Supporting Information

Oxidative C–S Bond Cleavage Reaction of DMSO for C–N and C–C Bond Formation: New Mannich-type Reaction for β-amino Ketones

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Table of Contents

I. General remarks ..................................................................................................................................................1

II. Optimization study for ruthenium catalyzed mannich reaction.................................................................1

III. The KIE for reactions between 1d and saccharin......................................................................................2

IV. General procedure for the preparation of 2 and 4.....................................................................................3

V. Analytical data of products obtained in this study..................................................................................3-11

VI. $^1$H NMR and $^{13}$C NMR spectra copies of compounds 2, 4, C and H...........................................12-44
I. General Remarks:
Unless otherwise stated, all commercial reagents and solvents were used without additional purification. All the reactions were carried out under air atmosphere. $^1$H NMR spectra were recorded at 25 ºC on a Bruker Ascend™ 400 spectrometer (Germany), $^{13}$C NMR spectra were recorded at 25 ºC on a Bruker 100 MHz, and TMS as internal standard. Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. HRMS data were obtained on a Waters LCT Premierxe™ (USA). All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

II. Optimization Study for Ruthenium catalyzed manich reaction

Table 1: Screening of Reaction Conditions $^{[a, b]}$

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<th>Entry</th>
<th>Catalyst</th>
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<th>Oxidant</th>
<th>Additive</th>
<th>Yield</th>
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$^{[a]}$ Reaction conditions: 1a (0.5 mmol), saccharin (1.0 mmol), RuCl$_3$ (5 mol%), 1,10-phen (0.025 mmol), selectflour (1.0 mmol), Na$_2$CO$_3$ (1.0 mmol) and DMSO (2 mL) at 120 ºC for 3 h. $^{[b]}$ Yield of the isolated products. $^{[c]}$ 1,10-phen = 1,10-phenanthroline. $^{[d]}$ 2,2-bipyl = 2,2-bipyridine.
III. The KIE for reactions between 1d and saccharin.

To a solution of 1-(p-toly)ethanone (1d) (67.0 mg, 0.5 mmol) in DMSO (1.0 mL) and DMSO-d$_6$ (1.0 mL) was added RuCl$_3$ (4.3 mg, 0.025 mmol), 1,10-phen (4.95 mg, 0.025 mmol), selectflour (354 mg, 1.0 mmol), Na$_2$CO$_3$ (108 mg, 1.0 mmol) and saccharin (183.2 mg, 1.0 mmol). The mixture was stirred at 120 °C for 0.5 h (monitored by TLC), quenched with water, extracted with dichloromethane (5 × 3 mL), and dried over anhydrous Na$_2$SO$_4$. The solvent was removed under reduced pressure, and the residue was purified by flash column chromatography. The KIE value was determined by average of two runs and representative $^1$HNMR spectrum was provided as follows:

To a solution of 1-(p-toly)ethanone (1d) (67.0 mg, 0.5 mmol) in DMSO (1.0 mL) and DMSO-d$_6$ (1.0 mL) was added RuCl$_3$ (4.3 mg, 0.025 mmol), 1,10-phen (4.95 mg, 0.025 mmol), selectflour (354 mg, 1.0 mmol), Na$_2$CO$_3$ (108 mg, 1.0 mmol) and saccharin (183.2 mg, 1.0 mmol). The mixture was stirred at 120 °C for 3.0 h (monitored by TLC), quenched with water, extracted with dichloromethane (5 × 3 mL), and dried over anhydrous Na$_2$SO$_4$. The solvent was removed under reduced pressure, and the residue was purified by flash column chromatography. The KIE value was determined by average of two runs and representative $^1$HNMR spectrum was provided as follows:
IV. General procedure for the preparation of 2 and 4 (2a as an example).

To a solution of acetophenone (1a) (60.1 mg, 0.5 mmol) in DMSO (2.0 mL) was added RuCl$_3$ (4.3 mg, 0.025 mmol), 1,10-phen (4.95 mg, 0.025 mmol), selectflour (354 mg, 1.0 mmol) and Na$_2$CO$_3$ (108 mg, 1.0 mmol). The mixture was stirred at 120 °C for 3.0 h (monitored by TLC), quenched with water, extracted with dichloromethane (5 × 3 mL), and dried over anhydrous Na$_2$SO$_4$. The solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (EtOAc/petro ether=1:6) to give compound 2a as a white solid (143.3 mg, 91%).

V. Analytical data of products obtained in this study

2-(3-oxo-3-phenylpropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2a

White solid. Mp: 138-140 °C; $^1$H NMR (400 MHz; CDCl$_3$): δ = 3.59 (t, $J$ = 7.6 Hz, 2H), 4.28 (t, $J$ = 7.6 Hz, 2H), 7.48 (t, $J$ = 7.6 Hz, 2H), 7.58 (d, $J$ = 7.2 Hz, 1H), 7.86 (d, $J$ = 8.6 Hz, 2H), 7.89-7.95 (m, 3H), 7.98 (dd, $J_1$ = 2.8 Hz, $J_2$ = 6.8 Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): δ = 34.5, 36.8, 121.0, 125.2, 127.4, 128.1, 128.7, 133.5, 134.4, 134.8, 136.2, 137.8, 158.8, 196.8. HRMS
(ESI-TOF) Calcd for C_{10}H_{18}NO_4S [M+H]^+ 316.0644; Found 316.0641.

2-(3-oxo-3-(o-tolyl)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2b
White solid. Mp: 134-135 °C; ^1H NMR (400 MHz; CDCl_3): δ = 2.56 (s, 3H), 3.52 (t, J = 7.6 Hz, 2H), 4.25 (t, J = 7.6 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 8.6 Hz, 1H), 7.88 (dd, J = 2.4 Hz, J = 7.6 Hz, 2H), 7.94 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 7.2 Hz, 1H). ^13C NMR (100 MHz; CDCl_3): δ = 21.5, 34.6, 39.2, 121.0, 125.2, 125.8, 127.4, 128.9, 131.9, 132.2, 134.4, 134.8, 137.8, 138.9, 158.8, 200.0. HRMS (ESI-TOF) Calcd for C_{17}H_{16}NO_4S [M+H]^+ 330.0794; Found 330.0797.

2-(3-oxo-3-(m-tolyl)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2c
White solid. Mp: 106-107 °C; ^1H NMR (400 MHz; CDCl_3): δ = 2.41 (s, 3H), 3.56 (t, J = 7.6 Hz, 2H), 4.26 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 8.0 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.76 (d, J = 9.2 Hz, 2H), 7.85-7.90 (m, 2H), 7.91-8.09 (m, 2H). ^13C NMR (100 MHz; CDCl_3): δ = 21.3, 34.5, 36.9, 121.0, 125.2, 125.3, 127.4, 128.9, 134.3, 134.4, 134.8, 136.2, 137.7, 138.5, 158.8, 197.0. HRMS (ESI-TOF) Calcd for C_{17}H_{16}NO_4S [M+H]^+ 330.0794; Found 330.0784.

2-(3-oxo-3-(p-tolyl)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2d
White solid. Mp: 132-133 °C; ^1H NMR (400 MHz; CDCl_3): δ = 2.42 (s, 3H), 3.55 (dd, J = 1.2 Hz, J = 8.0 Hz, 2H), 4.25 (dd, J = 1.2 Hz, J = 7.6 Hz, 2H), 7.26 (d, J = 6.8 Hz, 2H), 7.85-7.91 (m, 4H), 8.08 (d, J = 8.0 Hz, 1H). ^13C NMR (100 MHz; CDCl_3): δ = 21.7, 34.6, 36.7, 121.0, 125.2, 127.4, 128.2, 129.4, 133.8, 134.4, 134.8, 137.8, 144.4, 158.8, 196.4. HRMS (ESI-TOF) Calcd for C_{17}H_{16}NO_4S [M+H]^+ 330.0794; Found 330.0793.

2-(3-(2-chlorophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2e
White solid. Mp: 132-134 °C; ^1H NMR (400 MHz; CDCl_3): δ = 3.58 (t, J = 7.5 Hz, 2H), 4.25 (t, J = 7.5 Hz, 2H), 7.33 (dd, J = 2.4 Hz, J = 6.4 Hz, 1H), 7.35-7.59 (m, 2H), 7.60 (d, J = 6.8 Hz, 1H), 7.85-8.08 (m, 3H), 8.09 (d, J = 6.0 Hz, 1H). ^13C NMR (100 MHz; CDCl_3): δ = 34.2, 41.0, 121.0, 132.8, 133.6, 134.8, 135.0, 138.0, 144.4, 158.8.
2-(3-(3-chlorophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2f
White solid. Mp: 105-106 °C; ^1H NMR (400 MHz; CDCl₃): δ = 3.56 (t, J = 8.0 Hz, 2H), 4.27 (t, J = 8.0 Hz, 2H), 7.29 (t, J = 8.0 Hz, 1H), 7.55-7.58 (m, 1H), 7.84-7.88 (m, 3H), 7.90-7.95 (m, 2H), 8.08 (s, 1H). ^13C NMR (100 MHz; CDCl₃): δ = 34.3, 36.9, 121.0, 125.2, 126.1, 127.3, 128.2, 130.1, 133.5, 134.4, 134.9, 135.1, 137.7, 158.8, 195.5. HRMS (ESI-TOF) Calcd for C₇H₇ClNO₄S [M+H]^+ 350.0251; Found 350.0247.

2-(3-(4-chlorophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2g
White solid. Mp: 153-154 °C; ^1H NMR (400 MHz; CDCl₃): δ = 3.54 (t, J = 8.0 Hz, 2H), 4.26 (t, J = 8.0 Hz, 2H), 7.46 (dd, J₁ = 2.0 Hz, J₂ = 6.8 Hz, 2H), 7.86-8.08 (m, 5H), 8.09 (d, J = 6.8 Hz, 1H). ^13C NMR (100 MHz; CDCl₃): δ = 34.3, 36.8, 120.9, 125.2, 127.3, 129.1, 129.5, 134.4, 134.5, 134.9, 137.7, 140.1, 195.6. HRMS (ESI-TOF) Calcd for C₁₀H₇ClNO₄S [M+H]^+ 350.0251; Found 350.0254.

2-(3-(2-nitrophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2h
White solid. Mp: 131-132 °C; ^1H NMR (400 MHz; CDCl₃): δ = 3.39 (t, J = 7.6 Hz, 2H), 4.32 (t, J = 7.6 Hz, 2H), 7.48 (dd, J₁ = 1.2 Hz, J₂ = 7.6 Hz, 1H), 7.61-7.65 (m, 1H), 7.75 (dd, J₁ = 1.2 Hz, J₂ = 7.6 Hz, 1H), 7.83-8.07 (m, 3H), 8.08 (d, J = 7.5 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H). ^13C NMR (100 MHz; CDCl₃): δ = 34.0, 40.9, 121.0, 124.5, 125.3, 127.3, 127.5, 130.9, 134.4, 134.5, 134.9, 137.0, 137.7, 158.7, 198.8. HRMS (ESI-TOF) Calcd for C₁₀H₈N₂O₆S [M+H]^+ 361.0486; Found 361.0483.

2-(3-(3-nitrophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2i
White solid. Mp: 89-91 °C; ^1H NMR (400 MHz; CDCl₃): δ = 3.64 (t, J = 6.8 Hz, 2H), 4.31 (t, J = 6.8 Hz, 2H), 7.10 (d, J = 8.0 Hz, 1H), 7.81-7.96 (m, 3H), 8.10 (d, J = 8.0 Hz, 1H), 8.30 (d, J = 7.6...
Hz, 1H), 8.46 (dd, J₁ = 2.0 Hz, J₂ = 8.0 Hz, 1H), 8.79 (s, 1H). ¹³C NMR (100 MHz; CDCl₃): δ = 34.0, 37.1, 121.0, 122.9, 125.3, 127.2, 127.8, 130.0, 133.5, 134.5, 134.9, 137.4, 148.5, 158.8, 194.7. HRMS (ESI-TOF) Calcd for C₁₆H₁₃N₂O₈S [M+H]^⁺ = 361.0486; Found 361.0481.

2-(3-(4-methoxyphenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2j
White solid. Mp: 127-128 °C; ¹H NMR (400 MHz; CDCl₃): δ = 3.52 (t, J = 7.6 Hz, 2H), 3.88 (s, 3H), 4.26 (t, J = 7.6 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H), 7.85-7.96 (m, 5H), 8.08 (d, J = 7.2 Hz, 1H). ¹³C NMR (100 MHz; CDCl₃): δ = 34.6, 36.4, 55.5, 113.8, 121.0, 125.2, 127.3, 129.3, 130.3, 134.4, 134.8, 137.7, 158.8, 163.8, 196.3. HRMS (ESI-TOF) Calcd for C₁₅H₁₃NO₈S [M+H]^⁺ = 346.0741; Found 346.0748.

2-(3-(4-cyclohexylphenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2k
White solid. Mp: 153-154 °C; ¹H NMR (400 MHz; CDCl₃): δ = 1.28-1.45 (m, 5H), 1.59-1.88 (m, 5H), 2.56 (q, J = 4.4 Hz, 1H), 3.55 (t, J = 7.6 Hz, 2H), 4.26 (t, J = 7.6 Hz, 2H), 7.30 (d, J = 8.4 Hz, 2H), 7.85-7.95 (m, 5H), 8.09 (d, J = 7.2 Hz, 1H). ¹³C NMR (100 MHz; CDCl₃): δ = 26.0, 26.7, 34.1, 34.6, 36.7, 44.7, 121.0, 125.2, 127.2, 127.4, 128.3, 134.1, 134.4, 134.8, 137.8, 154.2, 158.8, 196.4. HRMS (ESI-TOF) Calcd for C₂₃H₂₄NO₈S [M+H]^⁺ = 398.1418; Found 398.1413.

2-(3-[[1,1'-biphenyl]-4-yl]-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2l
White solid. Mp: 151-152 °C; ¹H NMR (400 MHz; CDCl₃): δ = 3.62 (t, J = 7.6 Hz, 2H), 4.30 (t, J = 7.6 Hz, 2H), 7.41-7.63 (m, 3H), 7.65 (d, J = 6.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.86-7.89 (m, 3H), 7.90-8.11 (m, 3H). ¹³C NMR (100 MHz; CDCl₃): δ = 34.5, 36.9, 121.0, 125.2, 127.3, 127.4, 128.3, 128.7, 129.0, 134.4, 134.8, 134.9, 137.7, 139.8, 146.2, 158.8, 196.4. HRMS (ESI-TOF) Calcd for C₂₂H₁₈NO₈S [M+H]^⁺ = 392.0968; Found 392.0966.

2-(3-(4-fluorophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2m
White solid. Mp: 150-151 °C; \(^1\)H NMR (400 MHz; CDCl\(_3\)): \(\delta = 3.55\) (t, \(J = 7.6\) Hz, 2H), 4.28 (t, \(J = 7.6\) Hz, 2H), 7.15 (dd, \(J_1 = 2.4\) Hz, \(J_2 = 8.4\) Hz, 2H), 7.86-7.93 (m, 3H), 7.94-8.02 (m, 2H), 8.07 (dd, \(J_1 = 1.6\) Hz, \(J_2 = 6.8\) Hz, 1H). \(^{13}\)C NMR (100 MHz; CDCl\(_3\)): \(\delta = 34.4, 36.7, 115.7, 116.0, 121.0, 125.2, 127.3, 130.7, 130.8, 132.7, 134.4, 134.9, 137.7, 158.8, 164.7, 167.3, 195.2. HRMS (ESI-TOF) Calcd for C\(_{16}\)H\(_7\)FNO\(_3\)S \([M+H]^+\) 334.0549; Found 334.0546.

![Chemical structure](image)

2-(3-(4-bromophenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2n

White solid. Mp: 179-180 °C; \(^1\)H NMR (400 MHz; CDCl\(_3\)): \(\delta = 3.59\) (t, \(J = 8.0\) Hz, 2H), 4.29 (t, \(J = 7.6\) Hz, 2H), 7.73 (d, \(J = 8.4\) Hz, 2H), 7.83-7.87 (m, 2H), 7.88-7.91 (m, 1H), 7.93-8.08 (m, 3H). \(^{13}\)C NMR (100 MHz; CDCl\(_3\)): \(\delta = 34.2, 37.1, 121.0, 121.1, 125.3, 125.4, 125.7, 125.8, 127.2, 128.4, 134.3, 134.5, 134.9, 135.2, 137.6, 138.8, 158.8, 195.9. HRMS (ESI-TOF) Calcd for C\(_{16}\)H\(_7\)BrNO\(_3\)S \([M+H]^+\) 393.9749; Found 393.9747.

![Chemical structure](image)

4-(3-(1,1-dioxido-3-oxobenzo[d]isothiazol-2(3H)-yl)propanoyl)benzonitrile 2o

White solid. Mp: 177-178 °C; \(^1\)H NMR (400 MHz; CDCl\(_3\)): \(\delta = 3.59\) (t, \(J = 7.2\) Hz, 2H), 4.28 (s, 2H), 7.79 (d, \(J = 8.4\) Hz, 2H), 7.89-7.94 (m, 3H), 8.05-8.11 (m, 3H). \(^{13}\)C NMR (100 MHz; CDCl\(_3\)): \(\delta = 34.1, 37.1, 116.9, 117.8, 121.0, 125.3, 127.2, 128.5, 129.9, 132.2, 134.5, 134.9, 137.7, 139.1, 158.8, 195.5. HRMS (ESI-TOF) Calcd for C\(_{17}\)H\(_2\)N\(_2\)O\(_3\)S \([M+H]^+\) 341.0591; Found 341.0596.

![Chemical structure](image)

2-(3-oxo-3-(4-(trifluoromethyl)phenyl)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2p

White solid. Mp: 123-124 °C; \(^1\)H NMR (400 MHz; CDCl\(_3\)): \(\delta = 3.59\) (t, \(J = 7.6\) Hz, 2H), 4.28 (t, \(J = 7.6\) Hz, 2H), 7.73 (d, \(J = 8.4\) Hz, 2H), 7.85 (dd, \(J_1 = 1.2\) Hz, \(J_2 = 7.6\) Hz, 2H), 7.87-7.91 (m, 1H), 7.93-8.08 (m, 3H). \(^{13}\)C NMR (100 MHz; CDCl\(_3\)): \(\delta = 34.2, 37.1, 121.0, 121.1, 125.3, 125.4, 125.7, 125.8, 127.2, 128.4, 134.3, 134.5, 134.9, 135.2, 137.6, 138.8, 158.8, 159.9. HRMS (ESI-TOF) Calcd for C\(_{17}\)H\(_3\)F\(_3\)NO\(_3\)S \([M+H]^+\) 384.0517; Found 384.0516.

![Chemical structure](image)

methyl 4-(3-(1,1-dioxido-3-oxobenzo[d]isothiazol-2(3H)-yl)propanoyl)benzoate 2q
White solid. Mp: 132-133 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 3.60$ (t, $J = 8.0$ Hz, 2H), 3.95 (s, 3H), 4.27 (t, $J = 8.0$ Hz, 2H), 7.85-8.91 (m, 3H), 7.94 (d, $J = 7.2$ Hz, 2H). 8.01 (d, $J = 8.4$ Hz, 1H), 8.07-8.13 (m, 2H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 34.3$, 37.2, 52.5, 121.1, 125.2, 127.3, 127.9, 129.9, 134.2, 134.3, 134.5, 137.7, 139.3, 158.8, 166.1, 196.4. HRMS (ESI-TOF) Calcd for C$_{18}$H$_{18}$NO$_6$S$_2$ [M+H]$^+$ 374.0696; Found 374.0693.

2-(3-(3,4-dimethylphenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2r

White solid. Mp: 126-128 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 2.31$ (s, 3H), 2.32 (s, 3H), 3.55 (dd, $J_I = 1.2$ Hz, $J_J = 8.0$ Hz, 2H), 4.25 (q, $J = 6.4$ Hz, 2H), 7.22 (d, $J = 8.0$ Hz, 1H), 7.69 (d, $J = 6.4$ Hz, 1H), 7.74 (s, 1H), 7.83-7.89 (m, 3H), 7.91 (d, $J = 6.4$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta =$ 19.7, 20.2, 34.6, 36.7, 120.9, 125.2, 125.8, 127.4, 129.2, 134.2, 134.3, 137.0, 137.8, 143.1, 158.8, 196.7. HRMS (ESI-TOF) Calcd for C$_{18}$H$_{18}$NO$_6$S$_2$ [M+H]$^+$ 344.0951; Found 344.0953.

2-(3-(3,5-bis(trifluoromethyl)phenyl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2s

White solid. Mp: 129-130 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 3.63$ (t, $J = 7.6$ Hz, 2H), 4.31 (t, $J = 7.6$ Hz, 2H), 7.87-7.97 (m, 3H), 8.10 (t, $J = 6.8$ Hz, 2H), 8.37 (s, 2H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta =$ 33.9, 37.1, 121.0, 121.4, 124.1, 125.3, 126.7, 127.2, 128.1, 132.1, 132.4, 132.7, 133.1, 134.5, 134.9, 137.6, 137.7, 158.8, 194.1. HRMS (ESI-TOF) Calcd for C$_{18}$H$_{12}$F$_6$NO$_6$S$_2$ [M+H]$^+$ 452.0383; Found 452.0382.

2-(3-oxo-3-(2,3,4-trichlorophenyl)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2t

White solid. Mp: 142-143 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 3.52$ (t, $J = 6.8$ Hz, 2H), 4.25 (t, $J = 6.8$ Hz, 2H), 7.39 (d, $J = 8.4$ Hz, 1H), 7.47 (d, $J = 8.4$ Hz, 1H), 7.86-8.08 (m, 3H), 8.09 (d, $J = 6.8$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta =$ 34.0, 41.0, 121.0, 125.3, 127.1, 127.2, 128.7, 131.3, 133.2, 134.5, 134.9, 137.1, 137.7, 138.6, 158.7, 198.0. HRMS (ESI-TOF) Calcd for C$_{16}$H$_{12}$Cl$_3$NO$_6$S$_2$[M+H]$^+$ 417.9486; Found 417.9491.
2-(3-(naphthalen-1-yl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2u
White solid. Mp: 146-148 °C; ¹H NMR (400 MHz; CDCl₃): δ = 3.68 (t, J = 7.6 Hz, 2H), 4.35 (t, J = 7.6 Hz, 2H), 7.48-7.63 (m, 6H), 7.83-8.03 (m, 4H), 8.07 (dd, J₁ = 1.6 Hz, J₂ = 7.2 Hz, 1H). ¹³C NMR (100 MHz; CDCl₃): δ = 34.7, 39.7, 121.0, 124.3, 125.2, 125.9, 126.6, 127.3, 128.3, 128.4, 128.5, 130.2, 133.5, 134.0, 134.8, 137.7, 158.8, 200.2. HRMS (ESI-TOF) Calcd for C₂₉H₁₈NO₅S, [M+H]⁺ 366.0876; Found 366.0873.

2-(3-(naphthalen-2-yl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2v
White solid. Mp: 138-138 °C; ¹H NMR (400 MHz; CDCl₃): δ = 3.73 (t, J = 7.6 Hz, 2H), 4.34 (t, J = 7.6 Hz, 2H), 7.57-7.60 (m, 2H), 7.62-8.06 (m, 8H), 8.10 (dd, J₁ = 1.2 Hz, J₂ = 7.2 Hz, 1H). ¹³C NMR (100 MHz; CDCl₃): δ = 34.6, 36.9, 121.0, 123.6, 125.2, 126.9, 127.4, 127.8, 128.6, 128.7, 129.6, 130.0, 132.5, 133.6, 134.4, 134.8, 135.8, 137.8, 158.8, 196.7. HRMS (ESI-TOF) Calcd for C₂₉H₁₆NO₅S, [M+H]⁺ 366.0876; Found 366.0874.

2-(3-(furan-2-yl)-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 2w
White solid. Mp: 103-105 °C; ¹H NMR (400 MHz; CDCl₃): δ = 3.44 (dd, J₁ = 1.2 Hz, J₂ = 8.0 Hz, 2H), 4.24 (dd, J₁ = 1.2 Hz, J₂ = 7.6 Hz, 2H), 6.55 (dd, J₁ = 1.2 Hz, J₂ = 7.6 Hz, 1H), 7.25 (dd, J₁ = 0.8 Hz, J₂ = 6.4 Hz, 1H), 7.60 (t, J = 1.6 Hz, 1H), 7.85-7.95 (m, 3H), 8.07-8.09 (m, 1H). ¹³C NMR (100 MHz; CDCl₃): δ = 34.0, 36.7, 112.4, 117.5, 121.0, 125.2, 127.3, 134.4, 134.8, 137.7, 146.7, 152.2, 158.7, 185.6. HRMS (ESI-TOF) Calcd for C₁₄H₁₂NO₃S, [M+H]⁺ 306.0438; Found 306.0436.

(R)-2-(2-methyl-3-oxo-3-phenylpropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4a
White solid. Mp: 113-114 °C; ¹H NMR (400 MHz; CDCl₃): δ = 1.35 (d, J = 7.2 Hz, 3H), 3.99 (t, J = 6.4 Hz, 1H), 4.24 (dd, J₁ = 3.2 Hz, J₂ = 7.2 Hz, 2H), 7.26 (d, J = 8.8 Hz, 2H), 7.57 (d, J = 7.2 Hz, 1H), 7.84-7.88 (m, 2H), 7.88-7.94 (m, 1H), 8.01-8.08 (m, 3H). ¹³C NMR (100 MHz; CDCl₃): δ = 16.3, 39.5, 41.6, 121.0, 125.3, 127.2, 128.5, 128.8, 133.4, 134.4, 134.8, 135.7, 137.6, 159.1, 201.0.
HRMS (ESI-TOF) Calcd for $C_{17}H_{16}NO_3S\,[M+H]^+$ 330.0800; Found 330.0803.

(R)-2-(3-(4-chlorophenyl)-2-methyl-3-oxopropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4b
White solid. Mp: 160-161 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 1.33$ (d, $J = 7.2$ Hz, 3H), 3.96 (m, 1H), 4.16-4.26 (m, 2H), 7.44-7.47 (m, 2H), 8.46 (dd, $J_1 = 1.6$ Hz, $J_2 = 7.2$ Hz, 3H), 7.88-7.93 (m, 2H), 7.94-8.06 (m, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 16.2$, 39.5, 41.5, 121.0, 125.3, 127.2, 134.0, 134.4, 134.9, 159.1, 199.8. HRMS (ESI-TOF) Calcd for $C_{17}H_{15}ClNO_3S\,[M+H]^+$ 364.0409; Found 364.0405.

(R)-2-(2-methyl-3-oxo-3-(p-tolyl)propyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4c
White solid. Mp: 131-133 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 1.33$ (d, $J = 7.2$ Hz, 3H), 2.41 (s, 3H), 3.98 (t, $J = 6.4$ Hz, 1H), 4.19-4.24 (m, 2H), 7.28 (d, $J = 6.4$ Hz, 2H), 7.84 (dd, $J_1 = 1.6$ Hz, $J_2 = 7.2$ Hz, 2H), 7.87-7.83 (m, 3H), 8.06 (dd, $J_1 = 1.2$ Hz, $J_2 = 6.4$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 16.3$, 21.6, 39.3, 41.6, 120.9, 125.3, 127.2, 128.7, 129.5, 133.1, 134.4, 134.8, 137.6, 144.3, 159.1, 200.7. HRMS (ESI-TOF) Calcd for $C_{18}H_{16}NO_3S\,[M+H]^+$ 344.0951; Found 344.0954.

2-(3-oxobutyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4d
White solid. Mp: 113-115 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 2.21$ (s, 3H), 3.03 (t, $J = 7.6$ Hz, 2H), 4.05 (t, $J = 7.6$ Hz, 2H), 7.83-7.89 (m, 3H), 7.91-8.07 (m, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 30.1$, 33.8, 41.2, 121.0, 125.2, 127.2, 134.4, 134.9, 137.6, 158.7, 205.4. HRMS (ESI-TOF) Calcd for $C_{11}H_{12}NO_3S\,[M+H]^+$ 254.0479; Found 254.0472.

(R)-2-(2-methyl-3-oxopentyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4e
White solid. Mp: 90-91 °C; $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 1.08$ (t, $J = 7.2$ Hz, 3H), 1.24 (d, $J = 7.2$ Hz, 3H), 2.50 (q, $J = 7.2$ Hz, 1H), 2.63 (q, $J = 7.2$ Hz, 1H), 3.27 (q, $J = 7.6$ Hz, 1H), 3.80 (q, $J = 7.2$ Hz, 1H), 4.10 (q, $J = 7.6$ Hz, 1H), 7.84-7.94 (m, 3H), 8.08 (dd, $J_1 = 1.6$ Hz, $J_2 = 6.8$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 7.5$, 15.3, 34.7, 41.0, 44.2, 120.9, 125.3, 127.2, 134.4, 134.8,
137.6, 159.0, 211.8. HRMS (ESI-TOF) Calcd for C_{13}H_{16}NO_{4}S, [M+H]^+ 282.0792; Found 282.0794.

![Structure of 2-(4-methyl-3-oxopentyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4f](image)

2-(4-methyl-3-oxopentyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4f
Yellow liquid. $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 1.14$ (d, $J = 7.2$ Hz, 6H), 2.59-2.66 (m, 1H), 3.05 (t, $J = 7.6$ Hz, 2H), 4.08 (t, $J = 7.6$ Hz, 2H), 7.84-7.94 (m, 3H), 8.08 (dd, $J_1 = 1.2$ Hz, $J_2 = 6.4$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 18.0$, 34.1, 38.2, 41.0, 120.9, 125.2, 127.4, 134.3, 134.8, 137.8, 158.7, 211.1. HRMS (ESI-TOF) Calcd for C$_{13}$H$_{16}$NO$_4$S, [M+H]$^+$ 281.0722; Found 282.0795.

![Structure of 2-(2-nitroethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4g](image)

2-(2-nitroethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4g
Yellow liquid. $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 4.43$ (t, $J = 6.4$ Hz, 2H), 4.80 (t, $J = 6.4$ Hz, 2H), 7.88-7.96 (m, 3H), 8.09 (d, $J = 6.8$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 35.4$, 71.7, 121.2, 125.6, 126.8, 134.7, 135.3, 137.5, 158.7. HRMS (ESI-TOF) Calcd for C$_9$H$_9$N$_2$O$_5$S, [M+H]$^+$ 257.0232; Found 257.0235.

![Structure of (R)-2-(2-nitropropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4h](image)

(R)-2-(2-nitropropyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 4h
Yellow liquid. $^1$H NMR (400 MHz; CDCl$_3$): $\delta = 1.69$ (d, $J = 6.8$ Hz, 3H), 4.03-4.17 (m, 1H), 4.41-4.49 (m, 1H), 5.07-5.12 (m, 1H), 7.88-8.04 (m, 3H), 8.09 (d, $J = 6.8$ Hz, 1H). $^{13}$C NMR (100 MHz; CDCl$_3$): $\delta = 17.3$, 41.6, 80.0, 121.2, 125.6, 126.1, 134.7, 135.3, 137.4, 158.9. HRMS (ESI-TOF) Calcd for C$_{10}$H$_{11}$N$_2$O$_5$S, [M+H]$^+$ 271.0381; Found 271.0385.
VI. $^1$H NMR and $^{13}$C NMR spectra copies of compounds 2, 4, C and H.

Compound 2a
Compound 2b
Compound 2c
Compound 2d
Compound 2e
Compound 2f
Compound 2g
Compound 2h
Compound 2i
Compound 2j
Compound 2k
Compound 21
Compound 2m
Compound 2n
Compound 2o
Compound 2p
Compound 2q
Compound 2r
Compound 2s
Compound 2t
Compound 2u
Compound 2v
Compound 2w
Compound 4a
Compound 4b
Compound 4c
Compound 4d
Compound 4e
Compound 4f
Compound 4g
Compound 4h
Compound C
Compound H