

Supporting Information

Triazole-dithiocarbamate based LSD1 selective inactivators inhibit gastric cancer cell growth, invasion and migration

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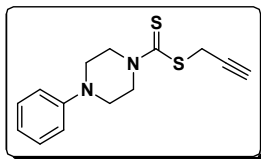
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Compound characterization

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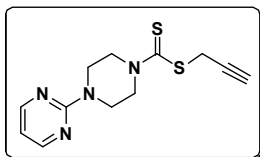
Prop-2-ynyl 4-phenylpiperazine-1-carbodithioate (**4g**):



found: 277.0835.

Yield 72.4%, red oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.31-7.35 (m, 2H), 6.93-6.96 (m, 3H), 4.49 (brs, 2H), 4.17 (d, $J = 2.7$ Hz, 2H), 4.11 (brs, 2H), 3.35 (t, $J = 5.3$ Hz, 4H), 2.30 (t, $J = 2.7$ Hz, 1H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 194.79, 150.22, 129.38, 120.67, 116.38, 78.34, 71.83, 48.76, 26.02; HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{S}_2$ $[\text{M} + \text{H}]^+$: 277.0833,

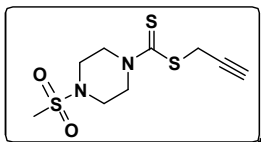
Prop-2-ynyl 4-(pyrimidin-2-yl)piperazine-1-carbodithioate (**4h**):



301.0558, found: 301.0559.

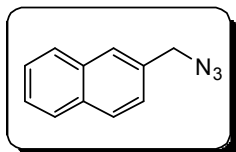
Yield 81.0%, white solid. Mp: 111-112°C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.35 (d, $J = 4.8$ Hz, 2H), 6.59 (t, $J = 4.8$ Hz, 1H), 4.40 (brs, 2H), 4.15 (d, $J = 2.7$ Hz, 2H), 3.95-4.00 (m, 6H), 2.28 (t, $J = 2.7$ Hz, 1H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 194.98, 161.25, 157.84, 110.79, 78.29, 71.81, 42.93, 25.97; HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{14}\text{N}_4\text{NaS}_2$ $[\text{M} + \text{Na}]^+$:

Prop-2-ynyl 4-(methylsulfonyl)piperazine-1-carbodithioate (**4i**):



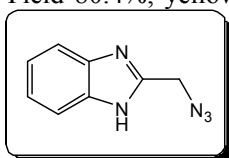
Yield 77.2%, white solid. Mp: 106-107°C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 4.27 (brs, 4H), 4.12 (d, $J = 2.6$ Hz, 2H), 3.36 (t, $J = 5.2$ Hz, 4H), 2.82 (s, 3H), 2.28 (t, $J = 2.6$ Hz, 1H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 195.81, 77.91, 72.04, 45.24, 35.14, 26.23; HRMS (ESI) calcd for $\text{C}_9\text{H}_{14}\text{N}_2\text{NaO}_2\text{S}_3$ $[\text{M} + \text{Na}]^+$: 301.0115, found: 301.0114.

2-(azidomethyl)naphthalene (**5e**):



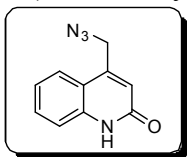
Yield 81.5%, yellow white solid. Mp: 34-35°C; $^1\text{HNMR}$ (400 MHz, Acetone- d_6 , ppm): δ 7.93-7.98 (m, 4H), 7.52-7.56 (m, 3H), 4.63 (s, 2H); $^{13}\text{C NMR}$ (100 MHz, Acetone- d_6 , ppm): δ 133.5, 133.4, 133.2, 128.6, 127.9, 127.7, 127.2, 126.4, 126.3, 126.2, 54.4; HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{10}\text{N}_3$ $[\text{M} + \text{H}]^+$: 184.0875, found: 184.0877.

2-(azidomethyl)-1H-benzo[d]imidazole (**5f**):



Yield 80.4%, yellow white solid. Mp: 118-119°C; $^1\text{H NMR}$ (400 MHz, Acetone- d_6 , ppm): δ 11.7 (brs, 1H), 7.60 (dd, $J_1 = 3.2$ Hz, $J_2 = 6.0$ Hz, 2H), 7.24 (dd, $J_1 = 3.2$ Hz, $J_2 = 6.0$ Hz, 2H), 4.73 (s, 2H); $^{13}\text{C NMR}$ (100 MHz, Acetone- d_6 , ppm): δ 149.2, 139.0, 122.3, 115.3, 47.8; HRMS (ESI) calcd for $\text{C}_8\text{H}_8\text{N}_5$ $[\text{M} + \text{H}]^+$: 174.0780, found: 174.0782.

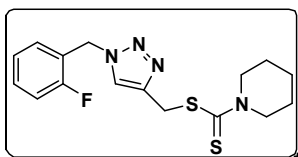
4-(azidomethyl)quinolin-2(1H)-one (**5g**):



201.0775.

Yield 79.9%, yellow white solid Mp: 155-156°C; $^1\text{HNMR}$ (400 MHz, Acetone- d_6 , ppm): δ 10.92 (brs, 1H), 7.78 (dd, $J_1 = 1.0$ Hz, $J_2 = 8.1$ Hz, 1H), 7.54-7.59 (m, 1H), 7.46 (d, $J_1 = 8.1$ Hz, 1H), 7.23-7.27 (m, 1H), 6.66 (s, 1H), 4.81 (s, 2H); $^{13}\text{C NMR}$ (100 MHz, Acetone- d_6 , ppm): δ 161.5, 145.1, 139.4, 130.7, 124.3, 122.1, 121.00, 117.8, 115.8, 50.9; HRMS (ESI) calcd for $\text{C}_{10}\text{H}_9\text{N}_4\text{O}$ $[\text{M} + \text{H}]^+$: 201.0776, found:

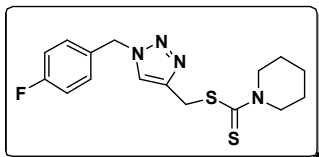
(1-(2-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl piperidine-1-carbodithioate (**12**):



Yield 71.8%, white solid. Mp: 94-95°C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.68 (s, 1H), 7.31-7.35 (m, 1H), 7.21-7.25 (m, 1H), 7.08-7.15 (m, 2H), 5.54 (s, 2H), 4.67 (s, 2H), 4.26 (brs, 2H), 3.84 (brs, 2H), 1.70-

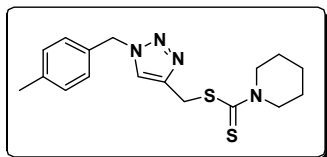
1.78 (m, 2H), 1.61-1.67 (m, 4H); HRMS (ESI) calcd for $C_{16}H_{20}FN_4S_2$ $[M + Na]^+$: 373.0933, found: 373.0924.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl piperidine-1-carbodithioate (13):



Yield 89.9%, white solid. Mp: 93-94°C; 1H NMR (400 MHz, Acetone) δ 7.99 (s, 1H), 7.45-7.48 (m, 2H), 7.15-7.20 (m, 2H), 5.63 (s, 2H), 4.62 (s, 2H), 4.29 (brs, 2H), 3.90 (brs, 2H), 1.72-1.78 (m, 2H), 1.62-1.67 (m, 4H); HRMS (ESI) calcd for $C_{16}H_{19}FN_4NaS_2$ $[M + Na]^+$: 373.0933, found: 373.0935.

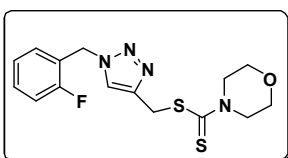
(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl piperidine-1-carbodithioate (14):



Yield 75.9%, white solid. Mp: 107-108°C; 1H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.17 (s, 4H), 5.44 (s, 2H), 4.68 (s, 2H), 4.28 (brs, 2H), 3.85 (brs, 2H), 2.36 (s, 3H), 1.72-1.79 (m, 2H), 1.61-1.68 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.56, 138.58, 131.66, 129.72, 128.07, 122.72, 53.94, 31.95, 25.99, 25.47, 24.23, 21.16;

HRMS (ESI) calcd for $C_{17}H_{22}N_4NaS_2$ $[M + Na]^+$: 369.1184, found: 369.1183.

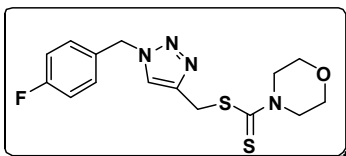
(1-(2-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl morpholine-4-carbodithioate (18):



Yield 75.4%, white solid. Mp: 112-113°C; 1H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.34-7.38 (m, 1H), 7.24-7.27 (m, 1H), 7.11-7.18 (m, 1H), 5.56 (s, 2H), 4.71 (s, 2H), 4.33 (brs, 2H), 3.94 (brs, 2H), 3.76 (s, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.47, 161.73, 159.26, 144.09, 130.90, 130.82, 130.52, 130.49, 124.83, 124.79, 122.98, 121.98, 121.84, 115.93, 115.72, 66.19, 47.67, 47.62, 31.68;

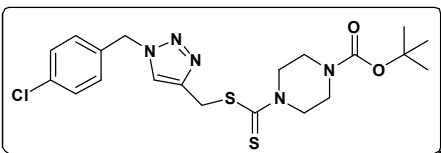
HRMS (ESI) calcd for $C_{15}H_{17}FN_4NaOS_2$ $[M + Na]^+$: 375.0726, found: 375.0725.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl morpholine-4-carbodithioate (19):



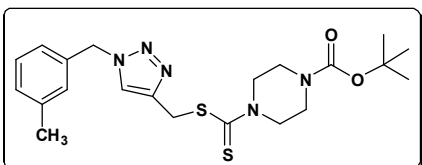
Yield 79.3%, white solid. Mp: 136-137°C; 1H NMR (400 MHz, Acetone) δ 8.00 (s, 1H), 7.44-7.49 (m, 2H), 7.15-7.21 (m, 2H), 5.64 (s, 2H), 4.64 (s, 2H), 4.28 (brs, 2H), 3.96 (brs, 2H), 3.74 (t, $J = 4.9$ Hz, 4H); HRMS (ESI) calcd for $C_{15}H_{17}FN_4NaOS_2$ $[M + Na]^+$: 375.0726, found: 375.0727.

tert Butyl 4-(((1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl)-piperazine-1-carboxylate (25):



Yield 85.5%, white solid. Mp: 177-178°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.59 (s, 1H), 7.35 (d, 2H, $J = 8.4$ Hz), 7.20 (d, $J = 8.4$ Hz, 2H), 5.45 (s, 2H), 4.68 (s, 2H), 4.29 (brs, 2H), 3.90 (brs, 2H), 3.54 (t, $J = 5.2$ Hz, 4H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.39, 154.42, 144.35, 134.78, 133.11, 129.36, 129.31, 122.79, 80.69, 53.40, 31.72, 28.35; HRMS (ESI) calcd for $C_{20}H_{27}ClN_5O_2S_2$ $[M + H]^+$: 468.1295, found: 468.1291.

tert Butyl 4-(((1-(3-methylbenzyl)-1H-1,2,3-triazol-4-yl)methylthio) carbonothioyl)-piperazine-1-carboxylate (28):

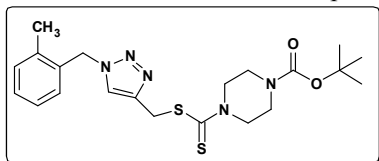


Yield 87.8%, white solid. Mp: 151-152°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.61 (s, 1H), 7.25 (d, $J = 7.5$ Hz, 1H), 7.16 (d, $J = 7.5$ Hz, 1H), 7.07 (s, 2H), 5.44 (s, 2H), 4.68 (s, 2H), 4.30 (brs, 2H), 3.90 (brs, 2H), 3.52 (s, 4H), 2.34 (s, 3H),

1.47 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 196.43, 154.41, 138.94, 134.50, 129.48, 128.96, 128.77, 125.10, 80.64, 54.22, 31.90, 28.36, 21.36; HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{30}\text{N}_5\text{O}_2\text{S}_2$ [$\text{M} + \text{H}$] $^+$: 448.1841, found: 448.1844.

tert Butyl 4-(((1-(2-methylbenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl)-piperazine-1-carboxylate (**29**):

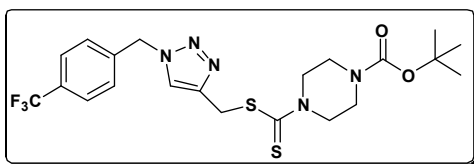
Yield 82.9%, white solid. Mp: 110-111°C; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 7.48 (s, 1H), 7.12-



7.29 (m, 4H), 5.50 (s, 2H), 4.67 (s, 2H), 4.30 (brs, 2H), 3.91 (brs, 2H), 3.54 (t, $J = 5.0$ Hz, 3H), 2.29 (s, 3H), 1.48 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 196.39, 154.41, 136.84, 132.51, 130.99, 129.31, 129.09, 126.65, 80.63, 52.36, 31.91, 28.36, 19.05; HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{30}\text{N}_5\text{O}_2\text{S}_2$ [$\text{M} + \text{H}$] $^+$: 448.1841, found:

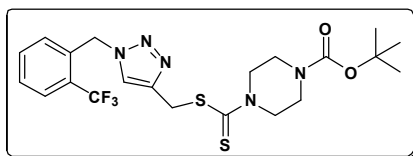
448.1842.

tert Butyl 4-(((1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**30**):



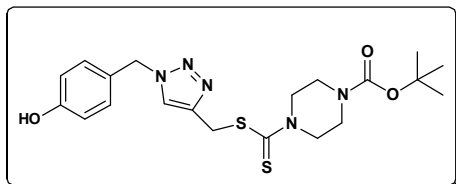
Yield 88.1%, white solid. Mp: 151-152°C; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 7.65 (s, 1H), 7.64 (d, $J = 8.0$ Hz, 2H), 7.37 (d, $J = 8.0$ Hz, 2H), 5.55 (s, 2H), 4.70 (s, 2H), 4.31 (brs, 2H), 3.91 (brs, 2H), 3.53 (s, 4H), 1.47 (s, 9H); HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{27}\text{F}_3\text{N}_5\text{O}_2\text{S}_2$ [$\text{M} + \text{H}$] $^+$: 502.1558, found: 502.1559.

tert Butyl 4-(((1-(2-(trifluoromethyl)benzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**31**):



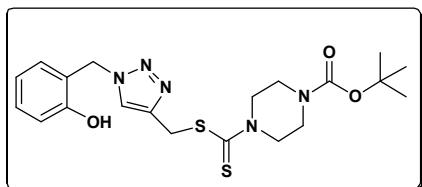
Yield 87.5%, white solid. Mp: 73-74°C; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 7.73 (d, $J = 7.7$ Hz, 1H), 7.63 (s, 1H), 7.43-7.5 (m, 2H), 7.15 (d, $J = 7.7$ Hz, 1H), 5.71 (s, 2H), 4.71 (s, 2H), 4.30 (brs, 2H), 3.91 (brs, 2H), 3.54 (t, $J = 5.0$ Hz, 4H), 1.47 (s, 9H); HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{27}\text{F}_3\text{N}_5\text{O}_2\text{S}_2$ [$\text{M} + \text{H}$] $^+$: 502.1558, found: 502.1560.

tert Butyl 4-(((1-(4-hydroxybenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**33**):



Yield 77.3%, white solid. Mp: 181-182°C; ^1H NMR (400 MHz, DMSO-d_6) δ 9.54 (s, 1H), 8.04 (s, 1H), 7.18 (d, $J = 8.3$ Hz, 2H), 6.75 (d, $J = 8.3$ Hz, 2H), 5.41 (s, 2H), 4.55 (s, 2H), 4.22 (brs, 2H), 3.89 (brs, 2H), 3.44 (s, 4H), 1.41 (s, 9H); ^{13}C NMR (101 MHz, DMSO) δ 195.01, 157.84, 154.13, 142.50, 130.17, 126.59, 123.85, 115.87, 79.86, 52.98, 31.97, 28.48; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{27}\text{N}_5\text{NaO}_3\text{S}_2$ [$\text{M} + \text{Na}$] $^+$: 472.1453, found: 472.1450.

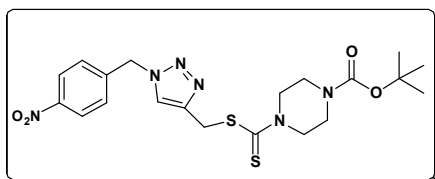
tert Butyl 4-(((1-(2-hydroxybenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**34**):



Yield 82.4%, white solid. Mp: 115-116°C; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (s, 1H), 7.20-7.24 (m, 1H), 6.86-6.88 (m, 2H), 6.82 (d, $J = 7.7$ Hz, 1H), 5.41 (s, 2H), 4.65 (s, 2H), 4.29 (brs, 2H), 3.87 (brs, 2H), 3.51 (s, 4H), 1.47 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 196.19, 157.55, 154.52, 144.10, 135.80, 130.23, 123.09, 119.46, 116.41, 114.92, 80.80, 54.31, 31.44, 28.36; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{27}\text{N}_5\text{NaO}_3\text{S}_2$ [$\text{M} + \text{Na}$] $^+$:

472.1453, found: 472.1455.

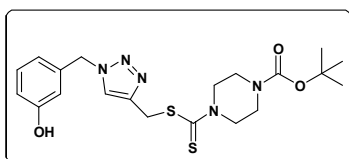
tert Butyl 4-(((1-(4-nitrobenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**35**):



Yield 81.1%, white solid. Mp: 155-156°C; ¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, J = 8.8 Hz, 2H), 7.70 (s, 1H), 7.41 (d, J = 8.8 Hz, 2H), 5.61 (s, 2H), 4.70 (s, 2H), 4.29 (brs, 2H), 3.91 (brs, 2H), 3.55 (t, J = 5.3 Hz, 4H), 1.47 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 196.26, 154.39, 148.06, 144.84, 141.66, 128.56, 124.28, 123.21, 80.69, 53.08, 31.58, 28.34; HRMS (ESI) calcd for C₂₀H₂₆N₆NaO₄S₂ [M + Na]⁺:

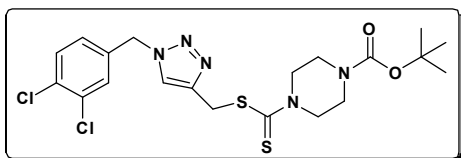
501.1355, found: 501.1357.

tert Butyl 4-(((1-(3-hydroxybenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**36**):



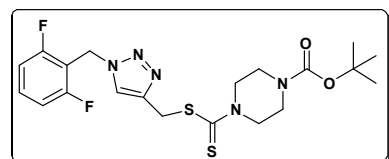
Yield 72.8%, white solid. Mp: 61-62°C; ¹H NMR (400 MHz, CDCl₃) δ 10.30 (s, 1H), 7.64 (s, 1H), 7.45-7.71 (m, 5H), 5.49 (s, 2H), 4.62 (s, 2H), 4.30 (brs, 2H), 3.87 (brs, 2H), 3.51 (s, 4H), 1.48 (s, 9H); HRMS (ESI) calcd for C₂₀H₂₇N₅NaO₃S₂ [M + Na]⁺: 472.1453, found: 472.1452.

tert Butyl 4-(((1-(3,4-dichlorobenzyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl) piperazine-1-carboxylate (**38**):



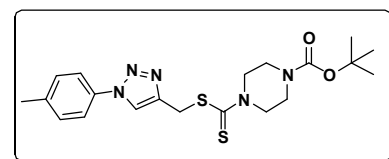
Yield 90.2%, white solid. Mp: 153-154°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.64 (s, 1H), 7.43 (d, J = 8.2 Hz, 1H), 7.35 (d, J = 2.0 Hz, 1H), 7.08 (dd, J₁ = 2.0 Hz, J₂ = 8.2 Hz, 1H), 5.44 (s, 2H), 4.70 (s, 2H), 4.30 (brs, 2H), 3.91 (brs, 2H), 3.52 (t, J = 5.1 Hz, 4H), 1.47 (s, 9H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 196.29, 154.39, 144.59, 134.77, 133.26, 133.08, 131.08, 129.86, 127.18, 122.94, 80.65, 52.82, 31.65, 28.34; HRMS (ESI) calcd for C₂₀H₂₆Cl₂N₅O₂S₂ [M + H]⁺: 502.0905, found: 502.0900.

tert Butyl 4-(((1-(2,6-difluorobenzyl)-1H-1,2,3-triazol-4-yl) methylthio) carbonthioyl)- piperazine-1- carboxylate (**39**):



Yield 77.8%, white solid. Mp: 129-130°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.71 (brs, 1H), 7.32-7.41 (m, 1H), 6.94-6.99 (m, 2H), 5.58 (s, 2H), 4.67 (s, 2H), 4.30 (brs, 2H), 3.91 (brs, 2H), 3.53 (s, 4H), 1.47 (s, 9H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 196.43, 162.66, 162.59, 160.16, 160.10, 154.41, 131.51, 131.40, 131.30, 111.94, 111.88, 111.75, 111.69, 110.95, 110.76, 110.57, 80.62, 41.39, 31.85, 28.35; HRMS (ESI) calcd for C₂₀H₂₆F₂N₅O₂S₂ [M + H]⁺: 470.1496, found: 470.1498.

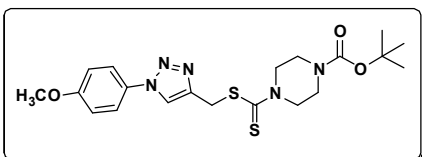
tert Butyl 4-(((1-(p-tolyl)-1H-1,2,3-triazol-4-yl)methylthio) carbonothioyl) piperazine -1-carboxylate (**41**):



Yield 78.4%, white solid. Mp: 130-131°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 8.08 (s, 1H), 7.59 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.4 Hz, 2H), 4.79 (s, 2H), 4.32 (brs, 2H), 3.93 (brs, 2H), 3.56 (t, J = 5.2 Hz, 4H), 2.41 (s, 3H), 1.47 (s, 9H); ¹³C NMR (100 MHz, DMSO-d₆, ppm): δ 196.39, 154.40, 138.81, 134.73, 130.17, 120.43, 80.62, 31.71, 28.35, 21.09; HRMS (ESI) calcd

for $C_{20}H_{28}N_5O_2S_2 [M + H]^+$: 434.1684, found: 434.1681.

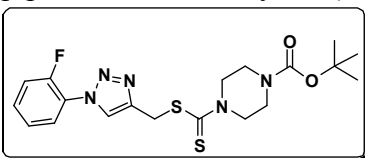
tert Butyl 4-(((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonthioyl)-piperazine-1-carboxylate (**42**):



Yield 83.0%, white solid. Mp: 133-134°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.04 (s, 1H), 7.61 (d, $J = 9.0$ Hz, 2H), 7.01 (d, $J = 9.0$ Hz, 2H), 4.79 (s, 2H), 4.32 (brs, 2H), 3.94 (brs, 2H), 3.86 (s, 3H), 3.56 (t, $J = 5.3$ Hz, 4H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.43, 159.80, 154.41, 144.33, 130.48, 122.17, 121.24, 114.72, 80.64, 55.63, 31.72,

28.35; HRMS (ESI) calcd for $C_{20}H_{28}N_5O_3S_2 [M + H]^+$: 450.1634, found: 450.1638.

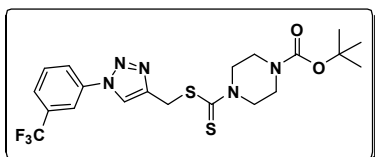
tert Butyl 4-(((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methylthio) carbonthioyl)-piperazine-1-carboxylate (**43**):



Yield 77.5%, white solid. Mp: 178-179°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.09 (s, 1H), 7.18-7.71 (m, 4H), 4.79 (s, 2H), 4.32 (brs, 2H), 3.93 (brs, 2H), 3.56 (t, $J = 5.2$ Hz, 4H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.30, 163.64, 161.17, 154.40, 133.32, 122.56, 122.48, 116.78, 116.55, 80.67, 31.56, 28.35;

HRMS (ESI) calcd for $C_{19}H_{25}FN_5O_2S_2 [M + H]^+$: 438.1434, found: 438.1437.

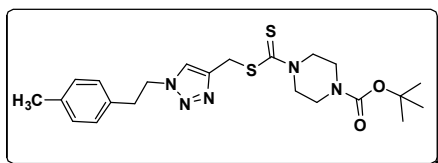
tert Butyl 4-(((1-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)methylthio)-carbonthioyl) piperazine-1-carboxylate (**44**):



Yield 87.6%, white solid. Mp: 109-110°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.21 (s, 1H), 8.01 (s, 1H), 7.96 (d, $J = 7.6$ Hz, 1H), 7.66-7.73 (m, 2H), 4.82 (s, 2H), 4.34 (brs, 2H), 3.95 (brs, 2H), 3.57 (t, $J = 5.2$ Hz, 4H), 1.48 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.13, 154.39, 145.29, 137.34, 132.87, 132.54, 132.21, 131.88, 130.51, 127.38, 125.37, 125.34, 125.30, 125.26,

124.67, 123.56, 121.96, 121.10, 119.25, 117.49, 117.46, 117.42, 117.38, 80.67, 31.45, 28.33; HRMS (ESI) calcd for $C_{20}H_{25}F_3N_5O_2S_2 [M + H]^+$: 488.1402, found: 488.1398.

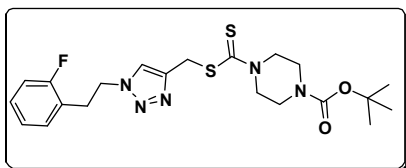
tert Butyl 4-(((1-(4-methylphenethyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonthioyl) piperazine-1-carboxylate(**45**):



Yield 79.1%, white solid. Mp: 119-120°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.47 (s, 1H), 7.13 (d, $J = 7.8$ Hz, 2H), 7.02 (d, $J = 7.8$ Hz, 2H), 4.69 (s, 2H), 4.55 (t, $J = 7.3$ Hz, 2H), 4.33 (brs, 2H), 3.94 (brs, 2H), 3.57 (t, $J = 5.1$ Hz, 4H), 3.18 (t, $J = 7.2$ Hz, 2H), 2.35 (s, 3H), 1.49 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.51, 154.41, 143.31, 136.69,

133.84, 129.51, 128.56, 123.08, 80.66, 51.78, 36.34, 31.81, 28.36, 21.10; HRMS (ESI) calcd for $C_{22}H_{31}N_5NaO_2S_2 [M + Na]^+$: 484.1817, found: 484.1815.

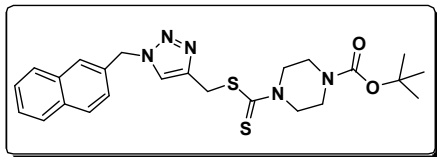
tert Butyl 4-(((1-(2-fluorophenethyl)-1H-1,2,3-triazol-4-yl)methylthio) carbonthioyl)piperazine-1-carboxylate (**46**):



Yield 69.0%, white solid. Mp: 85-86°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.49 (s, 1H), 7.00-7.25 (m, 4H), 4.67 (s, 2H), 4.58 (t, $J = 7.3$ Hz, 2H), 4.33 (brs, 2H), 3.92 (brs, 2H), 3.57 (t, $J = 5.2$ Hz, 4H), 3.26 (t, $J = 7.3$ Hz, 2H), 1.48 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.47, 162.36, 159.92, 154.41, 131.17, 131.12, 129.14, 129.06, 124.43, 124.40,

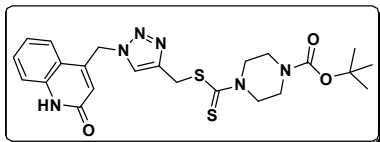
123.89, 123.73, 115.66, 115.44, 80.66, 50.05, 31.75, 30.61, 30.59, 28.36; HRMS (ESI) calcd for $C_{21}H_{28}FN_5NaO_2S_2$ $[M + Na]^+$: 488.1566, found: 488.1565.

tert Butyl 4-(((1-(naphthalen-2-ylmethyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl)piperazine-1-carboxylate (**48**):



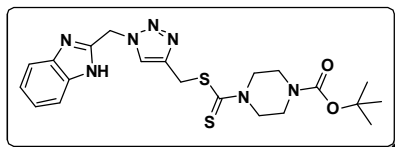
Yield 82.0%, white solid. Mp: 134-135°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.83-7.88 (m, 4H), 7.76 (s, 1H), 7.52-7.56 (m, 2H), 7.38 (dd, $J_1 = 1.2$ Hz, $J_2 = 8.4$ Hz, 1H), 5.67 (s, 2H), 4.71 (s, 2H), 4.31 (brs, 2H), 3.92 (brs, 2H), 3.54 (s, 4H), 1.49 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.42, 154.41, 133.20, 133.17, 131.97, 129.13, 127.96, 127.79, 127.37, 126.74, 125.34, 80.63, 54.41, 31.88, 28.36; HRMS (ESI) calcd for $C_{24}H_{30}N_5O_2S_2$ $[M + H]^+$: 484.1841, found: 484.1840.

tert Butyl 4-(((1-((2-oxo-1,2-dihydroquinolin-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl)piperazine-1-carboxylate (**49**):



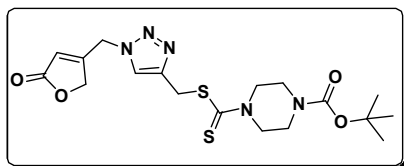
Yield 79.8%, white solid. Mp: 207-208 °C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 11.86 (s, 1H), 8.24 (s, 1H), 7.83 (d, $J = 5.0$ Hz, 1H), 7.55 (s, 1H), 7.36 (dd, $J_1 = 3.2$ Hz, $J_2 = 5.0$ Hz, 1H), 7.23 (d, $J = 3.2$ Hz, 1H), 5.95 (s, 1H), 5.92 (s, 2H), 4.62 (s, 2H), 4.32 (brs, 2H), 3.92 (brs, 2H), 3.46 (s, 4H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 194.90, 161.67, 154.15, 145.94, 139.39, 131.34, 125.23, 124.54, 122.45, 120.71, 117.53, 116.24, 79.88, 50.12, 31.83, 28.48; HRMS (ESI) calcd for $C_{23}H_{28}N_6NaO_3S_2$ $[M + Na]^+$: 523.1562, found: 523.1562.

tert Butyl 4-(((1-((1H-benzodimidazol-2-yl)methyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl)piperazine-1-carboxylate (**50**):



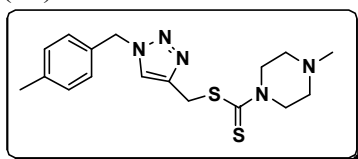
Yield 84.7%, white solid. Mp: 93-94 °C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.88 (s, 1H), 7.63 (dd, $J_1 = 3.1$ Hz, $J_2 = 6.0$ Hz, 2H), 7.30 (dd, $J_1 = 3.1$ Hz, $J_2 = 6.0$ Hz, 2H), 5.84 (s, 2H), 4.68 (s, 2H), 4.25 (brs, 2H), 3.83 (brs, 2H), 3.49 (s, 4H), 1.46 (s, 9H); NMR (100 MHz, $CDCl_3$, ppm): δ 195.72, 154.40, 146.85, 144.50, 123.90, 123.31, 80.68, 48.41, 31.48, 28.35; HRMS (ESI) calcd for $C_{24}H_{30}N_5O_2S_2$ $[M + H]^+$: 484.1841, found: 484.1840.

tert Butyl 4-(((1-((5-oxo-2,5-dihydrofuran-3-yl)methyl)-1H-1,2,3-triazol-4-yl)methylthio)carbonothioyl)piperazine-1-carboxylate (**51**):



Yield 74%, white solid. Mp: 146-147°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 8.11 (s, 1H), 5.84 (s, 2H), 5.65 (s, 1H), 4.96 (s, 2H), 4.69 (s, 2H), 4.30 (brs, 2H), 3.99 (brs, 2H), 3.76 (s, $J = 4.9$ Hz, 4H), 1.47 (s, 9H); HRMS (ESI) calcd for $C_{18}H_{25}N_5NaO_4S_2$ $[M + Na]^+$: 462.1246, found: 462.1247.

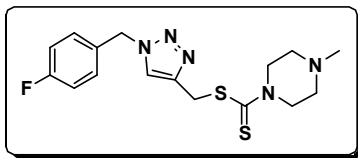
(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl4-methylpiperazine-1-carbodithioae (**54**):



Yield 90.1%, white solid. Mp: 90-91°C; 1H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.16 (s, 4H), 5.43 (s, 2H), 4.67 (s, 2H), 4.33 (brs, 2H), 3.91 (brs, 2H), 2.47 (s, 4H), 2.34 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.90, 144.12, 138.59, 131.62, 129.73, 128.07, 122.66, 54.34, 53.93, 45.60, 31.89,

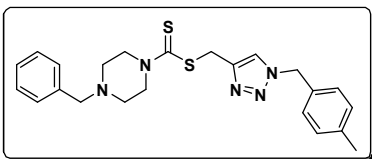
21.17; HRMS (ESI) calcd for $C_{17}H_{23}N_5NaS_2 [M + Na]^+$: 384.1293, found: 384.1290.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl methylpiperazine-1-carbodithioate (**55**):



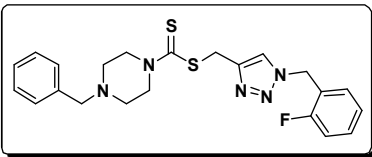
Yield 87.4%, white solid. Mp: 100-101°C; 1H NMR (400 MHz, Acetone) δ 8.00 (s, 1H), 7.45-7.48 (m, 2H), 7.15-7.20 (m, 2H), 5.63 (s, 2H), 4.63 (s, 2H), 4.30 (brs, 2H), 3.92 (brs, 2H), 2.45 (s, 4H), 2.28 (s, 3H); HRMS (ESI) calcd for $C_{16}H_{20}FN_5NaS_2 [M + Na]^+$: 388.1042, found: 388.1045.

(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-benzylpiperazine-1-carbodithioate (**59**):



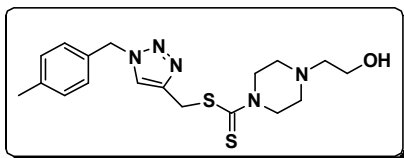
Yield 84%, white solid. Mp: 100-101°C; 1H NMR (400 MHz, $CDCl_3$, ppm): δ 7.68 (s, 1H), 7.09-7.31 (m, 9H), 5.54 (s, 2H), 4.69 (s, 2H), 4.34 (brs, 2H), 3.91 (brs, 2H), 3.53 (s, 2H), 2.52 (s, 4H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.4, 154.5, 136.8, 132.5, 131.1, 129.3, 129.1, 126.7, 124.83, 124.79, 123.00, 122.04, 121.89, 115.92, 115.71, 62.46, 52.35, 47.64, 47.60, 31.83, 28.44; HRMS (ESI) calcd for $C_{23}H_{27}N_5NaS_2 [M + Na]^+$: 460.1606, found: 460.1607.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-benzylpiperazine-1-carbodithioate (**60**):



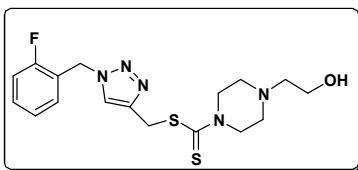
Yield 81.0%, white solid. Mp: 143-144°C. 1H NMR (400 MHz, $CDCl_3$, δ , ppm): 7.67 (s, 1H), 7.09-7.31 (m, 9H), 5.54 (s, 2H), 4.68 (s, 2H), 4.34 (brs, 2H), 3.90 (brs, 2H), 3.53 (s, 2H), 2.52 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, δ , ppm): 195.63, 161.71, 159.24, 144.29, 137.25, 130.87, 130.78, 130.49, 130.46, 129.14, 128.43, 127.45, 124.83, 124.79, 123.00, 122.04, 121.89, 115.92, 115.71, 62.46, 52.35, 47.64, 47.60, 31.83; HRMS (ESI) calcd for $C_{22}H_{24}FN_5NaS_2 [M + Na]^+$: 464.1355, found: 464.1357.

(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(2-hydroxyethyl)piperazine-1-carbodithioate (**61**):



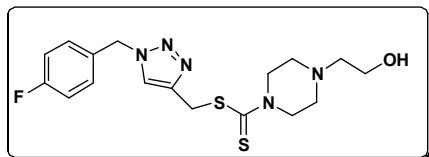
Yield 85.8%, white solid. Mp: 91-92°C; 1H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.18 (s, 4H), 5.46 (s, 2H), 4.69 (s, 2H), 4.36 (brs, 2H), 3.94 (brs, 2H), 3.69 (t, $J = 5.3$ Hz, 2H), 2.62 (t, $J = 5.3$ Hz, 6H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.96, 144.03, 138.63, 131.59, 129.74, 128.08, 122.67, 59.09, 58.00, 53.95, 52.33, 31.89, 21.17; HRMS (ESI) calcd for $C_{18}H_{26}N_5OS_2 [M + H]^+$: 392.1579, found: 392.1577.

(1-(2-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(2-hydroxyethyl)piperazine-1-carbodithioate (**62**):



Yield 71.0%, white solid. Mp: 101-102°C; 1H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.34-7.40 (m, 1H), 7.11-7.28 (m, 3H), 5.57 (s, 2H), 4.70 (s, 2H), 4.37 (brs, 2H), 3.95 (brs, 2H), 3.69 (t, $J = 5.3$ Hz, 2H), 2.62 (t, $J = 5.3$ Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.93, 161.72, 159.25, 144.16, 130.89, 130.81, 130.51, 130.48, 124.82, 124.79, 122.99, 121.98, 121.84, 115.92, 115.71, 59.06, 57.98, 52.32, 47.66, 47.62, 31.84; HRMS (ESI) calcd for $C_{17}H_{23}FN_5OS_2 [M + H]^+$: 396.1328, found: 396.1326.

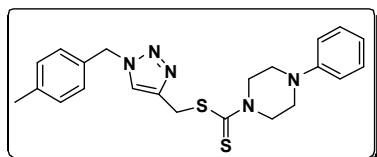
(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(2-hydroxyethyl)piperazine-1-carbodithioate (**63**):



396.1327.

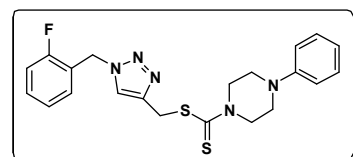
Yield 75.9%, white solid. Mp: 114-115 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.69 (s, 1H), 7.34-7.40 (m, 1H), 7.11-7.28 (m, 3H), 5.57 (s, 2H), 4.70 (s, 2H), 4.37 (brs, 2H), 3.95 (brs, 2H), 3.69 (t, J = 5.3 Hz, 2H), 2.62 (t, J = 5.3 Hz, 6H); HRMS (ESI) calcd for C₁₇H₂₃FN₅OS₂ [M + H]⁺: 396.1328, found:

(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-phenylpiperazine-1-carbodithioate (**64**):



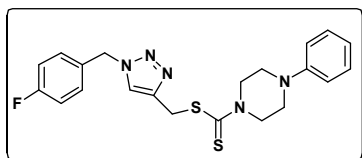
Yield 72.4%, white solid. Mp: 143-144°C; ¹H NMR (400 MHz, CDCl₃) δ 7.59 (s, 1H), 7.29-7.33 (m, 2H), 7.16-7.21 (m, 4H), 6.91-6.96 (m, 3H), 5.46 (s, 2H), 4.72 (s, 2H), 4.49 (brs, 2H), 4.11 (brs, 2H), 3.32 (t, J = 4.8 Hz, 4H), 2.37 (s, 3H); HRMS (ESI) calcd for C₂₂H₂₅N₅NaS₂ [M + Na]⁺: 446.1449, found: 446.1447.

(1-(2-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-phenylpiperazine-1-carbodithioate (**65**):



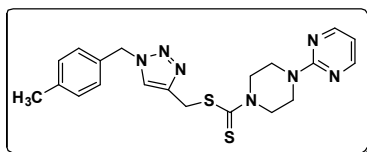
Yield 89.3%, white solid. Mp: 118-119°C; ¹H NMR (400 MHz, CDCl₃) δ 7.70 (s, 1H), 7.25-7.39 (m, 4H), 7.11-7.18 (m, 2H), 6.92-6.95 (m, 3H), 5.57 (s, 2H), 4.73 (s, 2H), 4.49 (brs, 2H), 4.09 (brs, 2H), 3.30 (t, J = 4.9 Hz, 4H); HRMS (ESI) calcd for C₂₁H₂₂FN₅NaS₂ [M + Na]⁺: 450.1198, found: 450.1196.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-phenylpiperazine-1-carbodithioate (**66**):



Yield 77.7%, white solid. Mp: 128-129°C; ¹H NMR (400 MHz, CDCl₃) δ 7.62 (s, 1H), 7.25-7.33 (m, 4H), 7.05-7.10 (m, 2H), 6.91-6.96 (m, 3H), 5.48 (s, 2H), 4.73 (s, 2H), 4.50 (brs, 2H), 4.09 (brs, 2H), 3.32 (t, J = 4.9 Hz, 4H); HRMS (ESI) calcd for C₂₁H₂₃FN₅S₂ [M + H]⁺: 428.1379, found: 428.1376.

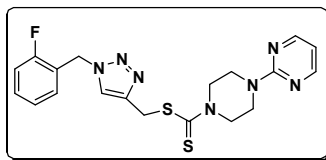
(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(pyrimidin-2-yl)piperazine-1-carbodithioate (**67**):



C₂₀H₂₄N₇S₂ [M + H]⁺: 426.1535, found: 426.1537.

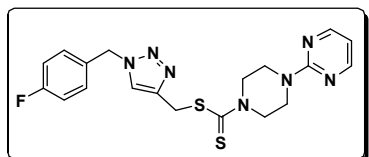
Yield 81.1%, white solid. Mp: 126-127°C; ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, J = 4.8 Hz, 2H), 7.59 (s, 1H), 7.18 (s, 4H), 6.59 (t, J = 4.8 Hz, 1H), 5.45 (s, 2H), 4.71 (s, 2H), 4.41 (brs, 2H), 4.00 (brs, 2H), 3.95 (t, J = 3.2 Hz, 4H), 2.35 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 196.29, 161.25, 157.82, 138.63, 131.60, 129.75, 128.09, 110.73, 53.97, 42.93, 31.87, 21.16; HRMS (ESI) calcd for

(1-(2-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(pyrimidin-2-yl)piperazine-1-carbodithioate (**68**):



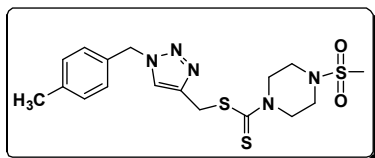
Yield 80.3%, white solid. Mp: 136-137°C; ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, $J = 4.8$ Hz, 2H), 7.70 (s, 1H), 7.33-7.40 (m, 1H), 7.24-7.27 (m, 1H), 7.11-7.18 (m, 2H), 6.60 (t, $J = 4.8$ Hz, 1H), 5.57 (s, 2H), 4.74 (s, 2H), 4.43 (brs, 2H), 4.02 (brs, 2H), 3.97 (t, $J = 3.2$ Hz, 4H); HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{FN}_7\text{NaS}_2$ [$\text{M} + \text{Na}$] $^+$: 452.1103, found: 452.1100.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(pyrimidin-2-yl)piperazine-1-carbodithioate (**69**):



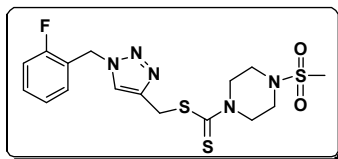
Yield 83.4%, white solid. Mp: 141-142°C; ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, $J = 4.8$ Hz, 2H), 7.62 (s, 1H), 7.26-7.30 (m, 2H), 7.05-7.10 (m, 2H), 6.60 (t, $J = 4.8$ Hz, 1H), 5.48 (s, 2H), 4.73 (s, 2H), 4.42 (brs, 2H), 4.03 (brs, 2H), 3.96 (t, $J = 3.2$ Hz, 4H); HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{FN}_7\text{NaS}_2$ [$\text{M} + \text{Na}$] $^+$: 452.1103, found: 452.1102.

(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(methylsulfonyl)piperazine-1-carbodithioate (**70**):



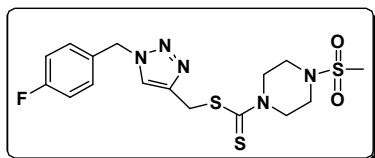
Yield 91.2%, white solid. Mp: 163-164°C; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (s, 1H), 7.19 (s, 4H), 5.46 (s, 2H), 4.67 (s, 2H), 4.25 (brs, 4H), 3.34 (t, $J = 5.0$ Hz, 4H), 2.82 (s, 3H), 2.37 (s, 3H); HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{23}\text{N}_5\text{NaO}_2\text{S}_3$ [$\text{M} + \text{Na}$] $^+$: 448.0912, found: 448.0914.

(1-(2-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(methylsulfonyl)piperazine-1-carbodithioate (**71**):



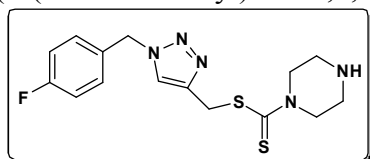
Yield 88.5%, white solid. Mp: 162-163°C. ^1H NMR (400 MHz, CDCl_3) δ 7.67 (s, 1H), 7.35-7.41 (m, 1H), 7.26-7.29 (m, 1H), 7.12-7.19 (m, 2H), 5.57 (s, 2H), 4.69 (s, 2H), 4.30 (brs, 2H), 4.17 (brs, 2H), 3.35 (t, $J = 5.1$ Hz, 4H), 2.82 (s, 3H); HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{20}\text{FN}_5\text{NaO}_2\text{S}_3$ [$\text{M} + \text{Na}$] $^+$: 452.0661, found: 452.0662.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-(methylsulfonyl)piperazine-1-carbodithioate (**72**):



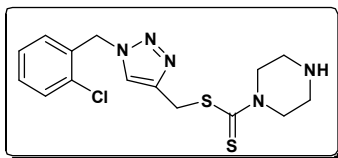
Yield 89.0%, white solid. Mp: 164-165°C. ^1H NMR (400 MHz, CDCl_3) δ 7.58 (s, 1H), 7.25-7.29 (m, 2H), 7.05-7.09 (m, 2H), 5.47 (s, 2H), 4.67 (s, 2H), 4.27 (brs, 4H), 3.34 (t, $J = 5.0$ Hz, 4H), 2.82 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 197.07, 164.08, 161.61, 143.78, 130.46, 130.42, 129.99, 129.91, 122.72, 116.22, 116.01, 53.42, 45.23, 35.15, 32.03; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{20}\text{FN}_5\text{NaO}_2\text{S}_3$ [$\text{M} + \text{Na}$] $^+$: 452.0661, found: 452.0662.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl piperazine-1-carbodithioate (**74**):



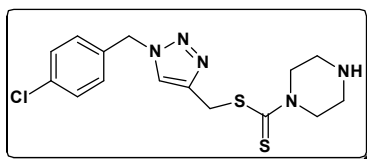
Yield 93.9%, white solid. Mp: 138-139°C; ^1H NMR (400 MHz, CDCl_3 , ppm): δ 7.60 (s, 1H), 7.04-7.27 (m, 4H), 5.45 (s, 2H), 4.69 (s, 2H), 4.31 (brs, 2H), 3.89 (brs, 2H), 2.93 (s, 4H); ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ 196.03, 164.07, 161.60, 144.33, 130.47, 130.44, 129.97, 129.88, 122.74, 116.21, 116.00, 53.41, 45.15, 31.76; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{19}\text{FN}_5\text{S}_2$ [$\text{M} + \text{H}$] $^+$: 352.1066, found: 352.1063.

(1-(2-Chlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl piperazine-1-carbodithioate (**75**):



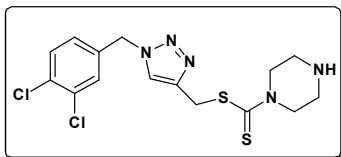
Yield 94.8%, white solid. Mp: 98-99°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.68 (s, 1H), 7.43 (dd, J₁ = 1.4 Hz, J₂ = 7.8 Hz, 1H), 7.24-7.33 (m, 2H), 7.18 (dd, J₁ = 1.6 Hz, J₂ = 7.4 Hz, 1H), 5.61 (s, 2H), 4.64 (s, 2H), 4.45 (brs, 4H), 3.34 (s, 4H); ¹³C NMR (100 MHz, CDCl₃, δ, ppm): 197.25, 143.28, 133.50, 132.25, 130.34, 130.19, 129.97, 127.65, 123.43, 51.57, 43.19, 32.18; HRMS (ESI) calcd for C₁₅H₁₉ClN₅S₂ [M + H]⁺: 368.0770, found: 368.0772.

(1-(4-Chlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl piperazine-1-carbodithioate (76):



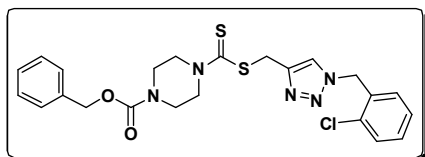
Yield 95.1%, white solid. Mp: 79-80°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.61 (s, 1H), 7.35 (d, J = 8.1 Hz, 2H), 7.20 (d, 2H, J = 8.1 Hz), 5.45 (s, 2H), 4.69 (s, 2H), 4.31 (brs, 2H), 3.90 (brs, 2H), 2.94 (s, 4H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 195.63, 144.54, 134.71, 133.17, 129.35, 129.27, 122.81, 53.36, 45.61, 31.65; HRMS (ESI) calcd for C₁₅H₁₉ClN₅S₂ [M + H]⁺: 368.0770, found: 368.0767.

(1-(3,4-Dichlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl piperazine-1-carbodithioate (81):



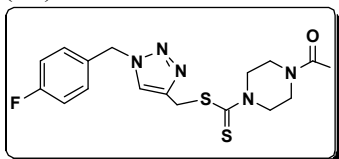
Yield 95.5%, white solid. Mp: 122-123°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.65 (s, 1H), 7.45 (d, J = 8.3 Hz, 1H), 7.35 (d, J = 2.0 Hz, 1H), 7.10 (dd, J₁ = 2.0 Hz, J₂ = 8.3 Hz, 1H), 5.44 (s, 2H), 4.70 (s, 2H), 4.31 (brs, 2H), 3.92 (brs, 2H), 2.95 (s, 4H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 195.62, 144.87, 134.79, 133.27, 133.07, 131.09, 129.86, 127.17, 122.92, 52.81, 45.63, 31.56; HRMS (ESI) calcd for C₁₅H₁₈Cl₂N₅S₂ [M + H]⁺: 402.0381, found: 402.0379.

Benzyl 4-(((1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methylthio) carbonothioyl) piperazine-1-carboxylate (85):



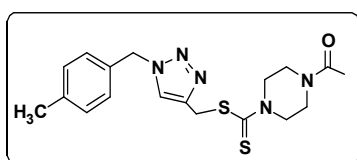
Yield 71.7%, white solid. Mp: 91-92°C; ¹H NMR (400 MHz, CDCl₃, ppm): δ 7.67 (s, 1H), 7.13-7.43 (m, 9H), 5.61 (s, 2H), 5.15 (s, 2H), 4.69 (s, 2H), 4.28 (brs, 2H), 3.95 (brs, 2H), 3.61 (t, J = 5.3 Hz, 4H); ¹³C NMR (100 MHz, CDCl₃, ppm): δ 196.60, 155.05, 143.86, 136.20, 133.42, 132.46, 130.20, 129.90, 128.61, 128.31, 128.10, 127.58, 126.98, 123.20, 67.65, 51.40, 43.04, 31.89; HRMS (ESI) calcd for C₂₃H₂₅ClN₅O₂S₂ [M + H]⁺: 502.1138, found: 502.1137.

(1-(4-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-acetylpiperazine-1-carbodithioate (94):



Yield 81.1%, white solid. Mp: 189-190°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.14 (s, 1H), 7.38-7.41 (m, 2H), 7.19-7.24 (m, 2H), 5.56 (s, 2H), 4.59 (s, 2H), 4.27 (brs, 2H), 3.90 (brs, 2H), 3.59 (t, J = 4.9 Hz, 4H), 2.03 (s, 3H); HRMS (ESI) calcd for C₁₇H₂₁FN₅OS₂ [M + H]⁺: 394.1172, found: 394.1173.

(1-(4-Methylbenzyl)-1H-1,2,3-triazol-4-yl)methyl 4-acetylpiperazine-1-carbodithioate (95):



Yield 76.2%, white solid. Mp: 137-138°C; ¹H NMR (400 MHz, CDCl₃) δ 7.57 (s, 1H), 7.17 (s, 4H), 5.44 (s, 2H), 4.67 (s, 2H), 4.30 (brs, 2H), 3.99 (brs, 2H), 3.74 (t, J = 5.6 Hz, 2H), 3.60 (t, J = 5.6 Hz, 2H), 2.36 (s, 3H), 2.13 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 196.81, 169.31, 138.68, 131.55, 129.75, 128.10, 53.99, 45.16,

40.56, 31.96, 21.36, 21.16; HRMS (ESI) calcd for $C_{18}H_{24}N_5OS_2$ $[M + H]^+$: 390.1422, found: 390.1424.