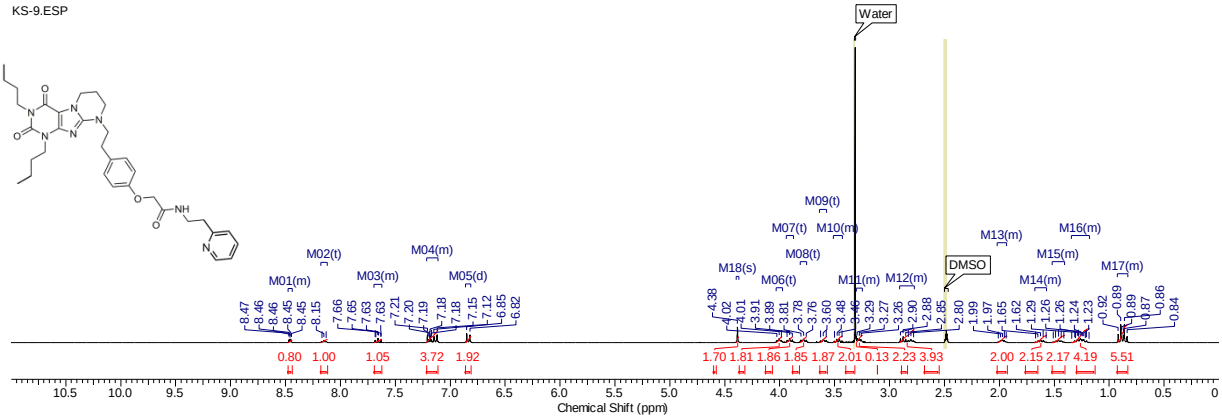
No.	(ppm)	(Hz)
16	44.45	3354.2
17	44.65	3369.2
18	51.21	3864.4
19	56.55	4267.5
20	63.85	4818.0

No.	(ppm)	(Hz)
21	67.57	5099.0
22	102.27	7717.9
23	115.09	8685.3
24	130.06	9815.1
25	132.12	9970.6

No.	(ppm)	(Hz)
26	148.59	11213.3
27	150.87	11384.9
28	151.67	11445.9
29	152.88	11536.9
30	156.65	11821.3

No.	(ppm)	(Hz)
31	167.93	12672.4

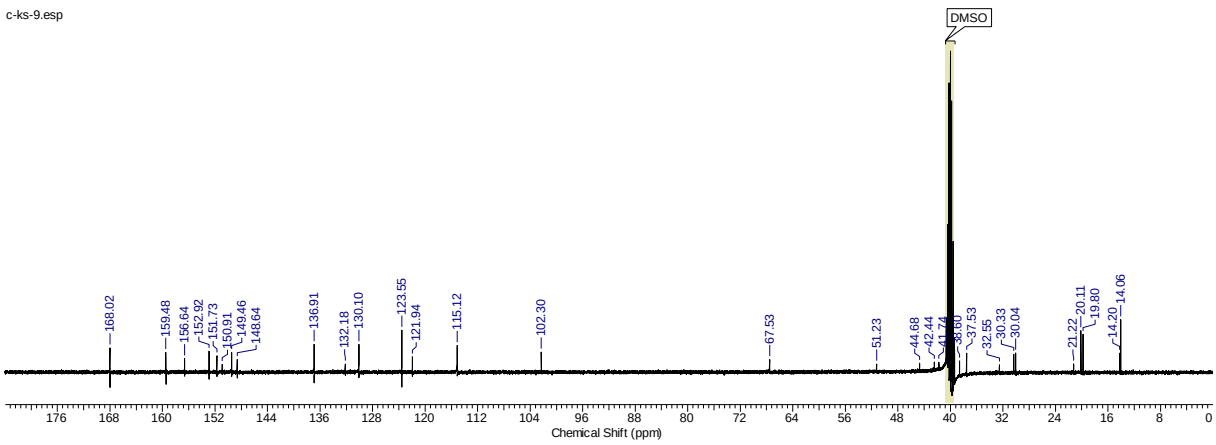
2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(pyridin-2-yl)ethyl)acetamide (34)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	0.84	251.3	13	1.26	379.3	25	1.60	480.1	37	2.85	856.0	49	3.63	1088.4	61	6.85	2055.5	73	7.65	2296.9
2	0.86	258.7	14	1.28	384.2	26	1.62	487.3	38	2.88	863.0	50	3.76	1127.9	62	7.12	2136.6	74	7.66	2298.7
3	0.87	260.8	15	1.29	386.7	27	1.65	494.4	39	2.90	870.4	51	3.78	1135.1	63	7.15	2145.3	75	7.68	2304.3
4	0.89	265.9	16	1.30	391.6	28	1.67	501.4	40	3.26	977.6	52	3.81	1142.5	64	7.17	2151.5	76	7.69	2306.4
5	0.89	268.2	17	1.31	394.4	29	1.94	581.4	41	3.27	982.2	53	3.89	1165.9	65	7.18	2153.8	77	8.13	2439.7
6	0.92	275.4	18	1.34	401.8	30	1.96	586.8	42	3.29	988.6	54	3.91	1173.0	66	7.18	2155.6	78	8.15	2445.4
7	1.18	354.7	19	1.41	423.6	31	1.97	591.6	43	3.43	1030.4	55	3.93	1180.0	67	7.19	2157.9	79	8.17	2451.0
8	1.21	361.8	20	1.44	431.6	32	1.99	597.3	44	3.46	1037.9	56	3.99	1196.1	68	7.19	2158.9	80	8.45	2534.4
9	1.22	364.9	21	1.46	438.5	33	2.01	603.2	45	3.48	1043.8	57	4.01	1202.0	69	7.20	2161.5	81	8.45	2536.2
10	1.23	369.0	22	1.49	446.2	34	2.78	834.5	46	3.50	1051.0	58	4.02	1207.7	70	7.21	2163.0	82	8.46	2538.0
11	1.24	372.1	23	1.51	453.1	35	2.80	841.4	47	3.58	1073.5	59	4.38	1315.6	71	7.63	2289.2	83	8.46	2540.0
12	1.26	376.7	24	1.58	472.6	36	2.83	849.1	48	3.60	1081.0	60	6.82	2046.8	72	7.63	2291.0	84	8.47	2541.8

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M17	[0.83 .. 0.93]
2	1.26	4	m	-	M16	[1.18 .. 1.34]
3	1.46	2	m	-	M15	[1.41 .. 1.52]
4	1.62	2	m	-	M14	[1.57 .. 1.68]
5	1.97	2	m	-	M13	[1.93 .. 2.02]
6	2.84	4	m	-	M12	[2.77 .. 2.91]
7	3.28	2	m	-	M11	[3.25 .. 3.30]
8	3.47	2	m	-	M10	[3.43 .. 3.51]
9	3.60	2	t	7.44	M09	[3.57 .. 3.64]
10	3.78	2	t	7.20	M08	[3.75 .. 3.81]
11	3.91	2	t	7.05	M07	[3.88 .. 3.94]
12	4.01	2	t	5.77	M06	[3.98 .. 4.03]
13	4.38	2	s	-	M18	[4.37 .. 4.40]
14	6.84	2	d	8.72	M05	[6.81 .. 6.86]
15	7.18	4	m	-	M04	[7.11 .. 7.21]
16	7.66	1	m	-	M03	[7.62 .. 7.69]
17	8.15	1	t	5.64	M02	[8.12 .. 8.18]
18	8.46	1	m	-	M01	[8.44 .. 8.48]

^{1}H NMR (300 MHz, DMSO-d_6) ⍰ ppm 0.83 - 0.93 (m, 6 H) 1.18 - 1.34 (m, 4 H) 1.41 - 1.52 (m, 2 H) 1.57 - 1.68 (m, 2 H) 1.93 - 2.02 (m, 2 H) 2.77 - 2.91 (m, 4 H) 3.25 - 3.30 (m, 2 H) 3.43 - 3.51 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.78 (t, *J*=7.20 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.38 (s, 2 H) 6.84 (d, *J*=8.72 Hz, 2 H) 7.11 - 7.21 (m, 4 H) 7.62 - 7.69 (m, 1 H) 8.15 (t, *J*=5.64 Hz, 1 H) 8.44 - 8.48 (m, 1 H)



No.	(ppm)	(Hz)
1	14.06	1414.8
2	14.20	1428.8
3	19.80	1992.2
4	20.11	2023.7
5	21.22	2135.2

No.	(ppm)	(Hz)
6	30.04	3022.9
7	30.33	3052.2
8	32.55	3275.2
9	37.53	3777.0
10	38.60	3884.8

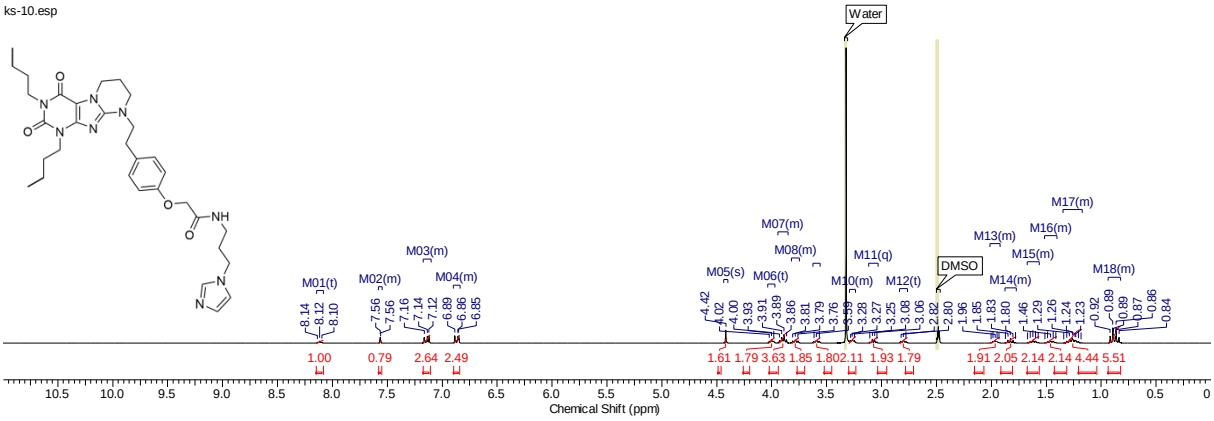
No.	(ppm)	(Hz)
11	41.74	4200.3
12	42.44	4270.7
13	44.68	4496.7
14	51.23	5155.4
15	67.53	6795.7

No.	(ppm)	(Hz)
16	102.30	10295.0
17	115.12	11584.7
18	121.94	12271.3
19	123.55	12433.4
20	130.10	13092.2

No.	(ppm)	(Hz)
21	132.18	13301.3
22	136.91	13777.4
23	148.64	14957.7
24	149.46	15040.6
25	150.91	15186.6

No.	(ppm)	(Hz)
26	151.73	15268.8
27	152.92	15388.3
28	156.64	15763.2
29	159.48	16049.3
30	168.02	16908.4

N-(3-(1H-imidazol-1-yl)propyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (35)



No.	(ppm)	(Hz)
1	0.84	251.6
2	0.86	259.0
3	0.87	260.8
4	0.89	266.2
5	0.89	268.2
6	0.92	275.7
7	1.18	354.7
8	1.21	361.8
9	1.23	369.0
10	1.24	371.8
11	1.26	378.8
12	1.29	386.5

No.	(ppm)	(Hz)
13	1.31	393.9
14	1.34	401.8
15	1.41	424.2
16	1.44	431.6
17	1.46	438.5
18	1.49	446.5
19	1.51	453.4
20	1.57	471.9
21	1.60	479.6
22	1.62	486.5
23	1.65	493.7
24	1.67	500.8

No.	(ppm)	(Hz)
25	1.78	534.4
26	1.80	541.1
27	1.83	548.0
28	1.85	554.7
29	1.87	561.6
30	1.93	579.1
31	1.95	584.5
32	1.96	589.6
33	1.98	595.5
34	2.00	601.1
35	2.78	833.0
36	2.80	840.1

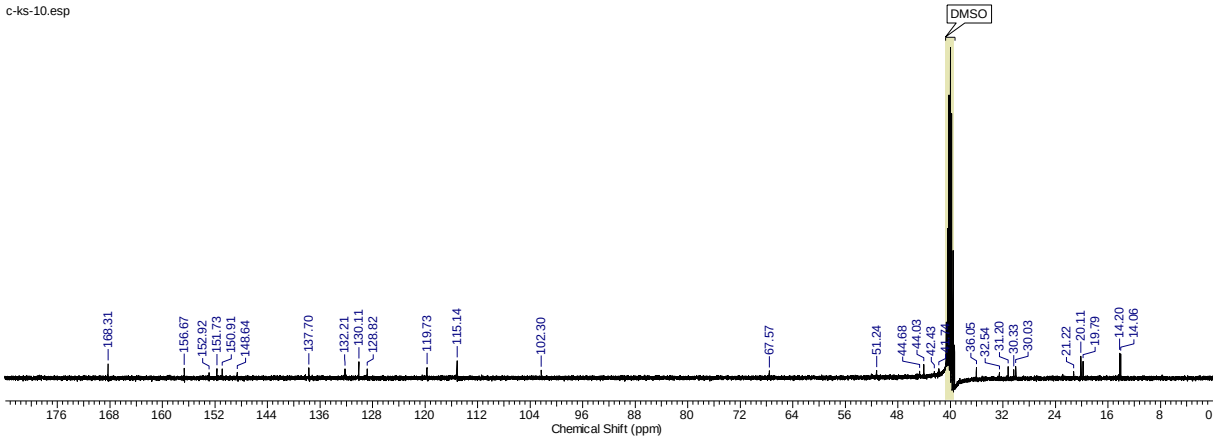
No.	(ppm)	(Hz)
37	2.82	847.3
38	3.04	912.5
39	3.06	919.1
40	3.08	925.3
41	3.11	932.0
42	3.25	974.5
43	3.27	980.4
44	3.28	985.1
45	3.57	1070.5
46	3.59	1078.1
47	3.62	1084.8
48	3.76	1128.4

No.	(ppm)	(Hz)
49	3.79	1135.9
50	3.81	1142.8
51	3.86	1159.7
52	3.89	1166.6
53	3.91	1173.3
54	3.93	1178.9
55	3.98	1195.1
56	4.00	1200.7
57	4.02	1206.6
58	4.42	1325.6
59	6.85	2055.5
60	6.86	2057.6

No.	(ppm)	(Hz)
61	6.89	2066.3
62	7.12	2136.8
63	7.14	2141.2
64	7.16	2149.9
65	7.56	2268.9
66	7.56	2269.9
67	8.10	2429.7
68	8.12	2435.4
69	8.14	2441.3

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M18	[0.82 .. 0.93]
2	1.26	4	m	-	M17	[1.17 .. 1.35]
3	1.46	2	m	-	M16	[1.40 .. 1.52]
4	1.62	2	m	-	M15	[1.56 .. 1.67]
5	1.83	2	m	-	M14	[1.77 .. 1.88]
6	1.97	2	m	-	M13	[1.92 .. 2.01]
7	2.80	2	t	7.18	M12	[2.76 .. 2.83]
8	3.07	2	q	6.67	M11	[3.03 .. 3.12]
9	3.27	2	m	-	M10	[3.24 .. 3.29]
10	3.59	2	t	7.18	M09	[3.56 .. 3.62]
11	3.78	2	m	-	M08	[3.75 .. 3.82]
12	3.90	4	m	-	M07	[3.85 .. 3.94]
13	4.00	2	t	5.77	M06	[3.97 .. 4.04]
14	4.42	2	s	-	M05	[4.40 .. 4.44]
15	6.86	3	m	-	M04	[6.84 .. 6.90]
16	7.14	3	m	-	M03	[7.10 .. 7.17]
17	7.56	1	m	-	M02	[7.55 .. 7.58]
18	8.12	1	t	5.77	M01	[8.08 .. 8.14]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.82 - 0.93 (m, 6 H) 1.17 - 1.35 (m, 4 H) 1.40 - 1.52 (m, 2 H) 1.56 - 1.67 (m, 2 H) 1.77 - 1.88 (m, 2 H) 1.92 - 2.01 (m, 2 H) 2.80 (t, *J*=7.18 Hz, 2 H) 3.07 (q, *J*=6.67 Hz, 2 H) 3.24 - 3.29 (m, 2 H) 3.59 (t, *J*=7.18 Hz, 2 H) 3.75 - 3.82 (m, 2 H) 3.85 - 3.94 (m, 4 H) 4.00 (t, *J*=5.77 Hz, 2 H) 4.42 (s, 2 H) 6.84 - 6.90 (m, 3 H) 7.10 - 7.17 (m, 3 H) 7.55 - 7.58 (m, 1 H) 8.12 (t, *J*=5.77 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.06	1414.8
2	14.20	1428.8
3	19.79	1991.4
4	20.11	2023.7
5	21.22	2135.2

No.	(ppm)	(Hz)
6	30.03	3022.1
7	30.33	3052.2
8	31.20	3139.5
9	32.54	3274.5
10	36.05	3627.3

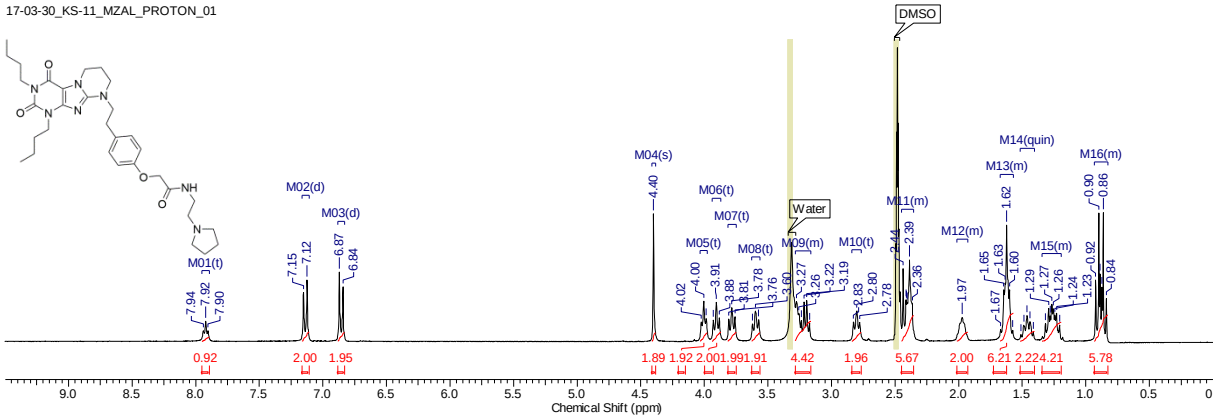
No.	(ppm)	(Hz)
11	41.74	4200.3
12	42.43	4270.0
13	44.03	4431.4
14	44.68	4496.7
15	51.24	5156.2

No.	(ppm)	(Hz)
16	67.57	6799.4
17	102.30	10295.0
18	115.14	11586.9
19	119.73	12048.3
20	128.82	12963.1

No.	(ppm)	(Hz)
21	130.11	13092.9
22	132.21	13304.2
23	137.70	13857.3
24	148.64	14957.7
25	150.91	15186.6

No.	(ppm)	(Hz)
26	151.73	15268.8
27	152.92	15389.1
28	156.67	15766.1
29	168.31	16937.7

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(2-(pyrrolidin-1-yl)ethyl)acetamide (36)



No.	(ppm)	(Hz)
1	0.84	251.7
2	0.86	258.7
3	0.87	262.3
4	0.89	266.4
5	0.90	269.3
6	0.92	276.9
7	1.21	361.9
8	1.23	368.9
9	1.24	373.0
10	1.26	377.1
11	1.27	380.1

No.	(ppm)	(Hz)
12	1.28	384.2
13	1.29	387.7
14	1.32	395.3
15	1.41	424.0
16	1.44	431.6
17	1.46	438.7
18	1.49	446.3
19	1.51	453.3
20	1.58	472.7
21	1.60	480.3
22	1.62	486.7

No.	(ppm)	(Hz)
23	1.63	490.3
24	1.65	493.8
25	1.67	500.8
26	1.97	591.7
27	2.36	709.5
28	2.39	715.9
29	2.40	721.2
30	2.41	722.9
31	2.41	724.1
32	2.44	731.1
33	2.78	833.7

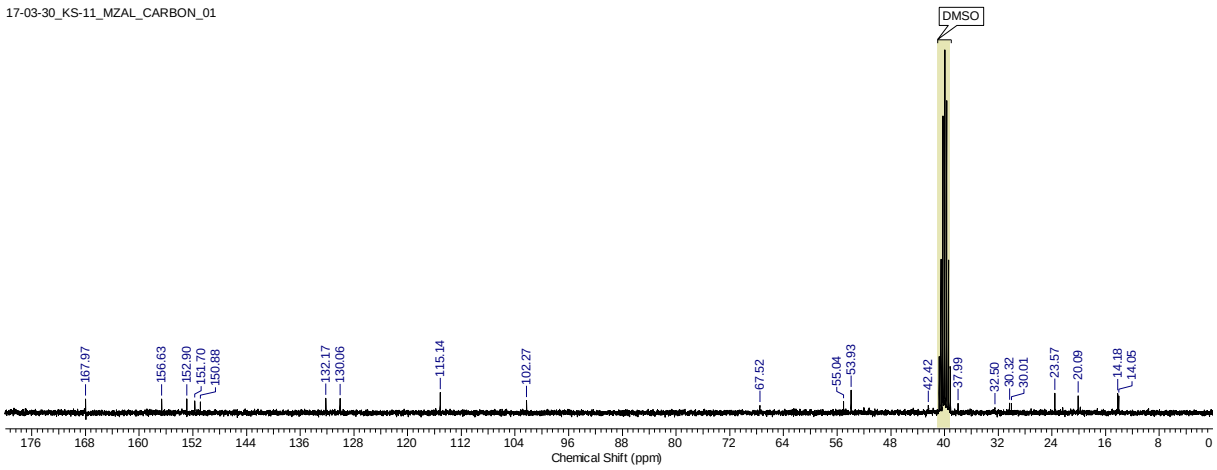
No.	(ppm)	(Hz)
34	2.80	840.7
35	2.83	848.4
36	3.17	952.1
37	3.19	958.6
38	3.22	965.0
39	3.24	971.4
40	3.26	977.3
41	3.27	982.6
42	3.57	1072.3
43	3.60	1079.9
44	3.62	1086.9

No.	(ppm)	(Hz)
45	3.76	1127.9
46	3.78	1135.6
47	3.81	1142.6
48	3.88	1164.9
49	3.91	1171.9
50	3.93	1178.9
51	3.99	1195.9
52	4.00	1201.8
53	4.02	1207.6
54	4.40	1320.2
55	6.84	2052.8

No.	(ppm)	(Hz)
56	6.87	2061.6
57	7.12	2137.8
58	7.15	2146.0
59	7.90	2371.6
60	7.92	2376.9
61	7.94	2382.8

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M16	[0.83 .. 0.93]
2	1.26	4	m	-	M15	[1.19 .. 1.34]
3	1.46	2	quin	7.33	M14	[1.40 .. 1.52]
4	1.62	6	m	-	M13	[1.57 .. 1.67]
5	1.97	2	m	-	M12	[1.93 .. 2.01]
6	2.40	6	m	-	M11	[2.36 .. 2.45]
7	2.80	2	t	7.33	M10	[2.77 .. 2.84]
8	3.23	4	m	-	M09	[3.16 .. 3.29]
9	3.60	2	t	7.33	M08	[3.56 .. 3.63]
10	3.78	2	t	7.33	M07	[3.75 .. 3.82]
11	3.91	2	t	7.03	M06	[3.87 .. 3.94]
12	4.00	2	t	5.86	M05	[3.98 .. 4.03]
13	4.40	2	s	-	M04	[4.38 .. 4.41]
14	6.86	2	d	8.79	M03	[6.83 .. 6.88]
15	7.14	2	d	8.21	M02	[7.11 .. 7.16]
16	7.92	1	t	5.57	M01	[7.89 .. 7.95]

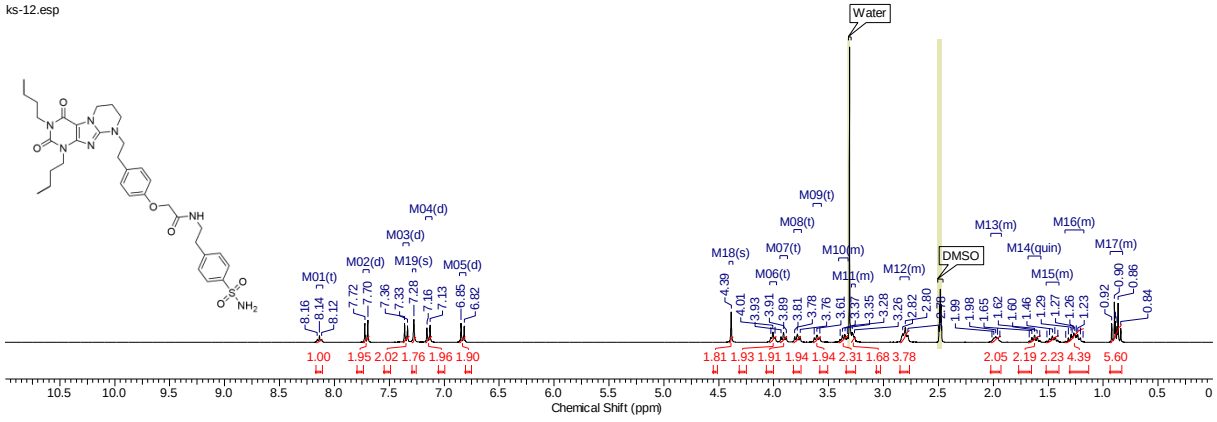
^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.83 - 0.93 (m, 6 H) 1.19 - 1.34 (m, 4 H) 1.46 (quin, *J*=7.33 Hz, 2 H) 1.57 - 1.67 (m, 6 H) 1.93 - 2.01 (m, 2 H) 2.36 - 2.45 (m, 6 H) 2.80 (t, *J*=7.33 Hz, 2 H) 3.16 - 3.29 (m, 4 H) 3.60 (t, *J*=7.33 Hz, 2 H) 3.78 (t, *J*=7.33 Hz, 2 H) 3.91 (t, *J*=7.03 Hz, 2 H) 4.00 (t, *J*=5.86 Hz, 2 H) 4.40 (s, 2 H) 6.86 (d, *J*=8.79 Hz, 2 H) 7.14 (d, *J*=8.21 Hz, 2 H) 7.92 (t, *J*=5.57 Hz, 1 H)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	14.05	1060.1	4	23.57	1778.7	7	32.50	2452.4	10	53.93	4069.4	13	102.27	7717.9	16	132.17	9974.1	19	152.90	11538.0
2	14.18	1070.4	5	30.01	2264.7	8	37.99	2867.1	11	55.04	4153.5	14	115.14	8688.8	17	150.88	11386.0	20	156.63	11820.2
3	20.09	1516.1	6	30.32	2287.8	9	42.42	3201.0	12	67.52	5095.5	15	130.06	9815.1	18	151.70	11448.2	21	167.97	12675.9

KS-12

2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)-N-(4-sulfamoylphenethyl)acetamide (37)



No.	(ppm)	(Hz)
1	0.84	252.1
2	0.86	259.5
3	0.87	262.1
4	0.89	266.7
5	0.90	269.5
6	0.92	276.7
7	1.18	355.2
8	1.21	362.4
9	1.23	369.3
10	1.24	373.1
11	1.26	377.2
12	1.27	380.3

No.	(ppm)	(Hz)
13	1.28	384.7
14	1.29	387.7
15	1.32	395.2
16	1.34	402.6
17	1.41	424.2
18	1.44	431.9
19	1.46	438.8
20	1.49	446.7
21	1.51	453.7
22	1.58	473.1
23	1.60	480.6
24	1.62	487.5

No.	(ppm)	(Hz)
25	1.65	494.4
26	1.67	501.9
27	1.94	582.7
28	1.96	588.3
29	1.98	593.7
30	1.99	598.6
31	2.01	604.2
32	2.78	833.7
33	2.80	840.7
34	2.82	847.6
35	3.26	979.4
36	3.28	985.3

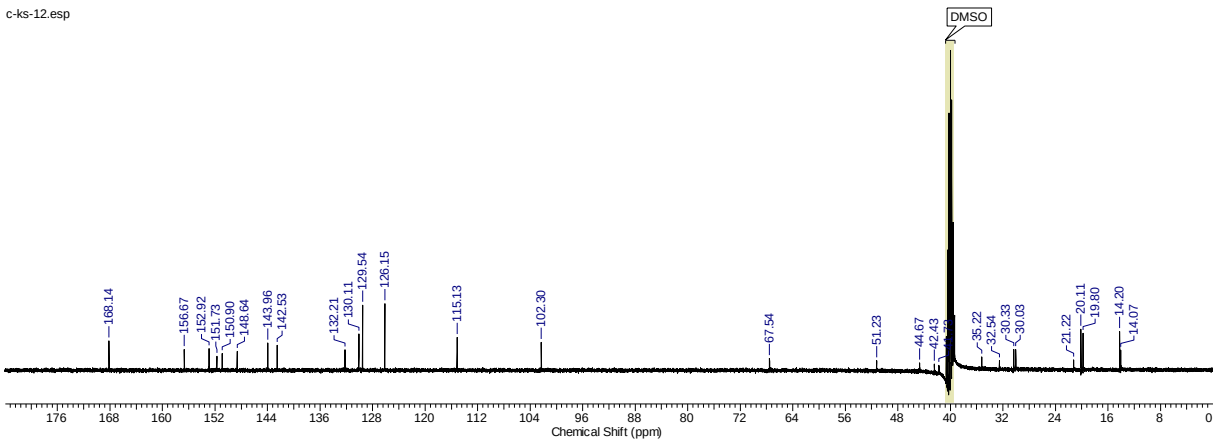
No.	(ppm)	(Hz)
37	3.33	998.6
38	3.35	1005.6
39	3.37	1012.5
40	3.40	1019.2
41	3.58	1074.6
42	3.61	1082.5
43	3.63	1089.2
44	3.76	1128.2
45	3.78	1135.6
46	3.81	1142.8
47	3.89	1166.1
48	3.91	1173.3

No.	(ppm)	(Hz)
49	3.93	1180.2
50	3.99	1196.6
51	4.01	1202.5
52	4.03	1208.2
53	4.39	1316.4
54	6.82	2046.1
55	6.85	2054.8
56	7.13	2139.4
57	7.16	2147.9
58	7.28	2183.5
59	7.33	2200.7
60	7.36	2209.2

No.	(ppm)	(Hz)
61	7.70	2309.2
62	7.72	2317.6
63	8.12	2435.6
64	8.14	2441.5
65	8.16	2447.4

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M17	[0.82 .. 0.93]
2	1.26	4	m	-	M16	[1.18 .. 1.35]
3	1.46	2	m	-	M15	[1.40 .. 1.52]
4	1.62	2	quin	7.18	M14	[1.57 .. 1.68]
5	1.98	2	m	-	M13	[1.93 .. 2.02]
6	2.80	4	m	-	M12	[2.77 .. 2.85]
7	3.27	2	m	-	M11	[3.26 .. 3.29]
8	3.36	2	m	-	M10	[3.32 .. 3.41]
9	3.61	2	t	7.31	M09	[3.57 .. 3.64]
10	3.78	2	t	7.20	M08	[3.75 .. 3.82]
11	3.91	2	t	7.05	M07	[3.87 .. 3.94]
12	4.01	2	t	5.77	M06	[3.97 .. 4.04]
13	4.39	2	s	-	M18	[4.37 .. 4.41]
14	6.83	2	d	8.72	M05	[6.80 .. 6.86]
15	7.14	2	d	8.46	M04	[7.11 .. 7.17]
16	7.28	2	s	-	M19	[7.26 .. 7.29]
17	7.35	2	d	8.46	M03	[7.32 .. 7.38]
18	7.71	2	d	8.46	M02	[7.68 .. 7.74]
19	8.14	1	t	5.90	M01	[8.11 .. 8.16]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.82 - 0.93 (m, 6 H) 1.18 - 1.35 (m, 4 H) 1.40 - 1.52 (m, 2 H) 1.62 (quin, *J*=7.18 Hz, 2 H) 1.93 - 2.02 (m, 2 H) 2.77 - 2.85 (m, 4 H) 3.26 - 3.29 (m, 2 H) 3.32 - 3.41 (m, 2 H) 3.61 (t, *J*=7.31 Hz, 2 H) 3.78 (t, *J*=7.20 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.77 Hz, 2 H) 4.39 (s, 2 H) 6.83 (d, *J*=8.72 Hz, 2 H) 7.14 (d, *J*=8.46 Hz, 2 H) 7.28 (s, 2 H) 7.35 (d, *J*=8.46 Hz, 2 H) 7.71 (d, *J*=8.46 Hz, 2 H) 8.14 (t, *J*=5.90 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.07	1415.6
2	14.20	1428.8
3	19.80	1992.2
4	20.11	2023.7

No.	(ppm)	(Hz)
5	21.22	2135.2
6	30.03	3022.1
7	30.33	3052.2
8	32.54	3274.5

No.	(ppm)	(Hz)
9	35.22	3544.4
10	41.73	4199.5
11	42.43	4270.0
12	44.67	4495.2

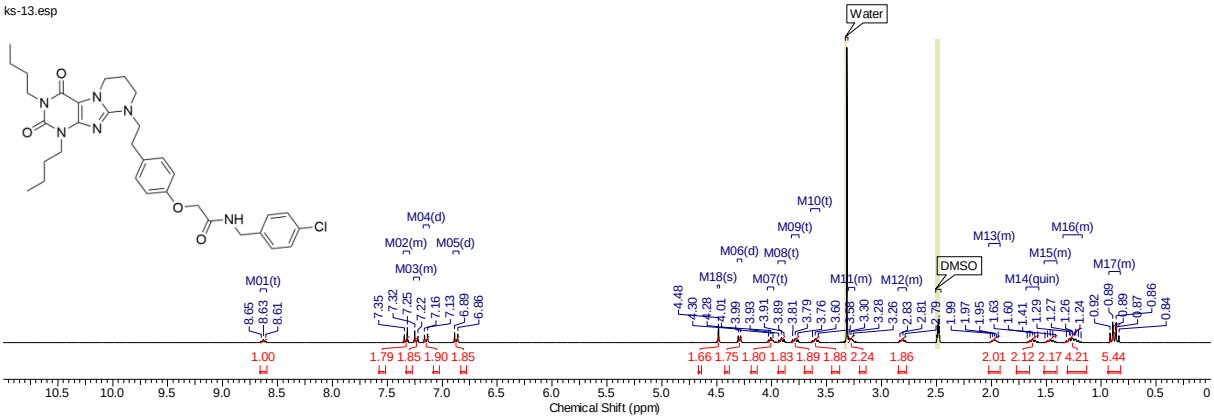
No.	(ppm)	(Hz)
13	51.23	5155.4
14	67.54	6797.2
15	102.30	10295.0
16	115.13	11585.4

No.	(ppm)	(Hz)
17	126.15	12695.3
18	129.54	13035.7
19	130.11	13092.9
20	132.21	13304.2

No.	(ppm)	(Hz)
21	142.53	14343.0
22	143.96	14487.5
23	148.64	14957.7
24	150.90	15185.9

No.	(ppm)	(Hz)
25	151.73	15268.8
26	152.92	15388.3
27	156.67	15766.1
28	168.14	16920.8

N-(4-chlorobenzyl)-2-(4-(2-(1,3-dibutyl-2,4-dioxo-1,2,3,4,7,8-hexahydropyrimido[2,1-*f*]purin-9(6*H*)-yl)ethyl)phenoxy)acetamide (38)



No.	(ppm)	(Hz)
1	0.84	251.6
2	0.86	259.0
3	0.87	261.0
4	0.89	266.4
5	0.89	268.5
6	0.92	275.7
7	1.18	355.2
8	1.21	362.4
9	1.23	369.5
10	1.24	372.6
11	1.26	377.2

No.	(ppm)	(Hz)
12	1.27	379.8
13	1.28	384.7
14	1.29	387.2
15	1.32	394.7
16	1.41	424.4
17	1.44	432.4
18	1.46	439.0
19	1.49	447.0
20	1.51	453.9
21	1.58	473.4
22	1.60	481.1

No.	(ppm)	(Hz)
23	1.63	488.0
24	1.65	494.9
25	1.67	502.1
26	1.94	580.9
27	1.95	586.5
28	1.97	591.9
29	1.99	597.3
30	2.01	603.2
31	2.79	835.8
32	2.81	842.2
33	2.83	850.4

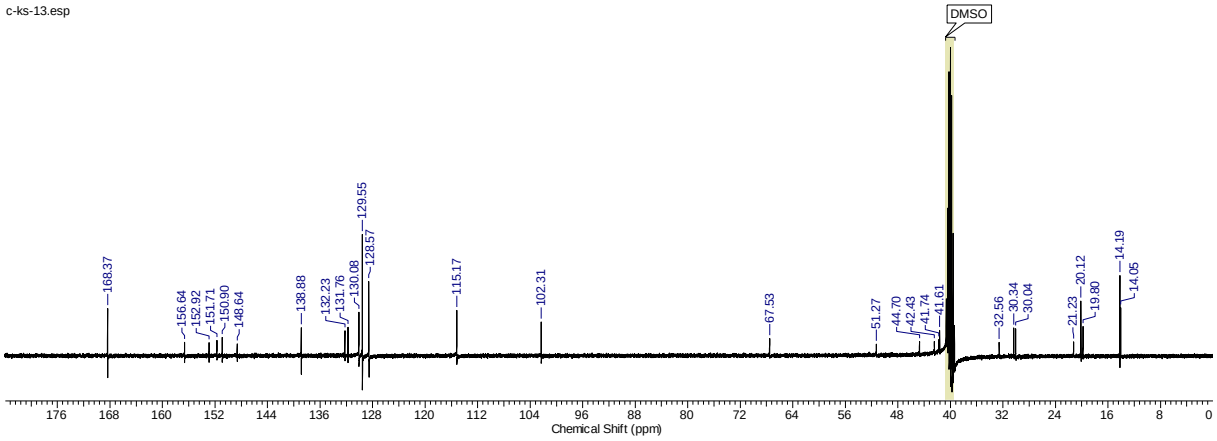
No.	(ppm)	(Hz)
34	3.26	977.9
35	3.28	983.5
36	3.30	988.9
37	3.58	1073.5
38	3.60	1081.2
39	3.63	1088.4
40	3.76	1128.7
41	3.79	1136.1
42	3.81	1143.3
43	3.89	1166.6
44	3.91	1173.8

No.	(ppm)	(Hz)
45	3.93	1180.7
46	3.99	1196.9
47	4.01	1202.8
48	4.03	1208.7
49	4.28	1285.4
50	4.30	1291.5
51	4.48	1345.6
52	6.86	2058.1
53	6.89	2066.8
54	7.13	2140.7
55	7.16	2149.1

No.	(ppm)	(Hz)
56	7.22	2167.1
57	7.25	2175.6
58	7.32	2195.8
59	7.35	2204.3
60	8.61	2583.1
61	8.63	2589.2
62	8.65	2595.4

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	0.88	6	m	-	M17	[0.83 .. 0.93]
2	1.25	4	m	-	M16	[1.17 .. 1.35]
3	1.46	2	m	-	M15	[1.40 .. 1.52]
4	1.63	2	quin	7.18	M14	[1.57 .. 1.68]
5	1.97	2	m	-	M13	[1.92 .. 2.02]
6	2.81	2	m	-	M12	[2.77 .. 2.85]
7	3.28	2	m	-	M11	[3.24 .. 3.30]
8	3.60	2	t	7.44	M10	[3.56 .. 3.64]
9	3.79	2	t	7.40	M09	[3.75 .. 3.82]
10	3.91	2	t	7.05	M08	[3.88 .. 3.94]
11	4.01	2	t	5.90	M07	[3.98 .. 4.04]
12	4.29	2	d	6.16	M06	[4.27 .. 4.31]
13	4.48	2	s	-	M18	[4.47 .. 4.50]
14	6.87	2	d	8.72	M05	[6.85 .. 6.90]
15	7.15	2	d	8.46	M04	[7.12 .. 7.17]
16	7.24	2	m	-	M03	[7.21 .. 7.26]
17	7.33	2	m	-	M02	[7.30 .. 7.36]
18	8.63	1	t	6.16	M01	[8.60 .. 8.66]

^{1}H NMR (300 MHz, DMSO-d_6) □ ppm 0.83 - 0.93 (m, 6 H) 1.17 - 1.35 (m, 4 H) 1.40 - 1.52 (m, 2 H) 1.63 (quin, *J*=7.18 Hz, 2 H) 1.92 - 2.02 (m, 2 H) 2.77 - 2.85 (m, 2 H) 3.24 - 3.30 (m, 2 H) 3.60 (t, *J*=7.44 Hz, 2 H) 3.79 (t, *J*=7.40 Hz, 2 H) 3.91 (t, *J*=7.05 Hz, 2 H) 4.01 (t, *J*=5.90 Hz, 2 H) 4.29 (d, *J*=6.16 Hz, 2 H) 4.48 (s, 2 H) 6.87 (d, *J*=8.72 Hz, 2 H) 7.15 (d, *J*=8.46 Hz, 2 H) 7.21 - 7.26 (m, 2 H) 7.30 - 7.36 (m, 2 H) 8.63 (t, *J*=6.16 Hz, 1 H)



No.	(ppm)	(Hz)
1	14.05	1414.1
2	14.19	1428.0
3	19.80	1992.9
4	20.12	2024.4

No.	(ppm)	(Hz)
5	21.23	2135.9
6	30.04	3022.9
7	30.34	3052.9
8	32.56	3276.7

No.	(ppm)	(Hz)
9	41.61	4187.8
10	41.74	4200.3
11	42.43	4270.0
12	44.70	4498.1

No.	(ppm)	(Hz)
13	51.27	5159.1
14	67.53	6795.7
15	102.31	10295.7
16	115.17	11589.8

No.	(ppm)	(Hz)
17	128.57	12938.1
18	129.55	13037.2
19	130.08	13090.7
20	131.76	13259.5

No.	(ppm)	(Hz)
21	132.23	13306.4
22	138.88	13975.4
23	148.64	14957.7
24	150.90	15185.9

No.	(ppm)	(Hz)
25	151.71	15267.3
26	152.92	15388.3
27	156.64	15763.2
28	168.37	16943.6