Exploration of Benzothiazole-Rhodocyanines as Allosteric Inhibitors of Protein-Protein Interactions with Heat Shock Protein 70 (Hsp70)

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Supporting Information

Compound Characterization

3-benzyl-2-((*Z*)-((*E*)-5-(6-bromo-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (Compound 1). Anal. RP-HPLC: t_R 2.07 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.27 (d, *J* = 4.0 Hz, 1H), 8.19 (d, *J* = 1.6 Hz, 1H), 7.91 (d, *J* = 4.0 Hz, 1H), 7.67 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.45 - 7.38 (m, 2H), 7.38 - 7.33 (m, 3H), 6.53 (s, 1H), 5.77 (s, 2H), 4.08 (s, 3H), 4.07 (q, *J* = 7.2 Hz, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.11, 161.78, 157.00, 153.74, 140.32, 135.77, 135.07, 130.48, 129.60, 128.92, 128.64, 127.89, 125.32, 116.29, 115.39, 114.36, 84.06, 81.47, 53.54, 39.01, 35.28, 12.28. ESI-MS: calculated for $C_{24}H_{21}BrN_3OS_3^+$ 542.00; found 541.86.

3-benzyl-2-((*Z*)-((*E*)-5-(5-bromo-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 2). Anal. RP-HPLC: t_R 2.05 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.27 (d, *J* = 4.0 Hz, 1H), 7.97 (d, *J* = 1.6 Hz, 1H), 7.91 (d, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.49 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.45-7.40 (m, 2H), 7.38-7.33 (m, 3H), 6.54 (s, 1H), 5.77 (s, 2H), 4.10 (s, 3H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.95, 161.67, 157.02, 153.42, 142.13, 135.77, 135.13, 129.56, 128.92, 127.99, 126.94, 125.66, 124.33, 120.73, 115.49, 115.35, 84.20, 81.57, 53.50, 39.04, 35.19, 12.27. ESI-MS: calculated for $C_{24}H_{21}BrN_3OS_3^+$ 542.00; found 541.96.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(3-methyl-6-nitrobenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (Compound 3). Anal. RP-HPLC: t_R 1.80 min, purity 95.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.90 (d, *J* = 2.4 Hz, 1H), 8.37 - 8.30 (m, 2H), 7.98 (dd, *J* = 4.0, 0.4 Hz, 1H), 7.82 (d, *J* = 9.2 Hz, 1H), 7.47 - 7.40 (m, 2H), 7.39 - 7.34 (m, 3H), 6.59 (s, 1H), 5.82 (s, 2H), 4.14 (s, 3H), 4.10 (q, *J* = 7.2 Hz, 2H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR

(125 MHz, DMSO) δ 164.46, 162.08, 157.62, 153.42, 145.75, 143.52, 135.98, 135.04, 129.61, 128.96, 127.93, 127.74, 123.80, 119.16, 116.14, 112.60, 84.66, 83.55, 53.64, 39.08, 35.60, 12.24. ESI-MS: calculated for $C_{24}H_{21}ClN_4O_3S_3^+$ 509.08; found 508.96.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(3-methyl-5-(methylsulfonyl)benzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 4). Anal. RP-HPLC: t_R 1.73 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.31 (d, *J* = 4.0 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 1.2 Hz, 1H), 7.93 (d, *J* = 4.0 Hz, 1H), 7.82 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.45 - 7.39 (m, 2H), 7.38 - 7.32 (m, 3H), 6.57 (s, 1H), 5.80 (s, 2H), 4.17 (s, 3H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.33 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.27, 161.87, 157.05, 153.44, 141.36, 140.38, 135.87, 135.10, 132.29, 129.58, 128.93, 127.96, 123.71, 122.38, 115.84, 110.94, 84.51, 82.19, 53.57, 44.08, 39.08, 35.38, 12.24. ESI-MS: calculated for $C_{25}H_{24}N_3O_3S_4^+$ 542.07; found 541.93.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(3-methyl-6-(trifluoromethyl)benzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 5). Anal. RP-HPLC: t_R 2.05 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.42 (s, 1H), 8.29 (d, *J* = 4.0 Hz, 1H), 7.94 (d, *J* = 4.0 Hz, 1H), 7.84 (t, *J* = 8.8 Hz, 2H), 7.45 - 7.40 (m, 2H), 7.38 - 7.33 (m, 3H), 6.57 (s, 1H), 5.78 (s, 2H), 4.15 (s, 3H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.29, 161.90, 157.50, 153.55, 143.74, 135.88, 135.10, 129.57, 128.92, 127.94, 127.38, 124.88, 124.60 (q, *J* = 270 Hz), 124.57 (q, *J* = 32 Hz) 120.54, 115.76, 113.03, 84.41, 82.28, 53.55, 39.05, 35.34, 12.25. ESI-MS: calculated for $C_{25}H_{21}F_3N_3OS_3^+$ 532.08; found 531.93.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(3-methyl-5-(trifluoromethoxy)benzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 6). Anal. RP-HPLC: t_R 2.07 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.30 (d, *J* = 4.4 Hz, 1H), 8.03 (d, *J* = 8.8

Hz, 1H), 7.92 (dd, *J* = 4.0, 0.8 Hz, 1H), 7.81 (d, *J* = 1.6 Hz, 1H), 7.46 - 7.39 (m, 2H), 7.39 - 7.31 (m, 4H), 6.56 (s, 1H), 5.79 (s, 2H), 4.11 (s, 3H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.96 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.05, 161.77, 157.83, 153.51, 148.25, 142.14, 135.81, 135.15, 129.55, 128.89, 127.96, 125.52, 124.23, 120.54 (q, *J* = 255 Hz), 117.11, 115.57, 106.52, 84.30, 81.84, 53.50, 39.03, 35.34, 12.25. ESI-MS: calculated for $C_{25}H_{21}F_3N_3O_2S_3^+$ 548.07; found 547.93.

3-benzyl-2-((Z)-((E)-3-ethyl-5-(3-methyl-6-(trifluoromethoxy)benzo[d]thiazol-2(3H)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 7). Anal. RP-HPLC: t_R 2.08 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.29 (d, *J* = 4.0 Hz, 1H), 8.10 (s, 1H), 7.93 (d, *J* = 4.0 Hz, 1H), 7.77 (d, *J* = 8.8 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.45 - 7.39 (m, 2H), 7.38 - 7.32 (m, 3H), 6.55 (s, 1H), 5.78 (s, 2H), 4.12 (s, 3H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.13, 161.76, 157.48, 153.60, 144.71, 139.91, 135.80, 135.13, 129.56, 128.90, 128.05, 127.95, 121.01, 120.55 (q, *J* = 254 Hz), 116.15, 115.50, 113.79, 84.22, 81.58, 53.50, 39.01, 35.41, 12.26. ESI-MS: calculated for $C_{25}H_{21}F_3N_3O_2S_3^+$ 548.07; found 547.93.

3-benzyl-2-((*Z*)-((*E*)-5-(3,5-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 8). Anal. RP-HPLC: t_R 2.01 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.24 (d, *J* = 4.0 Hz, 1H), 7.88 (d, *J* = 4.0 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.55 (s, 1H), 7.45 – 7.39 (m, 2H), 7.38 - 7.33 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 1H), 6.51 (s, 1H), 5.75 (s, 2H), 4.11 (s, 3H), 4.08 (q, *J* = 7.2 Hz, 3H), 2.45 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.65, 161.33, 157.23, 153.49, 140.77, 137.81, 135.57, 135.15, 129.54, 128.89, 127.99, 125.45, 123.12, 122.33, 114.99, 112.88, 83.75, 80.79, 53.37, 39.01, 34.98, 21.62, 12.28. ESI-MS: calculated for $C_{25}H_{24}N_3OS_3^+$ 478.11; found 478.00.

3-benzyl-2-((*Z*)-((*E*)-5-(3,6-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 9, JG-194). Anal. RP-HPLC: t_R 1.95 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.24 (d, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 4.0 Hz, 1H), 7.74 (s, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.45 - 7.39 (m, 2H), 7.38 – 7.33 (m, 4H), 6.51 (s, 1H), 5.75 (s, 2H), 4.11 (s, 3H), 4.08 (q, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{1}H-NMR (400 MHz, DMSO-d_6): δ 8.26 (d, J = 4.0 Hz, 1H), 7.89 (d, J = 4.0 Hz, 1H), 7.75 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.43 (t, J = 8.0 Hz, 2H), 7.39-7.33 (m, 4H), 6.52 (s, 1H), 5.76 (s, 2H), 4.14-4.05 (m, 5H), 2.40 (s, 3H), 0.98 (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.84, 161.56, 157.10, 153.86, 138.80, 135.63, 135.10, 134.33, 129.60, 128.91, 128.73, 127.88, 126.30, 122.78, 114.94, 112.52, 83.68, 80.67, 53.45, 38.97, 35.16, 21.06, 12.29. ESI-MS: calculated for $C_{25}H_{24}N_3OS_3^+$ 478.11; found 478.07.

3-benzyl-2-((*Z*)-((*E*)-5-(3,4-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 10). Anal. RP-HPLC: t_R 1.95 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.27 (d, *J* = 4.0 Hz, 1H), 7.93 (d, *J* = 3.6 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.46 - 7.32 (m, 5H), 7.29 - 7.19 (m, 2H), 6.53 (s, 1H), 5.77 (s, 2H), 4.21 (s, 3H), 4.08 (q, *J* = 7.2 Hz, 2H), 2.74 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.93, 161.49, 158.67, 153.58, 139.83, 135.69, 135.12, 131.60, 129.56, 128.90, 127.97, 127.00, 124.69, 124.00, 120.65, 115.16, 83.97, 81.49, 53.46, 39.03, 20.80, 12.29. ESI-MS: calculated for $C_{25}H_{24}N_3OS_3^+$ 478.11; found 477.94.

3-benzyl-2-((*Z*)-((*E*)-5-(3,7-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 11). Anal. RP-HPLC: t_R 1.97 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.26 (d, *J* = 4.0 Hz, 1H), 7.90 (d, *J* = 3.6 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.46 - 7.33 (m, 6H), 7.19 (d, *J* = 8.0 Hz, 1H), 6.53 (s, 1H), 5.76 (s, 2H), 4.13

(s, 3H), 4.08 (q, *J* = 7.2 Hz, 2H), 2.45 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 163.95, 161.68, 156.54, 153.73, 140.62, 135.74, 135.14, 132.09, 129.62, 128.94, 128.18, 127.94, 125.46, 125.25, 115.22, 110.48, 83.86, 81.03, 53.50, 39.04, 35.38, 19.52, 12.32. ESI-MS: calculated for $C_{25}H_{24}N_3OS_3^+$ 478.11; found 477.97.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(6-ethyl-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 12). Anal. RP-HPLC: t_R 2.08 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.26 (d, *J* = 4.0 Hz, 1H), 7.88 (d, *J* = 4.0 Hz, 1H), 7.77 (s, 1H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.47 - 7.39 (m, 2H), 7.39 - 7.32 (m, 4H), 6.51 (s, 1H), 5.76 (s, 2H), 4.11 (s, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.21 (d, *J* = 7.6 Hz, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.74, 161.45, 156.97, 153.66, 140.63, 138.85, 135.61, 135.16, 129.55, 128.88, 127.95, 127.62, 126.31, 121.55, 114.98, 112.53, 83.77, 80.64, 53.38, 38.98, 35.13, 28.17, 16.13, 12.29. ESI-MS: calculated for $C_{26}H_{26}N_3OS_3^+$ 492.12; found 492.00.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(5-methoxy-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 13). Anal. RP-HPLC: t_R 1.93 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.24 (d, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 4.0 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.38 - 7.32 (m, 3H), 7.28 (d, *J* = 2.4 Hz, 1H), 6.97 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.50 (s, 1H), 5.75 (s, 2H), 4.12 (s, 3H), 4.08 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.59, 161.38, 160.05, 158.14, 153.53, 142.03, 135.58, 135.15, 129.56, 128.89, 127.94, 123.37, 117.52, 114.98, 112.02, 98.27, 83.72, 80.96, 56.44, 53.40, 38.99, 35.17, 12.27. ESI-MS: calculated for $C_{25}H_{24}N_3O_2S_3^+$ 494.10; found 493.94.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(6-methoxy-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazo

lidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 14). Anal. RP-HPLC: t_R 1.88 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.25 (d, *J* = 4.0 Hz, 1H), 7.86 (d, *J* = 4.4 Hz, 1H), 7.61 (d, *J* = 9.2 Hz, 1H), 7.58 (d, *J* = 2.4 Hz, 1H), 7.45 - 7.39 (m, 2H), 7.38 - 7.33 (m, 3H), 7.10 (dd, *J* = 9.2, 2.4 Hz, 1H), 6.49 (s, 1H), 5.75 (s, 2H), 4.09 (s, 3H), 4.05 (q, *J* = 7.2 Hz, 2H), 3.79 (s, 3H), 0.96 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.70, 161.39, 156.91, 153.77, 135.58, 135.13, 134.69, 129.58, 128.89, 127.91, 127.71, 115.13, 114.79, 113.58, 107.08, 83.60, 80.33, 56.30, 53.41, 38.97, 35.28, 12.30. ESI-MS: calculated for $C_{25}H_{24}N_3O_2S_3^+$ 494.10; found 493.91.

3-benzyl-2-((*Z*)-((*E*)-3-ethyl-5-(3-methyl-6-(methylthio)benzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 15). Anal. RP-HPLC: t_R 2.03 min, purity 99.0 %.^{1}H NMR (400 MHz, DMSO) δ 8.25 (d, *J* = 4.0 Hz, 3H), 7.88 (dd, *J* = 4.8, 1.6 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 3H), 7.45 - 7.39 (m, 3H), 7.38 - 7.32 (m, 3H), 6.51 (s, 1H), 5.75 (s, 2H), 4.10 (s, 3H), 4.07 (q, *J* = 7.6 Hz, 2H), 2.52 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 163.81, 161.53, 156.55, 153.60, 138.52, 135.64, 135.10, 134.63, 129.58, 128.91, 127.93, 127.51, 126.05, 119.76, 115.05, 112.98, 83.85, 80.89, 53.45, 39.00, 35.16, 15.83, 12.27. ESI-MS: calculated for $C_{25}H_{24}N_3OS_4^+$ 510.08; found 509.91.

2-((*Z*)-((*E*)-3-allyl-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-benzylthiazol-3-ium chloride (compound 16). Anal. RP-HPLC: t_R 2.04 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.28 (d, *J* = 4.0 Hz, 1H), 8.06 (d, *J* = 2.0 Hz, 1H), 7.92 (d, *J* = 4.4 Hz, 1H), 7.68 (d, *J* = 9.2 Hz, 1H), 7.55 (dd, *J* = 9.2, 2.0 Hz, 1H), 7.45 - 7.33 (m, 3H), 7.30 (d, *J* = 7.2 Hz, 2H), 6.50 (s, 1H), 5.74 (s, 2H), 5.72 - 5.63 (m, 1H), 5.02 - 4.90 (m, 2H), 4.72 (d, *J* = 4.4 Hz, 2H), 4.10 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 163.98, 161.69, 157.08, 153.68, 139.84, 135.69, 134.82, 130.66, 129.49, 129.31, 129.12, 128.85, 128.58, 128.20, 127.92,

127.73, 122.46, 117.94, 115.65, 113.91, 84.73, 81.14, 53.43, 45.80, 35.30. ESI-MS: calculated for $C_{25}H_{21}ClN_3OS_3^+$ 510.05; found 509.86.

3-benzyl-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-cyclopropyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 17). Anal. RP-HPLC: t_R 1.99 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.34 (d, *J* = 4.0 Hz, 1H), 8.04 (d, *J* = 2.0 Hz, 1H), 7.96 (dd, *J* = 4.0, 1.2 Hz, 1H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.54 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.48 - 7.42 (m, 2H), 7.41 - 7.36 (m, 1H), 7.35 - 7.30 (m, 2H), 6.65 (d, *J* = 0.8 Hz, 1H), 5.74 (s, 2H), 4.07 (s, 3H), 2.83 - 2.74 (m, 1H), 1.07 (q, *J* = 7.2 Hz, 2H), 0.71 - 0.64 (m, 2H). ^{13}C NMR (100 MHz, DMSO) δ 164.80, 161.61, 156.75, 155.67, 139.94, 136.00, 134.62, 129.63, 128.93, 128.47, 128.25, 127.67, 122.48, 115.57, 113.87, 85.69, 81.13, 53.89, 35.32, 26.50, 7.73. ESI-MS: calculated for $C_{25}H_{21}ClN_3OS_3^+$ 510.05; found 509.96.

3-benzyl-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-(3-methoxy-3-oxopropyl)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 18). Anal. RP-HPLC: t_R 2.03 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.26 (d, *J* = 4.0 Hz, 1H), 8.10 (d, *J* = 2.0 Hz, 1H), 7.95 (d, *J* = 4.0 Hz, 1H), 7.72 (d, *J* = 9.2 Hz, 1H), 7.58 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.43 - 7.34 (m, 3H), 7.34 - 7.29 (m, 2H), 6.68 (s, 1H), 5.72 (s, 2H), 5.06 (s, 2H), 4.14 (s, 3H), 3.64 (s, 3H). ^{13}C NMR (100 MHz, DMSO) δ 171.13, 164.08, 161.77, 156.98, 153.63, 139.88, 135.74, 135.03, 129.54, 129.02, 128.57, 128.20, 128.15, 127.71, 122.50, 115.71, 113.96, 84.26, 81.06, 53.49, 52.21, 35.31, 31.03. ESI-MS: calculated for $C_{26}H_{23}ClN_3O_3S_3^+$ 556.06; found 555.96.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-fluorobenzyl)thiazol-3-ium chloride (compound 19). Anal. RP-HPLC: t_R 1.97 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.19 (dd, *J* = 4.0, 0.8 Hz, 1H), 8.06 (d, *J* =

2.4 Hz, 1H), 7.89 (dd, *J* = 4.0, 0.4 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.53 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.51 - 7.43 (m, 2H), 7.36 - 7.25 (m, 2H), 6.56 (s, 1H), 5.85 (s, 2H), 4.15 - 4.00 (m, 5H), 1.05 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.09, 162.00, 160.59 (d, *J* = 245.0 Hz), 157.23, 155.34, 154.01, 139.94, 135.65, 131.60 (d, *J* = 8.75 Hz), 130.53, 128.60, 128.27, 127.76, 125.63, 122.57, 121.77 (d, *J* = 15.0 Hz), 116.51 (d, *J* = 7.50 Hz), 115.17, 114.01, 83.69, 81.49, 48.57, 39.12, 35.35, 12.37. ESI-MS: calculated for $C_{24}H_{20}ClFN_3OS_3^+$ 516.04; found 515.85.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(3-fluorobenzyl)thiazol-3-ium chloride (compound 20). Anal. RP-HPLC: t_R 2.04 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.30 (d, *J* = 4.0 Hz, 1H), 8.06 (d, *J* = 2.0 Hz, 1H), 7.92 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.54 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.31 (d, *J* = 9.6 Hz, 1H), 7.25 - 7.15 (m, 2H), 6.53 (s, 1H), 5.81 (s, 2H), 4.11(q, *J* = 7.2 Hz, 2H), 4.09 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.09, 162.76 (d, *J* = 243.75 Hz), 161.87, 157.20, 153.95, 139.95, 137.80 (d, *J* = 7.5 Hz), 135.68, 131.75 (d, *J* = 8.75 Hz), 128.59, 128.27, 127.76, 123.97, 122.57, 115.83 (d, *J* = 21.25 Hz), 115.39, 115.11 (d, *J* = 22.5 Hz), 114.01, 83.95, 81.49, 52.83, 39.01, 35.34, 12.16. ESI-MS: calculated for $C_{24}H_{20}ClFN_3OS_3^+$ 516.04; found 515.91.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(4-fluorobenzyl)thiazol-3-ium chloride (compound 21). Anal. RP-HPLC: t_R 2.03 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.29 (d, *J* = 4.0 Hz, 1H), 8.06 (d, *J* = 2.0 Hz, 1H), 7.91 (d, *J* = 3.2 Hz, 1H), 7.68 (d, *J* = 9.2 Hz, 1H), 7.54 (dd, *J* = 8.8 , 2.0 Hz, 1H), 7.49-7.42 (m, 2H), 7.32-7.23 (m, 2H), 6.55 (s, 1H), 5.78 (s, 2H), 4.11(q, *J* = 7.2 Hz, 2H), 4.08 (s, 3H), 1.01 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.10, 162.40 (d, *J* = 242.5 Hz), 161.75,

157.15, 153.85, 139.95, 135.62, 131.312, 130.33 (d, J = 8.75 Hz), 128.57, 128.27, 127.75, 122.57, 116.46 (d, J = 21.25 Hz), 115.41, 114.00, 83.95, 81.46, 52.74, 39.04, 35.33, 12.34. ESI-MS: calculated for $C_{24}H_{20}ClFN_3OS_3^+$ 516.04; found 515.91.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-chlorobenzyl)thiazol-3-ium chloride (compound 22). Anal. RP-HPLC: t_R 2.06 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, J = 2.0 Hz, 1H), 8.07 (d, J = 4.0 Hz, 1H), 7.89 (dd, J = 4.0, 0.8 Hz, 1H), 7.71 (d, J = 8.8 Hz, 1H), 7.61 (dd, J = 8.0, 1.6 Hz, 1H), 7.57 (dd, J = 8.8, 2.0 Hz, 1H), 7.48 - 7.37 (m, 2H), 7.16 (dd, J = 7.6, 2.0 Hz, 1H), 6.44 (s, 1H), 5.82 (s, 2H), 4.12 (s, 3H), 4.03 (q, J = 7.2 Hz, 2H), 0.99 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.00, 162.16, 157.17, 154.04, 139.90, 135.52, 132.75, 132.06, 130.97, 130.57, 129.81, 128.60, 128.57, 128.25, 127.75, 122.55, 115.27, 113.99, 83.78, 81.46, 51.85, 39.13, 35.34, 12.31. ESI-MS: calculated for $C_{24}H_{20}Cl_2N_3OS_3^+$ 532.01; found 531.82.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(3-chlorobenzyl)thiazol-3-ium chloride (compound 23). Anal. RP-HPLC: t_R 2.12 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.30 (dd, J = 4.0, 0.8 Hz, 1H), 8.06 (dd, J = 2.4, 0.8 Hz, 1H), 7.91 (d, J = 4.0 Hz, 1H), 7.67 (d, J = 9.2 Hz, 1H), 7.57 (s, 1H), 7.56 - 7.51 (m, 1H), 7.48 - 7.41 (m, 2H), 7.31 - 7.24 (m, 1H), 6.53 (s, 1H), 5.79 (s, 2H), 4.21 - 4.10 (q, J = 7.2 Hz, 2H), 4.08 (s, 3H), 0.99 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.08, 161.82, 157.20, 154.00, 139.92, 137.51, 135.66, 134.11, 131.53, 128.95, 128.60, 128.14, 127.75, 126.59, 122.54, 115.37, 113.98, 83.89, 81.50, 52.71, 39.33, 35.31, 12.14. ESI-MS: calculated for $C_{24}H_{20}Cl_2N_3OS_3^+$ 532.01; found 531.82.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-yli-

dene)methyl)-3-(4-chlorobenzyl)thiazol-3-ium chloride (compound 24). Anal. RP-HPLC: t_R 2.09 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.25 (d, *J* = 4.0 Hz, 1H), 8.09 (s, 1H), 7.90 (d, *J* = 3.6 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 6.52 (s, 1H), 5.76 (s, 2H), 4.10 (s, 3H), 4.09 (q, *J* = 7.2 Hz, 2H), 1.00 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.11, 160.03, 157.21, 152.46, 139.96, 135.62, 134.11, 133.59, 131.22, 129.91, 129.55, 129.14, 128.59, 128.28, 127.77, 122.58, 115.41, 114.02, 83.90, 81.48, 52.72, 39.05, 35.34, 12.32. ESI-MS: calculated for $C_{24}H_{20}Cl_2N_3OS_3^+$ 532.01; found 531.80.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(trifluoromethyl)benzyl)thiazol-3-ium chloride (compound 25). Anal. RP-HPLC: t_R 2.11min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.11 (d, *J* = 2.4 Hz, 1H), 8.09 (d, *J* = 4.0 Hz, 1H), 7.95 (dd, *J* = 4.0, 0.8 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.75 - 7.67 (m, 2H), 7.66 - 7.54 (m, 2H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.16 (s, 1H), 5.91 (s, 2H), 4.13 (s, 3H), 3.89 (q, *J* = 7.2 Hz, 2H), 0.86 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.84, 162.04, 157.36, 154.08, 139.87, 135.54, 134.22, 132.75, 129.64, 128.65, 128.51, 128.24, 127.28 (q, *J* = 6.0 Hz), 126.71 (q, *J* = 30.0 Hz), 124.57 (q, *J* = 272.0 Hz), 122.55, 115.52, 114.03, 83.59, 81.38, 50.89, 38.98, 35.36, 11.78. ESI-MS: calculated for $C_{25}H_{20}ClF_3N_3OS_3^+$ 566.04; found 565.88.

3-(2-bromobenzyl)-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 26). Anal. RP-HPLC: t_R 2.09 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 2.0 Hz, 1H), 8.03 (d, *J* = 4.4 Hz, 1H), 7.90 (d, *J* = 4.0 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.57 (dd, *J* = 8.0, 2.4 Hz, 1H), 7.44 (td, *J* = 7.6, 1.2 Hz, 1H), 7.36 (td, *J* = 7.6, 1.6 Hz, 1H), 7.07 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.39 (s, 1H), 5.77 (s, 2H), 4.12 (s, 3H), 4.03 (q, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz,

3H).[13]C NMR (100 MHz, DMSO) δ 163.99, 162.15, 157.22, 154.05, 139.89, 135.37, 133.86, 133.61, 131.16, 129.75, 129.13, 128.63, 128.26, 127.76, 122.91, 122.55, 115.37, 114.00, 83.81, 81.46, 54.07, 39.15, 35.35, 12.32. ESI-MS: calculated for $C_{25}H_{20}ClF_3N_3OS_3^+$ 566.04; found 565.88. ESI-MS: calculated for $C_{24}H_{20}BrClN_3OS_3^+$ 575.96; found 575.86.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(methoxycarbonyl)benzyl)thiazol-3-ium chloride (compound 27). Anal. RP-HPLC: t_R 2.07 min, purity 96.0 %. [1]H NMR (400 MHz, DMSO) δ 8.15 - 7.99 (m, 3H), 7.90 (d, *J* = 4.4 Hz, 1H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.67 - 7.48 (m, 3H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.43 (s, 1H), 6.03 (s, 2H), 4.12 (s, 3H), 3.98 (q, *J* = 7.2 Hz, 2H), 3.90 (s, 3H), 0.86 (t, *J* = 7.2 Hz, 3H). [13]C NMR (100 MHz, DMSO) δ 167.18, 163.94, 162.09, 156.96, 153.72, 139.82, 135.56, 133.77, 131.51, 129.11, 129.04, 128.56, 128.21, 128.14, 127.69, 122.46, 115.42, 113.90, 84.04, 81.40, 53.06, 52.48, 38.96, 35.29, 12.03. ESI-MS: calculated for $C_{26}H_{23}ClN_3O_3S_3^+$ 556.06; found 555.88.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-methylbenzyl)thiazol-3-ium chloride (compound 28). Anal. RP-HPLC: t_R 2.04 min, purity 97.0 %. [1]H NMR (400 MHz, DMSO) δ 8.08 (d, *J* = 2.0 Hz, 1H), 8.02 (dd, *J* = 4.0, 0.8 Hz, 1H), 7.91 (d, *J* = 4.0 Hz, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.60 - 7.52 (m, 1H), 7.33 - 7.25 (m, 2H), 7.24 - 7.17 (m, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 6.41 (s, 1H), 5.73 (s, 2H), 4.11 (s, 3H), 4.01 (q, *J* = 7.2 Hz, 2H), 2.34 (s, 3H), 0.92 (t, *J* = 7.2 Hz, 3H). [13]C NMR (100 MHz, DMSO) δ 163.98, 162.05, 156.96, 153.62, 139.85, 136.47, 135.49, 132.86, 131.33, 128.83, 128.55, 128.23, 127.70, 127.02, 122.49, 115.52, 113.91, 84.12, 81.39, 52.44, 39.03, 35.29, 19.42, 12.13. ESI-MS: calculated for $C_{25}H_{23}ClN_3OS_3^+$ 512.07; found 511.94.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-yli-

dene)methyl)-3-(2-methoxybenzyl)thiazol-3-ium chloride (compound 29). Anal. RP-HPLC: t_R 2.06 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 4.0 Hz, 1H), 8.07 (d, *J* = 2.0 Hz, 1H), 7.83 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.55 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.43 - 7.36 (m, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.56 (s, 1H), 5.64 (s, 2H), 4.09 (s, 3H), 4.06 (t, *J* = 7.1 Hz, 2H), 3.82 (s, 3H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.03, 161.71, 157.56, 156.78, 153.34, 139.82, 136.23, 131.00, 130.16, 128.51, 128.20, 127.67, 122.44, 122.18, 121.27, 114.62, 113.83, 112.16, 83.86, 81.35, 56.17, 50.11, 39.09, 35.25, 12.39. ESI-MS: calculated for $C_{25}H_{23}ClN_3O_2S_3^+$ 528.06; found 527.85.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-((trifluoromethyl)thio)benzyl)thiazol-3-ium chloride (compound 30). Anal. RP-HPLC: t_R 2.17 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (t, *J* = 2.4 Hz, 1H), 8.08 (d, *J* = 4.4 Hz, 1H), 7.93 (d, *J* = 3.6 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.66 (td, *J* = 7.6, 1.6 Hz, 1H), 7.61 - 7.55 (m, 2H), 7.15 (d, *J* = 6.8 Hz, 1H), 6.34 (s, 1H), 5.97 (s, 2H), 4.13 (s, 3H), 3.99 (q, *J* = 7.2 Hz, 2H), 0.92 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.00, 162.24, 157.33, 154.07, 139.93, 139.53, 139.43, 135.56, 133.32, 130.52, 129.29, 128.63, 128.28, 127.78, 122.66, 122.59, 115.47, 114.05, 83.90, 81.46, 52.63, 39.04, 35.37, 12.09. ESI-MS: calculated for $C_{25}H_{20}ClF_3N_3OS_4^+$ 598.01; found 597.97.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(trifluoromethoxy)benzyl)thiazol-3-ium chloride (compound 31). Anal. RP-HPLC: t_R 2.13 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.12 (d, *J* = 4.0 Hz, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.90 (d, *J* = 4.0 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.62 - 7.52 (m, 2H), 7.53 -

7.43 (m, 2H), 7.41 - 7.35 (dd, *J* = 7.6, 1.2 Hz,1H), 6.42 (s, 1H), 5.84 (s, 2H), 4.11 (s, 3H), 4.02 (q, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.01, 162.05, 157.29, 154.03, 146.90, 139.92, 135.64, 131.39, 130.60, 128.61, 128.50, 128.26, 127.76, 126.74, 122.57, 121.01, 120.52 (q, *J* = 257 Hz), 115.20, 114.02, 83.70, 81.43, 49.37, 39.08, 35.34, 12.20. ESI-MS: calculated for $C_{25}H_{20}ClF_3N_3O_2S_3^+$ 582.04; found 581.97.

3-benzyl-2-((*Z*)-((*E*)-3'-ethyl-3-methyl-4'-oxo-3',4,4',5-tetrahydro-2'*H*,3*H*-[2,5'-bithiazolylidene]-2'-ylidene)methyl)thiazol-3-ium chloride (compound 32). Anal. RP-HPLC: t_R 1.54 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.26 (dd, *J* = 4.0, 0.8 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 1H), 7.48 - 7.38 (m, 2H), 7.37 - 7.31 (m, 3H), 6.46 (s, 1H), 5.75 (s, 2H), 4.06 - 3.88 (m, 4H), 3.48 (s, 3H), 3.25 (t, *J* = 7.6 Hz, 2H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.27, 162.68, 161.80, 154.06, 135.61, 135.14, 129.55, 128.87, 127.94, 114.91, 83.66, 80.33, 58.98, 53.41, 38.79, 37.47, 27.80, 12.22. ESI-MS: calculated for $C_{20}H_{22}N_3OS_3^+$ 416.09; found 416.02.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(2,6-dichlorobenzyl)thiazol-3-ium chloride (compound 33). Anal. RP-HPLC: t_R 2.12 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.11 (d, *J* = 2.4 Hz, 1H), 7.78 (dd, *J* = 4.4, 0.8 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 1.2 Hz, 1H), 7.67 (s, 1H), 7.63 (d, *J* = 4.0 Hz, 1H), 7.60 - 7.55 (m, 2H), 6.65 (s, 1H), 5.84 (s, 2H), 4.12 (s, 3H), 4.11 (q, *J* = 7.2 Hz, 2H), 1.18 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.12, 162.18, 157.34, 154.41, 139.95, 136.21, 133.90, 132.95, 130.14, 129.24, 128.64, 128.30, 127.79, 122.60, 115.27, 114.06, 83.58, 81.58, 50.27, 35.38, 12.76. ESI-MS: calculated for $C_{24}H_{19}Cl_3N_3OS_3^+$ 567.97; found 569.79.

3-((2-bromopyridin-3-yl)methyl)-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 34). Anal. RP-HPLC: t_R 1.85 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.42 (d, *J* = 4.4 Hz, 1H),

8.10 (s, 1H), 8.07 (d, *J* = 4.0 Hz, 1H), 7.91 (d, *J* = 3.6 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.58 (d, *J* = 9.2 Hz, 1H), 7.53 - 7.47 (m, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 6.44 (s, 1H), 5.77 (s, 2H), 4.13 (s, 3H), 4.07 (q, *J* = 7.6 Hz, 2H), 1.00 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.01, 162.43, 157.33, 154.37, 150.58, 142.26, 139.91, 138.19, 135.26, 131.42, 128.63, 128.26, 127.78, 124.53, 122.56, 115.45, 114.03, 83.73, 81.50, 52.92, 39.14, 35.38, 12.40. ESI-MS: calculated for $C_{23}H_{19}BrClN_4OS_3^+$ 578.96; found 578.91.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((2-chloropyridin-4-yl)methyl)thiazol-3-ium chloride (compound 35). Anal. RP-HPLC: t_R 1.87 min, purity 96.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.44 (d, *J* = 5.2 Hz, 1H), 8.23 (d, *J* = 4.0 Hz, 1H), 8.10 (d, *J* = 2.0 Hz, 1H), 7.92 (d, *J* = 4.0 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.65 - 7.53 (m, 2H), 7.23 (d, *J* = 5.2 Hz, 1H), 6.44 (s, 1H), 5.85 (s, 2H), 4.11 (s, 3H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.03, 162.20, 157.34, 154.34, 151.33, 151.16, 148.15, 139.93, 135.54, 128.63, 128.28, 127.79, 123.25, 122.59, 121.80, 115.48, 114.05, 83.80, 81.56, 51.71, 39.02, 35.36, 12.10. ESI-MS: calculated for $C_{23}H_{19}Cl_2N_4OS_3^+$ 533.01; found 532.80.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((5-(trifluoromethyl)furan-2-yl)methyl)thiazol-3-ium chloride (compound 36). Anal. RP-HPLC: t_R 2.10 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.21 (d, *J* = 4.0 Hz, 1H), 8.05 (d, *J* = 2.0 Hz, 1H), 7.88 (dd, *J* = 4.0, 0.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.53 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.31 - 7.27 (m, 1H), 6.94 (d, *J* = 4.0 Hz, 1H), 6.78 (s, 1H), 5.98 (s, 2H), 4.21 (q, *J* = 7.2 Hz, 2H), 4.10 (s, 3H), 1.19 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.10, 162.20, 157.31, 154.44, 151.85, 140.96 (q, *J* = 42.5 Hz) 139.92, 135.00, 128.62, 128.28, 127.77,

122.57, 119.23 (q, J = 266.25 Hz), 115.46, 114.78, 114.03, 112.31, 83.62, 81.60, 46.18, 39.19, 35.36, 12.45. ESI-MS: calculated for $C_{23}H_{18}ClF_3N_3O_2S_3^+$ 556.02; found 555.93.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((5-(methoxycarbonyl)furan-2-yl)methyl)thiazol-3-ium chloride (compound 37). Anal. RP-HPLC: t_R 1.92 min, purity 95.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.20 (d, J = 4.0 Hz, 1H), 8.05 (d, J = 2.0 Hz, 1H), 7.87 (d, J = 3.6 Hz, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.54 (dd, J = 8.8, 2.0 Hz, 1H), 7.34 (d, J = 3.6 Hz, 1H), 6.92 (d, J = 3.6 Hz, 1H), 6.77 (s, 1H), 5.95 (s, 2H), 4.20 (q, J = 7.2 Hz, 2H), 4.09 (s, 3H), 3.78 (s, 3H), 1.20 (t, J = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.09, 162.11, 158.42, 157.19, 154.30, 152.44, 144.80, 139.89, 135.10, 128.61, 128.25, 127.76, 122.53, 119.67, 115.39, 113.98, 113.34, 83.73, 81.56, 52.47, 46.56, 39.25, 35.34, 12.56. ESI-MS: calculated for $C_{24}H_{21}ClN_3O_4S_3^+$ 546.04; found 545.83.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((3-(methoxycarbonyl)furan-2-yl)methyl)thiazol-3-ium chloride (compound 38). Anal. RP-HPLC: t_R 1.98 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.17 (d, J = 4.4 Hz, 1H), 8.08 (d, J = 2.0 Hz, 1H), 7.90 - 7.85 (m, 2H), 7.70 (d, J = 8.8 Hz, 1H), 7.56 (dd, J = 8.8, 1.6 Hz, 1H), 6.86 (d, J = 2.0 Hz, 1H), 6.66 (s, 1H), 6.04 (s, 2H), 4.11 (s, 3H), 4.05 (q, J = 7.2 Hz, 2H), 3.89 (s, 3H), 1.15 (t, J = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.03, 163.70, 162.21, 157.37, 154.43, 152.74, 145.35, 139.92, 135.52, 128.65, 128.26, 127.79, 122.58, 116.80, 115.08, 114.06, 111.13, 83.26, 81.55, 52.70, 45.94, 39.26, 35.38, 12.48. ESI-MS: calculated for $C_{24}H_{21}ClN_3O_4S_3^+$ 546.04; found 545.85.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-(thiophen-3-ylmethyl)thiazol-3-ium chloride (compound 39). Anal. RP-HPLC: t_R 2.01 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.23 (d, J = 4.0 Hz, 1H), 8.10 (d, J =

2.0 Hz, 1H), 7.89 (d, *J* = 3.6 Hz, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.66 - 7.64 (m, 1H), 7.63 - 7.60 (dd, *J* = 5.2, 2.8 Hz, 1H), 7.58 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.09 (dd, *J* = 5.2, 1.2 Hz, 1H), 6.63 (s, 1H), 5.73 (s, 2H), 4.13 (d, *J* = 7.2 Hz, 2H), 4.11 (s, 3H), 1.08 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.17, 161.66, 157.10, 153.78, 139.97, 135.44, 135.35, 128.51, 128.28, 127.75, 127.30, 125.27, 122.55, 115.42, 113.98, 83.86, 81.46, 49.31, 39.09, 35.32, 12.44. ESI-MS: calculated for $C_{22}H_{19}ClN_3OS_4^+$ 504.01; found 503.80.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((2-(methoxycarbonyl)thiophen-3-yl)methyl)thiazol-3-ium chloride (compound 40). Anal. RP-HPLC: t_R 2.01 min, purity 95.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.20 (d, *J* = 4.4 Hz, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.95 (d, *J* = 5.2 Hz, 1H), 7.90 (d, *J* = 4.0 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.57 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.87 (d, *J* = 5.2 Hz, 1H), 6.49 (s, 1H), 6.01 (s, 2H), 4.11 (s, 3H), 4.00 (q, *J* = 7.2 Hz, 2H), 3.91 (s, 3H), 1.01 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.05, 162.71, 162.08, 157.25, 154.07, 142.03, 139.94, 135.50, 134.26, 129.17, 128.61, 128.26, 128.12, 127.75, 122.56, 115.39, 114.00, 83.49, 81.46, 53.10, 48.70, 39.09, 35.34, 12.23. ESI-MS: calculated for $C_{24}H_{21}ClN_3O_3S_4^+$ 562.01; found 561.80.

3-((2-bromothiophen-3-yl)methyl)-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 41). Anal. RP-HPLC: t_R 2.06 min, purity 96.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.13 (d, *J* = 4.4 Hz, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.88 (d, *J* = 4.0 Hz, 1H), 7.74 - 7.67 (m, 2H), 7.56 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.92 (d, *J* = 5.6 Hz, 1H), 6.39 (s, 1H), 5.64 (s, 2H), 4.11 (s, 3H), 4.06 (q, *J* = 7.2 Hz, 2H), 1.10 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.99, 161.79, 157.14, 153.98, 139.88,

135.47, 134.26, 129.57, 128.61, 128.24, 128.16, 127.74, 122.53, 115.26, 113.98, 111.95, 83.54, 81.42, 49.02, 35.33, 12.51. ESI-MS: calculated for $C_{22}H_{18}BrN_3OS_4^+$ 583.92; found 583.93.

3-((5-bromothiophen-2-yl)methyl)-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 42, JG-231). Anal. RP-HPLC: t_R 2.14 min, purity 98.0 %. ^{1}H-NMR (400 MHz, DMSO-d_6): δ 8.24 (d, J = 4.0 Hz, 1H), 8.07 (d, J = 2.4 Hz, 1H), 7.88 (d, J = 4.0 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.55 (dd, J = 8.8, 4.0 Hz, 1H), 7.20 (s, 2H), 6.75 (s, 1H), 5.94 (s, 2H), 4.20 (q, J = 7.2 Hz, 2H), 4.11 (s, 3H), 1.18 (t, J = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.17, 161.71, 157.28, 154.36, 139.96, 138.65, 134.78, 130.95, 130.23, 128.62, 128.29, 127.78, 122.59, 115.62, 114.05, 113.24, 83.67, 81.61, 48.33, 39.26, 35.36, 12.74. ESI-MS: calculated for $C_{22}H_{18}BrClN_3OS_4^+$ 581.92; found 581.89.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((2,5-dimethylthiophen-3-yl)methyl)thiazol-3-ium chloride (compound 43). Anal. RP-HPLC: t_R 2.11 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 2.0 Hz, 1H), 8.06 (d, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 4.0 Hz, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.57 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.52 (s, 1H), 6.50 (s, 1H), 5.54 (s, 2H), 4.11 (s, 3H), 4.08 (q, *J* = 7.2 Hz, 2H), 2.41 (s, 3H), 2.31 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 164.16, 161.61, 157.14, 153.68, 139.98, 137.19, 135.38, 135.07, 130.07, 128.58, 128.28, 127.76, 125.99, 122.57, 115.32, 114.00, 83.76, 81.42, 48.28, 39.36, 35.33, 15.20, 13.18, 12.32. ESI-MS: calculated for $C_{24}H_{23}ClN_3OS_4^+$ 532.04; found 531.83.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((2-methylthiazol-4-yl)methyl)thiazol-3-ium chloride (compound 44). Anal. RP-HPLC: t_R 1.93 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.21 (d, *J* = 4.0 Hz, 1H), 8.07

(s, 1H), 7.85 (d, *J* = 3.6 Hz, 1H), 7.76 (s, 1H), 7.68 (d, *J* = 9.2 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 6.81 (s, 1H), 5.77 (s, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 4.10 (s, 3H), 2.61 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 167.59, 164.09, 161.78, 156.88, 153.51, 148.57, 139.87, 135.69, 128.52, 128.23, 127.70, 122.46, 119.64, 115.12, 113.87, 84.30, 81.45, 49.71, 39.14, 35.28, 19.22, 12.51. ESI-MS: calculated for $C_{22}H_{20}ClN_4OS_4^+$ 519.02; found 518.80.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((2-chlorothiazol-5-yl)methyl)thiazol-3-ium chloride (compound 45). Anal. RP-HPLC: t_R 1.97 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.24 (d, *J* = 4.0 Hz, 1H), 8.09 (d, *J* = 2.4 Hz, 1H), 7.94 (s, 1H), 7.87 (d, *J* = 4.0 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.57 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.76 (s, 1H), 6.03 (s, 2H), 4.22 (q, *J* = 7.2 Hz, 2H), 4.11 (s, 3H), 1.19 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.16, 161.85, 157.37, 154.65, 152.41, 142.78, 139.95, 134.55, 134.49, 128.64, 128.29, 127.79, 122.60, 115.65, 114.07, 83.47, 81.65, 45.94, 35.38, 12.82. ESI-MS: calculated for $C_{21}H_{17}Cl_2N_4OS_4^+$ 538.97; found 540.80.

3-((2-acetamidothiazol-4-yl)methyl)-2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 46). Anal. RP-HPLC: t_R 1.82 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 12.14 (s, 1H), 8.16 (d, *J* = 4.0 Hz, 1H), 8.07 (s, *J* = 2.0 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.59 - 7.51 (m, 1H), 7.42 (s, 1H), 6.64 (s, 1H), 5.74 (s, 2H), 4.11 (q, *J* = 7.2 Hz, 2H), 4.09 (s, 3H), 2.09 (s, 3H), 1.10 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 169.23, 164.14, 161.75, 159.58, 157.02, 153.62, 143.73, 139.94, 135.96, 128.56, 128.26, 127.74, 122.54, 114.96, 113.94, 112.72, 84.01, 81.45, 50.21, 39.14, 35.31, 22.85, 12.46. ESI-MS: calculated for $C_{23}H_{21}Cl_2N_5O_2S_4^+$ 562.03; found 561.96.

2-((*Z*)-((*E*)-5-(6-chloro-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-yli-

dene)methyl)-3-((3,5-dimethylisoxazol-4-yl)methyl)thiazol-3-ium chloride (compound 47). ^{1}H NMR (400 MHz, DMSO) δ 8.08 (d, *J* = 2.0 Hz, 1H), 7.94 (d, *J* = 4.0 Hz, 1H), 7.85 (d, *J* = 4.0 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.56 (dd, *J* = 8.8, 1.6 Hz, 1H), 6.61 (s, 1H), 5.57 (s, 2H), 4.13 (q, *J* = 7.2 Hz, 2H), 4.11 (s, 3H), 2.45 (s, 3H), 2.07 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 168.73, 164.10, 161.93, 159.34, 157.10, 154.03, 139.89, 134.67, 128.59, 128.24, 127.74, 122.51, 115.35, 113.97, 108.45, 83.73, 81.45, 43.64, 35.34, 12.56, 11.30, 10.41. ESI-MS: calculated for $C_{23}H_{22}ClN_4O_2S_3^+$ 517.06; found 516.83.

2-((*Z*)-((*E*)-5-(3,5-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene) methyl)-3-(2-(trifluoromethoxy)benzyl)thiazol-3-ium chloride (compound 48). Anal. RP-HPLC: t_R 1.83 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 4.0 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.59 - 7.52 (m, 2H), 7.52 - 7.42 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 6.39 (s, 1H), 5.82 (s, 2H), 4.13 (s, 3H), 4.02 (q, *J* = 7.2 Hz, 2H), 2.46 (s, 3H), 0.99 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.69, 161.76, 157.64, 154.00, 146.89, 140.90, 137.90, 135.49, 131.38, 130.63, 128.50, 126.77, 125.61, 123.19, 122.48, 121.02, 120.52 (q, *J* = 257.0 Hz) 114.80, 113.05, 83.32, 80.86, 49.27, 39.05, 35.07, 21.61, 12.23. ESI-MS: calculated for $C_{26}H_{23}F_3N_3O_2S_3^+$ 562.09; found 561.89.

2-((*Z*)-((*E*)-5-(3,6-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene) methyl)-3-(2-(trifluoromethoxy)benzyl)thiazol-3-ium chloride (compound 49). Anal. RP-HPLC: t_R 2.10 min, purity 98.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.10 (dd, *J* = 4.0, 0.8 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 1H), 7.74 (s, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.55 (td, *J* = 8.0, 1.2 Hz, 1H), 7.51 - 7.46 (m, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.34 (dd, *J* = 8.8, 1.2 Hz, 1H), 6.38 (s, 1H), 5.82 (s, 2H), 4.11 (s, 3H), 4.01 (q, *J* = 7.2 Hz, 2H), 2.38 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, DMSO) δ 163.69, 161.75, 157.13, 154.06, 146.89, 138.73, 135.48, 134.33, 131.37, 130.60, 128.72, 128.50, 126.77, 126.29, 122.70, 120.52 (q, *J* = 256.0 Hz), 121.02, 114.76, 112.50, 83.30, 80.68, 49.24, 39.05, 35.16, 21.04, 12.22. ESI-MS: calculated for $C_{26}H_{23}F_3N_3O_2S_3^+$ 562.09; found 561.88.

2-((*Z*)-((*E*)-3-ethyl-5-(5-methoxy-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(trifluoromethoxy)benzyl)thiazol-3-ium chloride (compound 50). Anal. RP-HPLC: t_R 2.06 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (dd, *J* = 4.4, 2.0 Hz, 1H), 7.86 (d, *J* = 4.0 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.58 - 7.52 (m, 1 Hz, 1H), 7.51 - 7.42 (m, 2H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 2.0 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 1H), 6.38 (s, 1H), 5.82 (s, 2H), 4.14 (s, 3H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.88 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.60, 161.75, 160.12, 158.49, 153.98, 146.88, 142.12, 135.48, 131.36, 130.56, 128.51, 126.79, 123.48, 121.03, 120.53 (q, *J* = 257.0 Hz), 117.59, 114.79, 112.20, 98.37, 83.29, 81.01, 56.48, 49.26, 39.04, 35.24, 12.22. ESI-MS: calculated for $C_{26}H_{23}F_3N_3O_3S_3^+$ 578.08; found 578.04.

2-((*Z*)-((*E*)-3-ethyl-5-(6-methoxy-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(trifluoromethoxy)benzyl)thiazol-3-ium chloride (compound 51). Anal. RP-HPLC: t_R 2.03 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.10 (d, *J* = 4.4 Hz, 1H), 7.86 (d, *J* = 4.4 Hz, 1H), 7.63 (d, *J* = 9.2 Hz, 1H), 7.59 (d, *J* = 2.8 Hz, 1H), 7.58 - 7.52 (m, 1H), 7.52 - 7.42 (m, 2H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.10 (dd, *J* = 9.2, 3.0 Hz, 1H), 6.36 (s, 1H), 5.82 (s, 2H), 4.10 (s, 3H), 4.01 (q, *J* = 7.2 Hz, 2H), 3.80 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.61, 161.64, 156.98, 156.95, 154.07, 146.89, 135.44, 134.67, 131.35, 130.56, 128.50, 127.73, 126.79, 121.03, 120.53 (q, *J* = 257.0 Hz), 115.20, 114.60, 113.65, 107.04, 83.20,

80.36, 56.30, 49.21, 39.03, 35.32, 12.23. ESI-MS: calculated for $C_{26}H_{23}F_3N_3O_3S_3^+$ 578.08; found 578.16.

2-((*Z*)-((*E*)-3-ethyl-5-(6-isopropyl-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(trifluoromethoxy)benzyl)thiazol-3-ium chloride (compound 52). Anal. RP-HPLC: t_R 2.28 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.11 (d, *J* = 4.0 Hz, 1H), 7.88 (dd, *J* = 4.4, 0.8 Hz, 1H), 7.85 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.59 - 7.52 (m, 1H), 7.52 - 7.41 (m, 3H), 7.40 - 7.36 (m, 1H), 6.40 (s, 1H), 5.83 (s, 2H), 4.13 (s, 3H), 4.03 (q, *J* = 7.2 Hz, 2H), 3.06 - 2.94 (m, 1H), 1.24 (d, *J* = 7.2 Hz, 6H), 0.99 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.79, 161.82, 157.46, 154.14, 146.90, 145.52, 139.05, 135.52, 131.37, 130.56, 128.52, 126.80, 126.41, 121.04, 120.53 (q, *J* = 257.5, 1.4 Hz), 120.34, 114.78, 112.73, 83.35, 80.71, 49.29, 39.06, 35.23, 33.68, 24.46, 12.25. ESI-MS: calculated for $C_{28}H_{27}F_3N_3O_2S_3^+$ 590.12; found 590.11.

3-(2-chlorobenzyl)-2-((*Z*)-((*E*)-3-ethyl-5-(6-methoxy-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 53). Anal. RP-HPLC: t_R 1.94 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.05 (dd , *J* = 4.4, 0.8 Hz, 1H), 7.85 (d, *J* = 4.0 Hz, 1H), 7.68 - 7.56 (m, 3H), 7.49 - 7.37 (m, 2H), 7.19 - 7.08 (m, 2H), 6.38 (s, 1H), 5.79 (s, 2H), 4.11 (s, 3H), 4.03 (q, *J* = 7.2 Hz, 2H), 3.80 (s, 3H), 0.99 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ ^{13}C NMR (100 MHz, DMSO) δ 163.58, 161.72, 156.97, 154.03, 135.34, 134.63, 132.74, 132.11, 130.94, 130.57, 129.78, 128.57, 127.73, 115.20, 114.71, 113.60, 107.07, 83.28, 80.40, 56.29, 51.67, 39.09, 35.30, 12.34. ESI-MS: calculated for $C_{25}H_{23}ClN_3O_2S_3^+$ 528.06; found 527.86.

3-(2-chlorobenzyl)-2-((*Z*)-((*E*)-3-ethyl-5-(3-methyl-6-(methylthio)benzo[*d*]thiazol-2(3*H*)-yli-

dene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 54). Anal. RP-HPLC: t_R 2.08 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.07 (d, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 2.0 Hz, 2H), 7.61 (td, *J* = 8.8, 1.2 Hz, 2H), 7.48 - 7.37 (m, 3H), 7.16 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.39 (s, 1H), 5.80 (s, 2H), 4.11 (s, 3H), 4.02 (q, *J* = 7.2 Hz, 2H), 2.52 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 163.78, 161.94, 156.77, 154.05, 138.55, 135.42, 134.72, 132.75, 132.08, 130.96, 130.57, 129.78, 128.57, 127.55, 126.10, 119.81, 114.95, 113.08, 83.53, 80.98, 51.78, 39.12, 35.24, 15.88, 12.33. ESI-MS: calculated for $C_{25}H_{23}ClN_3OS_4^+$ 544.04; found 543.91.

2-((*Z*)-((*E*)-3-ethyl-5-(6-methoxy-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-(2-methoxybenzyl)thiazol-3-ium chloride (compound 55). Anal. RP-HPLC: t_R 1.92 min, purity 99.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.07 (d, *J* = 4.0 Hz, 1H), 7.78 (dd, *J* = 4.0, 0.4 Hz, 1H), 7.61 (d, *J* = 9.2 Hz, 1H), 7.59 (d, *J* = 2.8 Hz, 1H), 7.43 - 7.36 (m, 1H), 7.32 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.14 - 7.08 (m, 2H), 7.00 (td, *J* = 7.6, 1.2 Hz, 1H), 6.51 (s, 1H), 5.61 (s, 2H), 4.10 (s, 3H), 4.06 (q, *J* = 7.2 Hz, 2H), 3.83 (s, 3H), 3.80 (s, 3H), 1.08 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.68, 161.37, 157.53, 156.87, 156.63, 153.49, 136.02, 134.63, 130.95, 130.07, 127.68, 122.22, 121.27, 115.08, 114.03, 113.50, 112.15, 106.99, 83.31, 80.28, 56.26, 56.17, 49.92, 39.04, 35.24, 12.42. ESI-MS: calculated for $C_{26}H_{26}N_3O_3S_3^+$ 524.11; found 523.91.

2-((*Z*)-((*E*)-5-(3,6-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene) methyl)-3-(2-methoxybenzyl)thiazol-3-ium chloride (compound 56). Anal. RP-HPLC: t_R 2.06 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.07 (d, *J* = 4.0 Hz, 1H), 7.79 (d, *J* = 4.4 Hz, 1H), 7.74 (s, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.42 - 7.30 (m, 3H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.00 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.53 (s, 1H), 5.62 (s, 2H), 4.11 (s, 3H), 4.06 (q, *J* = 7.2, 2H), 3.83 (s,

3H), 2.39 (s, 3H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.75, 161.45, 157.55, 156.75, 153.46, 138.67, 136.06, 134.21, 130.98, 130.13, 128.64, 126.24, 122.60, 122.21, 121.27, 114.18, 112.35, 112.16, 83.42, 80.59, 56.17, 49.96, 39.06, 35.08, 21.01, 12.42. ESI-MS: calculated for $C_{26}H_{26}N_3O_2S_3^+$ 508.12; found 508.02.

2-((*Z*)-((*E*)-3-ethyl-5-(6-ethyl-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-(2-(methoxycarbonyl)benzyl)thiazol-3-ium chloride (compound 57). Anal. RP-HPLC: t_R 2.12 min, purity 97.0 %. ^{1}H-NMR (400 MHz, DMSO-d_6): δ 8.06 -7.99 (m, 2H), 7.87 (d, J = 4.4 Hz, 1H), 7.80 (s, 1H), 7.62 (t, J = 8.0 Hz, 2H), 7.52 (t, J = 8.0 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.41 (s, 1H), 6.02 (s, 2H), 4.14 (s, 3H), 3.99 (q, J = 7.2 Hz, 2H), 3.90 (s, 3H), 2.70 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H), 0.87 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 167.19, 163.72, 161.84, 157.09, 153.85, 140.70, 138.89, 135.60, 135.45, 133.76, 131.50, 129.07, 129.05, 128.06, 127.66, 126.33, 121.59, 114.96, 112.59, 83.67, 80.68, 53.05, 52.37, 38.92, 35.17, 28.19, 16.16, 12.06. ESI-MS: calculated for $C_{28}H_{28}N_3O_3S_3^+$ 550.13; found 550.05.

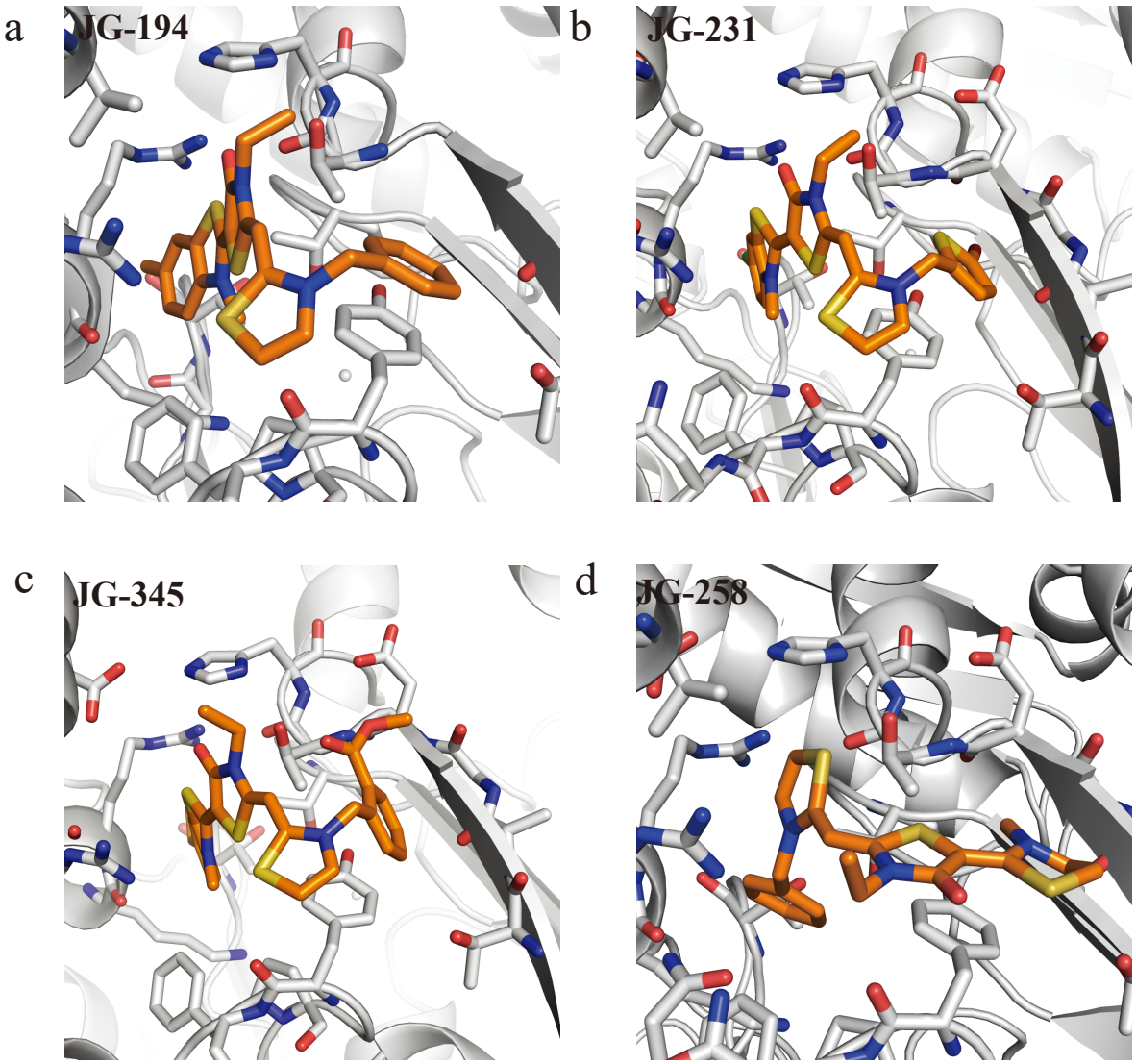
3-(2,6-dichlorobenzyl)-2-((*Z*)-((*E*)-5-(3,5-dimethylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 58). Anal. RP-HPLC: t_R 2.07 min, purity 97.0 %. ^{1}H NMR (400 MHz, DMSO) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 4.0 Hz, 1H), 7.70 - 7.65 (m, 2H), 7.62 - 7.54 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 1H), 6.62 (s, 1H), 5.82 (s, 2H), 4.14 (s, 3H), 4.11 (q, *J* = 7.2, 2H), 2.46 (s, 3H), 1.18 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO) δ 163.76, 161.84, 157.63, 154.32, 140.90, 137.93, 136.17, 133.80, 132.91, 130.14, 129.25, 125.63, 123.22, 122.50, 114.90, 113.04, 83.17, 81.00, 50.18, 35.10, 21.65, 12.78. ESI-MS: calculated for $C_{25}H_{22}Cl_2N_3OS_3^+$ 546.03; found 545.82.

3-(2,6-dichlorobenzyl)-2-((*Z*)-((*E*)-3-ethyl-5-(6-ethyl-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)thiazol-3-ium chloride (compound 59). Anal. RP-HPLC: t_R 2.22 min, purity 96.0 %. ^{1}H NMR (400 MHz, DMSO) δ 7.82 (d, *J* = 1.2 Hz, 1H), 7.75 (d, *J* = 4.0 Hz, 1H), 7.71 - 7.67 (m, 2H), 7.66 - 7.55 (m, 3H), 7.41 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.64 (s, 1H), 5.83 (s, 2H), 4.16 (s, 3H), 4.13 (q, *J* = 7.2 Hz, 2H), 2.71 (q, *J* = 7.2 Hz, 2H), 1.26 - 1.17 (m, 6H). ^{13}C NMR (100 MHz, DMSO) δ 163.82, 161.89, 157.29, 154.43, 140.79, 138.93, 136.18, 133.80, 132.91, 130.13, 129.26, 127.72, 126.37, 121.66, 114.85, 112.66, 83.18, 80.83, 50.19, 35.23, 28.22, 16.19, 12.78. ESI-MS: calculated for $C_{26}H_{24}Cl_2N_3OS_3^+$ 560.05; found 559.97.

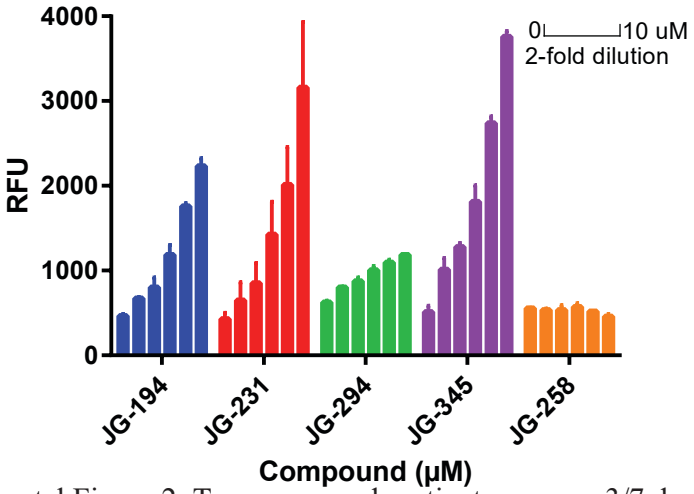
2-((*Z*)-((*E*)-5-(6-bromo-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-3-ethyl-4-oxothiazolidin-2-ylidene)methyl)-3-((5-(trifluoromethyl)furan-2-yl)methyl)thiazol-3-ium chloride (compound 60). Anal. RP-HPLC: t_R 2.14 min, purity 98.0 %. ^{1}H-NMR (400 MHz, DMSO-d_6): δ 8.21 (d, *J* = 2.0 Hz, 1H), 8.20 (d, *J* = 4.0 Hz, 1H), 7.88 (d, *J* = 4.0 Hz, 1H), 7.69 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.29 (d, *J* = 3.2 Hz, 1H), 6.93 (d, *J* = 3.2 Hz, 1H), 6.79 (s, 1H), 5.95 (s, 2H), 4.21 (q, *J* = 7.2 Hz, 2H), 4.11 (s, 3H), 1.19 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 164.11, 162.21, 154.43, 151.86, 140.97 (q, *J* = 41.25 Hz), 140.29, 135.01, 130.50, 128.65, 125.33, 119.23 (q, *J* = 266.25 Hz), 116.35, 115.47, 114.81, 114.38, 112.33, 83.64, 81.62, 46.19, 39.19, 35.30, 12.44. ESI-MS: calculated for $C_{23}H_{18}BrF_3N_3O_2S_3^+$ 599.97; found 599.99.

2-((*Z*)-((*E*)-3-ethyl-5-(6-ethyl-3-methylbenzo[*d*]thiazol-2(3*H*)-ylidene)-4-oxothiazolidin-2-ylidene)methyl)-3-((5-(trifluoromethyl)furan-2-yl)methyl)thiazol-3-ium chloride (compound 61). Anal. RP-HPLC: t_R 2.20 min, purity 95.0 %. ^{1}H NMR (400 MHz, DMSO) δ 8.14 (dd, *J* = 4.0, 1.6 Hz, 1H), 7.83 (d, *J* = 4.0 Hz, 1H), 7.81 (s, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.30 - 7.26 (m, 1H), 6.90 (s, 1H), 6.75 (s, 1H), 5.91 (s, 2H), 4.20 (q, *J* = 7.2 Hz, 2H), 4.14 (s, 3H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H), 1.19 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125

MHz, DMSO) δ 163.85, 161.96, 157.39, 154.57, 151.89, 140.94 (q, J = 42.5 Hz) 140.81, 138.98, 134.85, 127.74, 126.38, 121.71, 119.26 (q, J = 258.75 Hz), 115.01, 114.78, 112.70, 112.24, 83.23, 80.87, 46.11, 39.16, 35.23, 28.24, 16.24, 12.49.

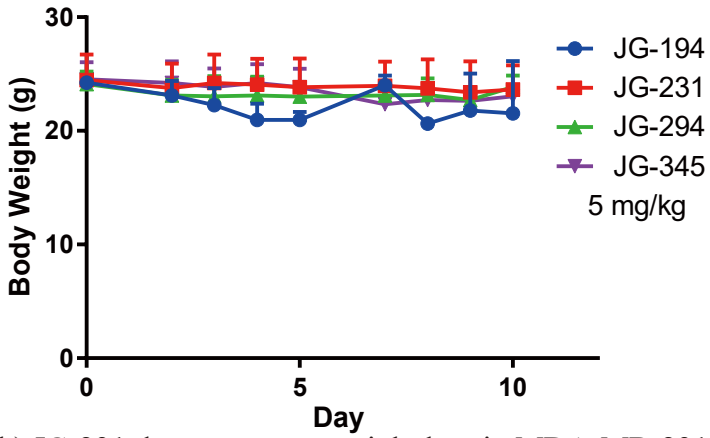


Supplemental Figure 1: the docked pose of top and negative control compounds. JG-194, JG-231 and JG-345 bind to Hsp70 similarly with JG-98, whereas JG-258 adopts a poor pose. (a) JG-194; (b) JG-294; (c) JG-345; (d) JG-258. The carbon atoms of the protein and inhibitor are shown in gray and orange respectively.

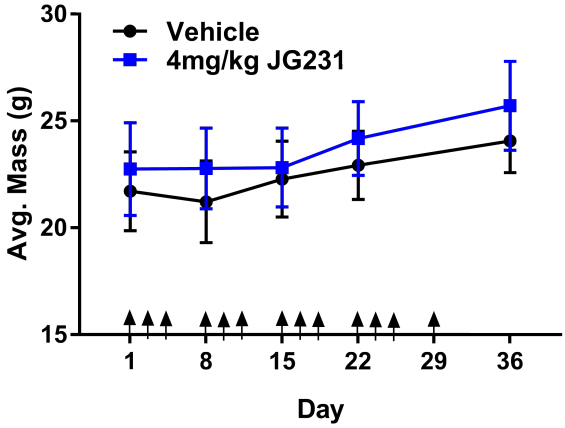


Supplemental Figure 2: Top compounds activate caspase 3/7 dose dependently. MCF-7 cells were treated with compound at indicated concentration for 24 h. Caspase-Glo reagent was added and luminescence was measured after 30 mins.

(a) Top compounds are well tolerated in NSG mice



(b) JG-231 does not cause weight loss in MDA-MB-231 xenografted mice



Supplemental Figure 3: Top compounds do not cause weight loss. (a) NSG mice were dosed with compounds at 5 mg/kg 4 times a week for 2 weeks. No signs of toxicity or discomfort were observed. (b) MDA-MB-231 xenografted mice were treated with JG-231 for 4 weeks. Arrows indicate treatments. No significant weight loss was observed.

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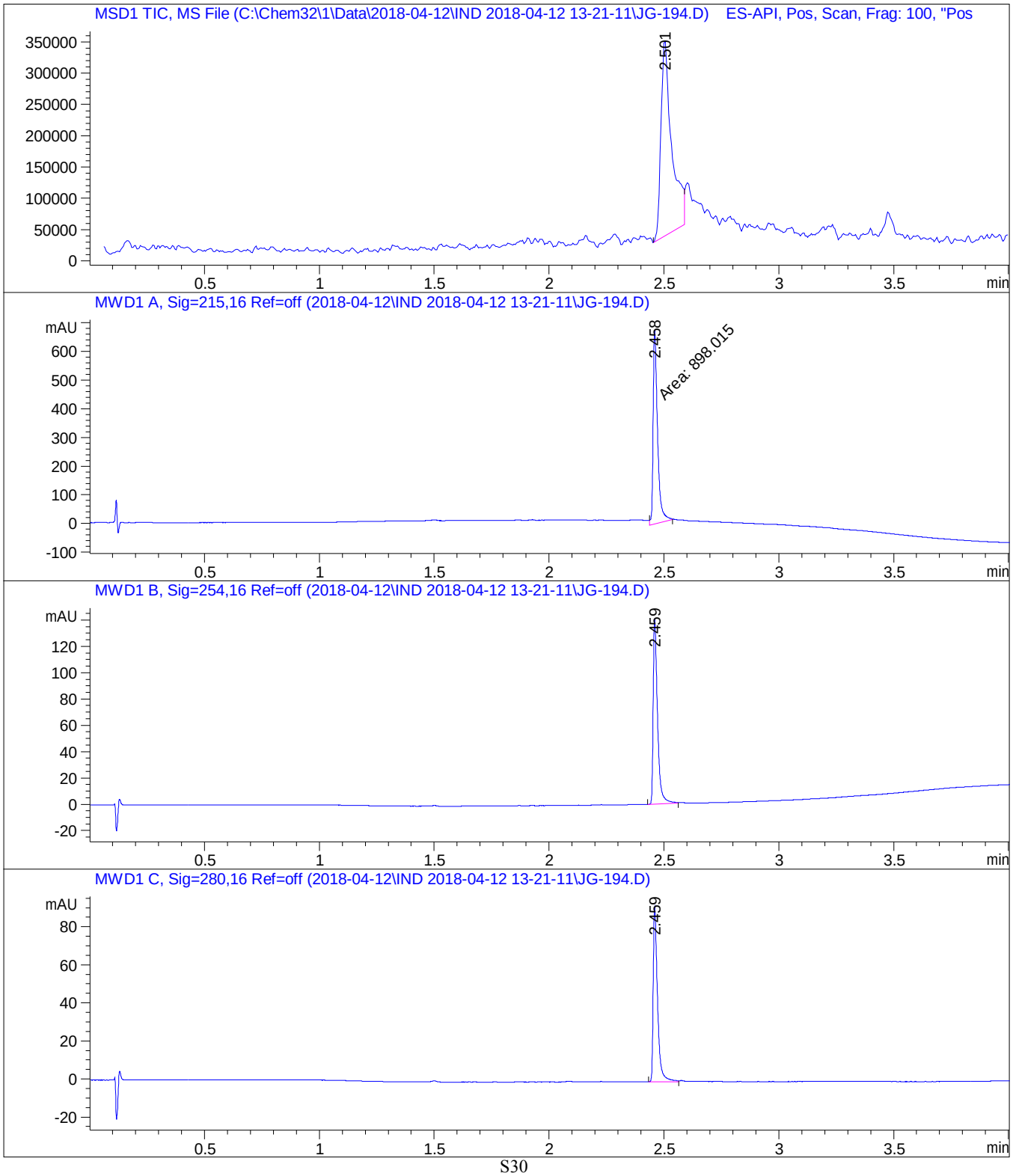

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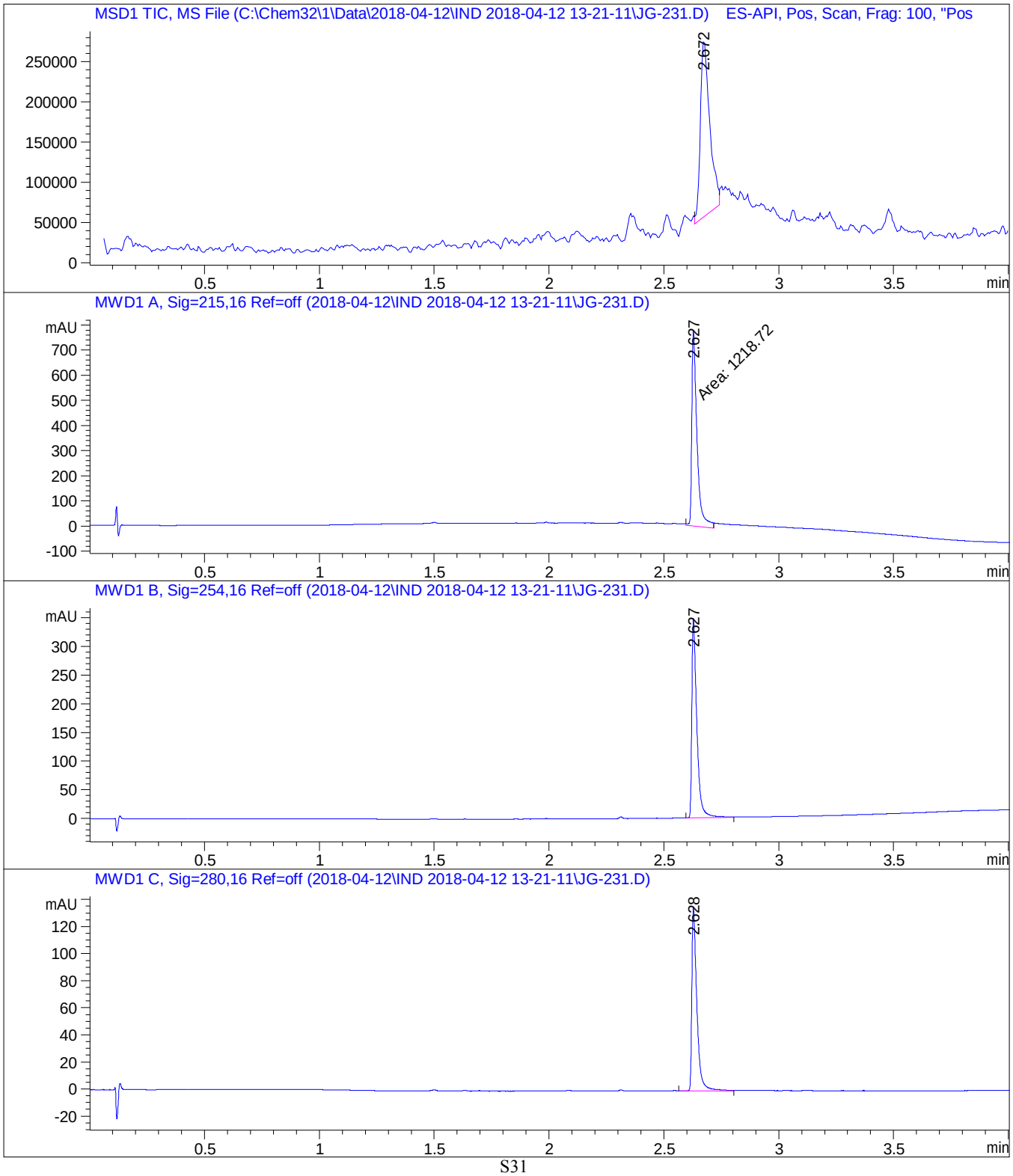

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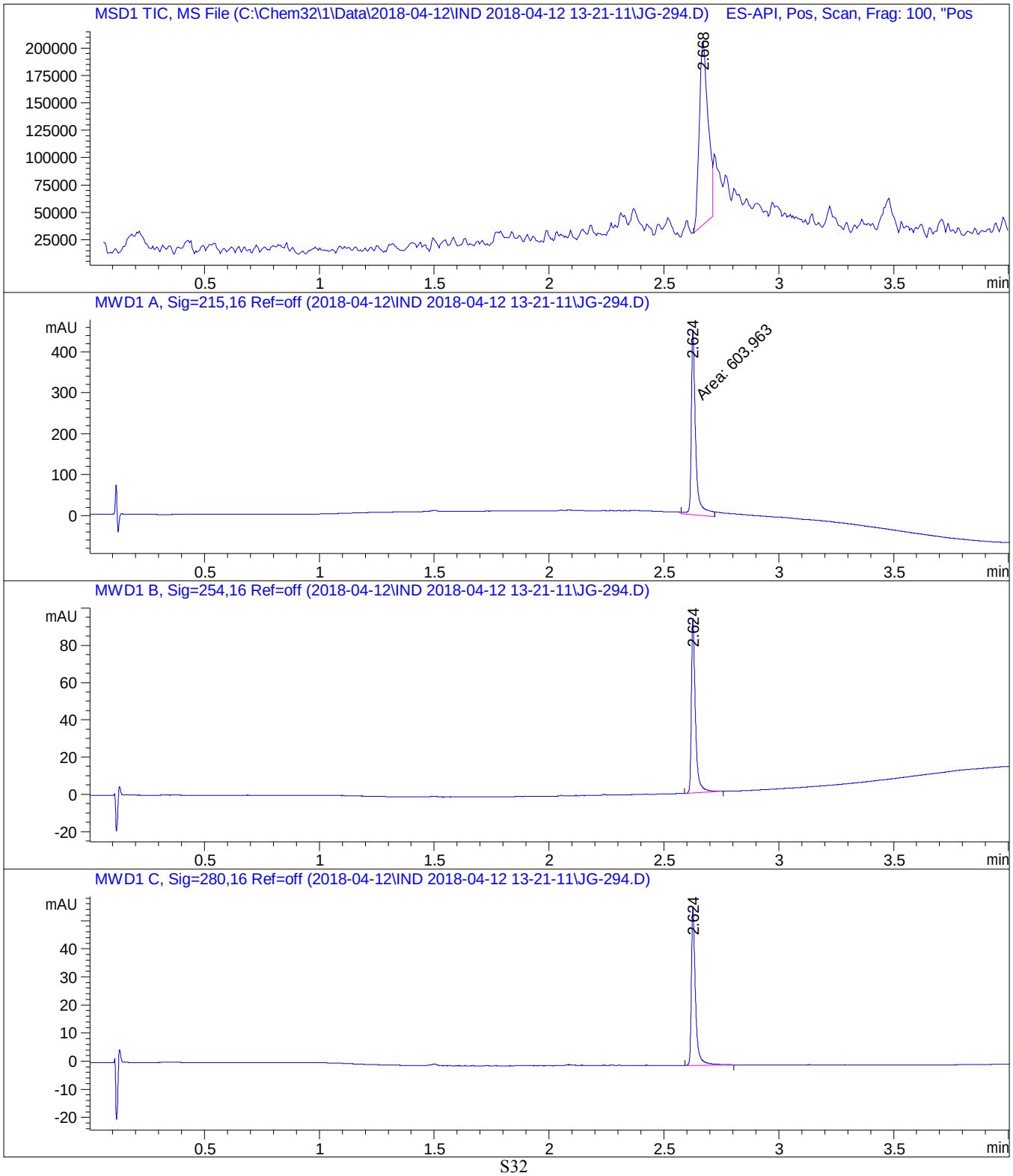
Additional Info : Peak(s) manually integrated

Current Chromatogram(s)



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Sample Name : JG-345

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Method Info : LCMS registration method for Open Access: HALO

Additional Info : Peak(s) manually integrated

Current Chromatogram(s)