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# **Supporting Information**

## Visible-light-driven relay redox deracemization of cyclic sulfonamides catalyzed by a bifunctional chiral iridium complex

## **Table of Contents**

1.	General and Materials	S1
2.	Synthesis of catalyst	S1
3.	Intermediate MS	
4.	Extra optimization of the reaction conditions	S2
5.	General Procedure for deracemization of sulfonamides	S3
6.	Synthesis of cyclic Sulfonamides 3	S3
7.	Characterization data	S3
8.	References	
9.	Copies of NMR and HPLC	

#### 1. General and Materials

**General:** All reactions were carried out under an atmosphere of air using the standard glass bottle, unless otherwise noted. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded at room temperature in CDCl<sub>3</sub>, DMSO- $d_6$  on 400 MHz instrument with tetramethylsilane (TMS) as internal standard. Enantiomeric excess was determined by HPLC analysis, using chiral column described below in detail. Optical rotations were measured by polarimeter. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis.

**Materials:** Commercially available reagents and solvents were used throughout without further purification. The catalysts  $\Delta$ -IrS and  $\Delta$ -IrO were prepared by following reported procedure<sup>1</sup>. The racemic cyclic *N*-sulfonylimines were prepared according to the known procedures reported in the literature<sup>2,3</sup>.

## 2. Synthesis of catalyst



5-(*tert*-butyl)-2-phenylbenzothiazole (197 mg, 0.74 mmol, 2 equiv.) was added to  $IrCl_3 \cdot 3H_2O$  (130 mg, 0.37 mmol, 1 equiv.) in a mixture of 2-ethoxyethanol/water (3:1, 15 mL). The reaction mixture was heated at 130 °C for 36 h under nitrogen. After the reaction was completed, the solvent was distilled off under reduced pressure. Add AgPF<sub>6</sub> (279 mg, 1.1 mmol, 3 equiv.) and 10 mL CH<sub>3</sub>CN (distilled) to the schlenk flask. Immerse the schlenk flask in a preheated oil bath at 60 °C for 14 h. Remove the schlenk flask from the oil bath and allow it to cool to room temperature. Filter off the solid and the filtrate was subjected to a flash silica gel chromatography (CH<sub>2</sub>Cl<sub>2</sub>/CH<sub>3</sub>CN = 30:1, R<sub>f</sub> = 0.3 in CH<sub>2</sub>Cl<sub>2</sub>/CH<sub>3</sub>CN = 20:1) to separate as yellow solids (300 mg, 0.31 mmol, 72% yield).



Add **S1** (250 mg, 0.26 mmol, 1 equiv.), Et<sub>3</sub>N (126 mg, 1.25 mmol, 2.5 equiv.) and **S2** (116 mg, 0.53 mmol, 2 equiv.) in CH<sub>2</sub>Cl<sub>2</sub>. Stir the reaction mixture for 4 h at room temperature. The reaction mixture was cooled to room temperature and concentrated to dryness. The residue was subjected to a flash silica gel chromatography (PE/EA) to separate the two diastereomers. Use PE:EA (25:1) as the eluent until the first diastereomer  $\Lambda$ -**S3** (118 mg, 0.12 mmol, 47% yield) and then use PE:EA (10:1) to elute the second diastereomer  $\Delta$ -**S3** (130 mg, 0.14mmol, 52% yield).



A suspension of the iridium auxiliary complexes  $\Delta$ -S3 (160 mg, 0.17 mmol, 1 equiv.) and TFA (78  $\mu$ L, 1 mmol, 6 equiv.) in CH<sub>3</sub>CN (HPLC, 10 mL) was stired for 30 minutes. Remove the volatiles in vacuo to obtain a yellow oil. Dissolve the yellow oil in 10 ml of CH<sub>3</sub>CN and add NH<sub>4</sub>PF<sub>6</sub> (554 mg, 3.4 mmol, 20 equiv.) in one portion. Stir at room temperature for another 30 min. The reaction mixture was concentrated to dryness and subjected to a flash silica gel chromatography (100% CH<sub>2</sub>Cl<sub>2</sub> to CH<sub>2</sub>Cl<sub>2</sub>/CH<sub>3</sub>CN = 30:1, R<sub>f</sub> = 0.3 in CH<sub>2</sub>Cl<sub>2</sub>/CH<sub>3</sub>CN = 20:1) to give the enantiopure catalysts  $\Delta$ -IrS (106 mg, 0.11 mmol, 66%) as yellow solids.

## 3. Intermediate MS



16-electron intermediate MS

## 4. Extra optimization of the reaction conditions

#### Table S1 Oxidation reaction solvent screening<sup>a</sup>



Entry <sup>a,c</sup>	Oxidant	Solvent	Yield <sup>b</sup>
1	air	MeCN	77%
2	air	DCM	81%
3	air	THF	76%
4	air	toluene	61%

5	air	acetone	58%
6	air	CHCl <sub>3</sub>	68%
7	air	1,4-dioxane	67%
8	air	CCl <sub>4</sub>	57%
9	air	DCE	>95%
10	air	DMSO	>95%
11	air	EA	>95%
12	air	DMF	>95%
13	None (in $N_2$ )	DMF	none

<sup>*a*</sup>Reaction conditions: (±)-4a (0.2 mmol),  $\Delta$ -IrS (1 mol%), TMG (0.1 mmol), solvent (2 mL), 390 nm LED, 8h. <sup>*b*</sup>Determined by <sup>1</sup>H NMR with 1,3,5-trimethoxybenzene as the internal standard; <sup>*c*</sup>None of the raw materials have been reacted.

#### 5. General procedure for deracemization of sulfonamides



Racemic sulfonamides 1 (0.2 mmol) were placed in a 10 mL glass bottle and then  $\Delta$ -IrS(1 mol%), TMG (0.5 equiv.), DMF (2 mL) was added in air. After this, the solution was irradiated under stirring with 40 W 390nm LEDs (distance approx. 4 cm) at room temperature for 8 h. After the reaction is completed, HCOONH<sub>4</sub> (9 equiv) and H<sub>2</sub>O (1 mL) are added to the system in air and heated at 60°C for 18 hours. The solvent was removed under reduced pressure and the crude product was purified by flash chromatography on silica gel (PE/DCM = 1:4) to provide pure products. Enantiomeric excess was established by HPLC analysis. Absolute configuration of the products were assigned as *S* by comparing their optical rotation with the literature.

#### 6. Synthesis of Cyclic Sulfonamides 3



A mixture of **1b** (115 mg, 0.3 mmol), iodomethane (47 mg, 0.33 mmol), dried potassium carbonate (54 mg, 0.39 mmol), and 18-crown-6 (54 mg, 0.03 mmol) in dry acetone (2 mL) was stirred at room temperature under nitrogen for 56 h. The mixture was evaporated to dryness and purified by flash chromatography on silica gel (EtOAc) to afford product **S4** as a white solid (117 mg, yield: 97%). A mixture of **S4** (55 mg, 0.137 mmol) and 3 mol/L HCl (137  $\mu$ L, 0.417 mmol) in MeOH (3 mL) was stirred at room temperature for 2 h. The mixture was evaporated to dryness and purified by flash chromatography on silica gel (EtOAc) to afford product **S4** as a white solid (36 mg, yield: 87%).

#### 7. Characterization Data

(S)-3-phenyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1a): 97% yield, 96% ee(S), known compound<sup>4</sup>, white solid,  $N_{\text{NH}}$   $N_{\text{NH}}$  $N_{$  220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.7 mL/min, retention time 20.6 min (maj) and 22.5 min.



**OTBS** 

(S)-3-(3-(((tert-butyldimethylsilyl)oxy)methyl)phenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1b): 66% yield, 91% ee(S), known compound<sup>4a</sup>, colorless oil,  $[\alpha]^{20} = +60.9$  (c 0.96, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.00 - 7.79 (m, 1H), 7.67 - 7.49 (m, 2H), 7.45 - 7.31 (m, 3H), 7.26 (d, J = 6.5 Hz, 1H), 7.19 – 7.12 (m, 1H), 5.74 (d, J = 4.0 Hz, 1H), 5.02 (d, J = 4.1 Hz, 1H), 4.75 (s, 2H), 0.93 (s, 9H), 0.10 (d, J = 2.2 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 142.7, 139.9, 138.8, 134.8, 133.3, 129.5, 129.2, 126.6, 126.2, 125.5, 125.1, 121.1, 64.6, 61.4, 26.0, 18.4, -5.2. HPLC: Chiracel OD column, 220 nm, 30 °C, n-hexane/i-propanol = 70/30, flow = 0.8 mL/min, retention time 7.4 min (maj) and 9.0 min.

(S)-3-(*m*-tolyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (1c): 97% yield, 92% ee(S), known compound<sup>4b</sup>, white solid, m.p.=  $124-126^{\circ}$ C,  $[\alpha]^{20}_{D} = +71.0$  (c 0.44, CH<sub>2</sub>Cl<sub>2</sub>) [lit.<sup>4</sup>  $[\alpha]^{20}_{D} = +96.1$  (c 0.28, CH<sub>2</sub>Cl<sub>2</sub>), 89% ee (S)]. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (t, J = 6.1 Hz, 1H), 7.55 (d, J = 15.1 Hz, 2H), 7.26 (d, J = 7.1ŇН Hz, 1H), 7.17 (d, J = 7.8 Hz, 4H), 5.68 (s, 1H), 5.32 (s, 1H), 2.35 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) (S) 8 140.0, 139.1, 138.8, 134.7, 133.3, 129.8, 129.4, 129.1, 128.1, 125.4, 124.7, 121.1, 77.5, 77.1, 76.8, 61.4, 21.4. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*- propanol = 80/20, flow = 1.0 Me mL/min, retention time 10.8 min and 12.0 min (maj).

(S)-3-(p-tolyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1d): 95% yield, 92% ee(S) known compound<sup>4b</sup>, white solid, m.p.=  $169-171^{\circ}$ C,  $[\alpha]^{20}_{D} = +58.1$  (c 0.58, CH<sub>2</sub>Cl<sub>2</sub>) [lit.<sup>4</sup>  $[\alpha]^{20}_{D} = +66.5$  (c 0.52, CH<sub>2</sub>Cl<sub>2</sub>), 90% ee (S)]. .0 <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.90–7.71 (m, 1H), 7.54 (qt, *J* = 6.7, 3.5 Hz, 2H), 7.31–7.23 (m, 2H), 7.19 ΝH (d, J = 7.7 Hz, 2H), 7.14 (d, J = 7.3 Hz, 1H), 5.69 (s, 1H), 2.36 (s, 3H).<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$ (S) 140.2, 139.0, 135.8, 134.8, 133.3, 129.9, 129.4, 127.6, 125.4, 121.1, 77.4, 77.1, 76.8, 61.2, 21.2. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.7 mL/min, retention time 20.2 min and 22.8 min (maj). Ме

(S)-3-(3,5-dimethylphenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1e): 93% yield, 95% ee(S), known compound<sup>6</sup>, white solid, m.p.= 204.5-206°C,  $[\alpha]^{20}$  = +74.1 (c 0.45, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, <sub>~</sub>0 CDCl<sub>3</sub>) & 7.93–7.74 (m, 1H), 7.54 (q, *J* = 7.7, 6.3 Hz, 2H), 7.16 (d, *J* = 6.4 Hz, 1H), 6.99 (d, *J* = 11.6 Hz, ΝH 3H), 5.65 (d, J = 3.2 Hz, 1H), 5.26–4.92 (m, 1H), 2.31 (s, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 140.1, (S) 139.0, 138.61, 134.8, 133.3, 130.7, 129.4, 125.4, 125.3, 121.1, 77.4, 77.1, 76.8, 61.4, 21.3. HPLC: Chiracel AD column, 220 nm, 30 °C, n-hexane/i-propanol = 80/20, flow = 0.6 mL/min, retention time Ме 17.5 min and 19.6 min (maj).

- (S)-3-(3-isopropylphenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1f): 99% yield, 93% ee(S), unknown compound, colorless liquid,  $[\alpha]^{20}_{D}$  = +56.1 (c 1.00, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.81 (d, J = 6.9 Hz, 1H), 7.54 (m, J = 6.1 Hz, 2H), 7.31 (t, J = 7.5 Hz, 1H), 7.25 (d, J = 9.1 Hz, 2H), 7.17 (t, J = 7.1 0 Hz, 2H), 5.72 (s, 1H), 5.30 (s, 1H), 2.92 (m, J = 6.9 Hz, 1H), 1.26 (d, J = 6.9 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 149.8, 140.1, 139.1, 134.5, 133.3, 129.4, 129.2, 126.8, 125.8, 125.5, 125.0, 120.9, 77.8, 77.5, 77.2, 61.4, 34.0, 24.0, 24.0. HRMS Calculated for C<sub>16</sub>H<sub>18</sub>NO<sub>2</sub>S [M+H]<sup>+</sup> 288.1053, found: 288.1053.
  - HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.7 mL/min, retention time 15.0 min and 21.4 min (maj).

(S)-3-(4-ethylphenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1g): 90% yield, 87% ee(S), known compound<sup>7</sup>, white solid, m.p.=  $123-124^{\circ}$ C,  $[\alpha]^{20}_{D}$ = +81.7 (c 0.61, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.95–7.74 0 (m, 1H), 7.65-7.39 (m, 2H), 7.29 (d, J = 8.1 Hz, 2H), 7.23 (d, J = 7.9 Hz, 2H), 7.17 (d, J = 8.4 Hz, 1H), 5.71 (s, 1H), 4.99 (s, 1H), 2.67 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.6 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) ŇΗ δ 145.4, 140.1, 136.0, 134.8, 133.4, 129.4, 128.8, 127.7, 125.5, 121.1, 61.2, 28.6, 15.5. HPLC: Chiracel (S) OD column, 220 nm, 30 °C, n-hexane/i-propanol = 80/20, flow = 0.6 mL/min, retention time 43.9 min (maj) and 50.3 min.

(S)-3-(4-(tert-butyl)phenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1h): 73% yield, 99% ee(S), known compound<sup>6</sup>, white solid, m.p.= 145.1-146.2 °C,  $[\alpha]^{20}_{D}$  = +63.3 (c 0.15, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz,  $CDCl_3$   $\delta$  7.83 (d, J = 7.1 Hz, 1H), 7.55 (t, J = 5.9 Hz, 2H), 7.41 (d, J = 8.1 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 7.2 Hz, 1H), 5.73 (s, 1H), 1.32 (s, 9H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  152.2, 140.1, ŇН 135.7, 134.9, 133.3, 129.4, 127.4, 126.2, 125.5, 121.1, 77.4, 77.1, 76.8, 61.2, 34.7, 31.3. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 80/20, flow = 0.6 mL/min, retention time 12.8 min (maj) and 14.9 min.

(S)-3-(4-butylphenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1i): 82% yield, 88% ee(S), unknown compound,



white solid, m.p.=  $87-89.4^{\circ}$ C,  $[\alpha]^{20}_{D}$ = +68.2 (c 0.5, CH<sub>3</sub>Cl). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (t, J = 6.6 Hz, 1H), 7.54 (q, J = 6.7, 6.2 Hz, 2H), 7.27 (d, J = 7.9 Hz, 2H), 7.17 (dd, J = 16.0, 7.3 Hz, 3H), 5.70 (s, 1H), 5.32 (s, 1H), 2.61 (t, J = 7.8 Hz, 2H), 1.60 (q, J = 7.4 Hz, 2H), 1.37 (m, J = 8.3, 7.3 Hz, 2H), 0.94 (t, J = 7.3 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  144.0, 140.1, 136.0, 134.7, 133.3, 129.4, 129.2, 127.6, 125.5, 121.1, 77.5, 77.2, 76.9, 61.2, 35.4, 33.5, 22.4, 14.0. HRMS Calculated for C<sub>17</sub>H<sub>20</sub>NO<sub>2</sub>S [M+H]<sup>+</sup> 302.1209, found: 302.1209. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.8 mL/min, retention time 10.3 min (maj) and 15.4 min.

(*S*)-3-(3,5-di-*tert*-butylphenyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (1j): 86% yield, 62% ee(*S*), unknown compound, white solid, m.p.= 160.6-162.8 °C,  $[\alpha]^{20}_{D}$ = +68.9 (c 0.27, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.93–7.74 (m, 1H), 7.54 (q, *J* = 7.7, 6.3 Hz, 2H), 7.16 (d, *J* = 6.4 Hz, 1H), 6.99 (d, *J* = 11.6 Hz, 3H), 5.65 (d, *J* = 3.2 Hz, 1H), 5.26–4.92 (m, 1H), 2.31 (s, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  152.0, 140.3, 137.8, 135.1, 133.2, 129.3, 125.4, 123.1, 121.7, 121.1, 77.4, 77.1, 76.8, 62.1, 35.0, 31.4. HRMS Calculated for C<sub>21</sub>H<sub>28</sub>NO<sub>2</sub>S [M+H]<sup>+</sup> 358.1835, found: 358.1835. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 90/10, flow = 0.7 mL/min, retention time 11.1 min and 12.5 min (maj).

(*S*)-3-(3-methoxyphenyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (1k): 84% yield, 81% ee(*S*), known compound<sup>6</sup>, white solid, m.p.= 116.7-118.1 °C,  $[\alpha]^{20}{}_{D}$ = +54.8 (c 0.2, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.88–7.82 (m, 1H), 7.57 (t, *J* = 3.6 Hz, 2H), 7.33 (t, *J* = 8.2 Hz, 1H), 7.19 (d, *J* = 8.1 Hz, 1H), 7.04–6.86 (m, 3H), 5.71 (s, 1H), 5.02 (s, 1H), 3.80 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  160.2, 140.4, 139.7, 134.6, 133.3, 130.3, 129.5, 125.4, 121.1, 119.7, 114.5, 113.0, 77.5, 77.1, 76.8, 61.2, 55.4. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 80/20, flow = 0.7 mL/min, retention time 22.1 min and 30.5 min (maj).

(S)-3-(4-methoxyphenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (11): 57% yield, 89% ee(S), known compound<sup>4b</sup>, white solid, m.p.= 151-154°C,  $[\alpha]^{20}_{D}$ = +32.7 (c 0.33, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.87–7.74 (m, 1H), 7.54 (q, J = 7.3, 6.2 Hz, 2H), 7.27 (d, J = 8.8 Hz, 2H), 7.18–7.10 (m, 1H), 6.90 (d, J = 8.7 Hz, 2H), 5.68 (d, J = 2.4 Hz, 1H), 5.14 (s, 1H), 3.81 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$ 160.1, 140.3, 135.0, 133.3, 130.7, 129.4, 129.0, 125.4, 121.1, 114.6, 77.4, 77.1, 76.8, 61.0, 55.4. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.8 mL/min, retention time 24.9 min (maj) and 38.2 min.

(*S*)-3-(3,5-dimethoxyphenyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (1m): 71% yield, 87% ee(*S*), known compound<sup>4c</sup>, white solid, m.p.= 167-168 °C,  $[\alpha]^{20}_{D}$ = +71.5 (c 0.35, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (d, *J* = 6.7 Hz, 1H), 7.53 (q, *J* = 7.0 Hz, 2H), 7.20 (d, *J* = 6.7 Hz, 1H), 6.53 (d, *J* = 2.2 Hz, 2H), 6.42 (t, *J* = 2.3 Hz, 1H), 5.63 (s, 1H), 5.44 (s, 1H), 3.75 (s, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  152.0, 140.3, 137.8, 135.1, 133.2, 129.3, 125.4, 123.1, 121.7, 121.1, 77.4, 77.1, 76.8, 62.1, 35.0, 31.4. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.7 mL/min, retention time 26.3 min (maj) and 30.8 min.

(S)-3-(3-fluorophenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1n): 76% yield, 91% ee(S), known compound<sup>6</sup>, white solid, m.p.= 113-118°C,  $[\alpha]^{20}_{D}$ = +74.0 (c 0.25, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (d, J = 6.9 Hz, 1H), 7.56 (p, J = 7.4 Hz, 2H), 7.44 – 7.29 (m, 1H), 7.25 – 6.98 (m, 4H), 5.75 (d, J = 3.1Hz, 1H), 5.58 (d, J = 4.4 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  161.8, 141.5, 139.1, 134.4, 133.5, 130.8, 129.7, 125.3, 123.2, 121.2, 116.1, 114.6, 77.4, 77.1, 76.8, 60.6. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 80/20, flow = 0.6 mL/min, retention time 23.5 min and 31.3 min (maj).

(S)-3-(4-fluorophenyl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (1o): 94% yield, 92% ee(*S*), known compound<sup>5</sup>, white solid, m.p.= 163-167°C,  $[\alpha]^{20}_{D}$ = +84.6 (c 0.46, CH<sub>2</sub>Cl<sub>2</sub>). [lit.<sup>4</sup>  $[\alpha]^{20}_{D}$  = +66.9 (c 0.76, CH<sub>2</sub>Cl<sub>2</sub>), 85% ee (*S*)]. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.91–7.77 (m, 1H), 7.66–7.52 (m, 2H), 7.37 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.22 – 6.97 (m, 3H), 5.74 (s, 1H), 5.14 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  164.3, 161.8, 139.6, 134.7, 133.5, 129.7, 129.5, 129.4, 125.3, 121.2, 116.4, 116.1, 60.6, 53.5. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.7 mL/min, retention time 12.8 min (maj) and 19.3 min.



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(S)-3-(3-chlorophenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1p): 79% yield, 95% ee(S), known compound<sup>8</sup>, white solid, m.p.= 137-138°C,  $[\alpha]^{20}$  = +101.15 (c 0.29, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92– 7.79 (m, 1H), 7.70–7.51 (m, 2H), 7.49–7.29 (m, 4H), 7.24–7.11 (m, 1H), 5.72 (s, 1H), 5.31 (d, J = 6.1 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 140.8, 139.0, 135.1, 134.5, 133.6, 130.6, 129.8, 129.3, 127.6, 125.8, 125.3, 121.3, 77.4, 77.1, 76.8, 60.6. HPLC: Chiracel OD column, 220 nm, 30 °C, n-hexane/ipropanol = 70/30, flow = 0.7 mL/min, retention time 16.1 min (maj) and 20.6 min.

(S)-3-(4-chlorophenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1q): 85% yield, 88% ee(S), known compound<sup>5</sup>, white solid, m.p.= 179-181 °C,  $[\alpha]^{20}_{D}$  = +83.2 (c 0.25, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.66 (s, 1H), 7.88 (d, J = 7.0 Hz, 1H), 7.71–7.55 (m, 2H), 7.53–7.41 (m, 4H), 7.30 (d, J = 7.5 Hz, 1H), 5.92 (s, 1H). ŇН <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 140.1, 140.0, 135.2, 133.7, 133.3, 130.1, 129.4, 129.2, 126.0, 121.1, 59.5, 40.6, 40.4, 40.2, 40.0, 39.8, 39.6, 39.4. HPLC: Chiracel OJ column, 220 nm, 30 °C, n-hexane/ipropanol = 70/30, flow = 0.7 mL/min, retention time 25.0 min (mai) and 29.7 min.

(S)-3-(4-phenoxyphenyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1r): 79% yield, 92% ee(S), unknown compound, white solid, m.p.= 101.5-104.8 °C,  $[\alpha]^{20}_{D}$  = +44.2 (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.83 (d, J = 7.4 Hz, 1H), 7.57 (p, J = 7.2 Hz, 2H), 7.45–7.29 (m, 4H), 7.17 (q, J = 7.4 Hz, 2H), 7.01 (dd, NH J = 15.6, 8.3 Hz, 4H), 5.74 (s, 1H), 5.31 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  158.1, 156.5, 139.9, 134.8, 133.4, 133.3, 130.0, 129.6, 129.2, 125.5, 123.9, 121.1, 119.4, 119.0, 77.5, 77.2, 76.8, 60.8. HRMS Calculated for C<sub>19</sub>H<sub>16</sub>NO<sub>3</sub>S [M+H]<sup>+</sup> 338.0845, found: 338.0845. HPLC: Chiracel AD column, 220 nm, 30  $^{\circ}$ C, *n*-hexane/*i*-propanol = 80/20, flow = 0.6 mL/min, retention time 30.9 min (maj) and 38.4 min.

(S)-3-(naphthalen-2-yl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1s): 92% yield, 96% ee(S), known compound<sup>5</sup>, white solid, m.p.=  $191.2-192.4^{\circ}$ C,  $[\alpha]^{20}$ D = +127.0 (c 0.37, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.06– -.0 7.74 (m, 5H), 7.53 (d, J = 4.2 Hz, 4H), 7.38 (d, J = 8.6 Hz, 1H), 7.13 (s, 1H), 5.87 (s, 1H), 5.34 (s, 1H). ŇН <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 139.7, 136.0, 134.7, 133.5, 133.4, 133.1, 129.6, 129.5, 128.1, 127.9, S) 127.2, 126.8, 126.8, 125.5, 124.5, 121.2, 77.4, 77.1, 76.8, 61.5. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 80/20, flow = 0.7 mL/min, retention time 30.4 min and 38.7 min (maj).

(S)-3-(benzofuran-5-yl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (1t): 86% yield, 88% ee(S), unknown compound, white solid, m.p.= 140-143.1°C,  $[\alpha]^{20}_{D} = +96.3$  (c 0.59, CH<sub>2</sub>Cl<sub>2</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.92– 7.72 (m, 1H), 7.71–7.57 (m, 2H), 7.57–7.39 (m, 3H), 7.31–7.19 (m, 1H), 7.17–7.04 (m, 1H), 6.75 (d, J ΝH = 2.2 Hz, 1H), 5.82 (s, 1H), 5.47 (s, 1H).  $^{13}$ C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  155.0, 146.1, 140.3, 134.6, 133.5, 133.4, 129.5, 128.1, 125.5, 123.8, 121.1, 120.7, 112.2, 106.7, 77.5, 77.2, 76.9, 61.5. HRMS Calculated for C<sub>15</sub>H<sub>12</sub>NO<sub>3</sub>S [M+H]<sup>+</sup> 286.0532, found: 286.0532. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.8 mL/min, retention time 38.0 min (maj) and 49.9 min.

(S)-5-methyl-3-phenyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (2a): 98% yield, 92% ee(S), known compound<sup>4d</sup>, white solid, m.p.=  $171-172^{\circ}$ C,  $[\alpha]^{20}_{D}$ = +63.8 (c 0.5, CH<sub>3</sub>Cl). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.70 (d, J -0 = 8.0 Hz, 1H), 7.39 (m, J = 2.4 Hz, 5H), 7.33 (d, J = 7.5 Hz, 1H), 6.92 (s, 1H), 5.69 (d, J = 4.1 Hz, ΝH 1H), 5.20 (s, 1H), 2.37 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 144.4, 140.2, 139.0, 132.1, 130.5, 129.2, (S) 129.0, 127.6, 125.5, 120.9, 77.4, 77.1, 76.8, 61.3, 21.7. HPLC: Chiracel AD column, 220 nm, 30 °C, n-hexane/*i*-propanol = 85/15, flow = 0.5 mL/min, retention time 37.3 min and 39.6 (maj) min.

(S)-5-methoxy-3-phenyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (2b): 94% yield, 85% ee(S), known compound<sup>4d</sup>, white solid, m.p.= 120-121 °C,  $[\alpha]^{20}_{D}$ = +61.4 (c 0.52, CH<sub>3</sub>Cl). <sup>1</sup>H NMR (400 MHz,



CDCl<sub>3</sub>)  $\delta$  7.71 (d, J = 8.7 Hz, 1H), 7.38 (m, 5H), 7.03 (d, J = 6.4 Hz, 1H), 6.53 (d, J = 2.2 Hz, 1H), 5.66 (d, J = 4.1 Hz, 1H), 5.21 (s, 1H), 3.77 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  163.8, 142.5, 138.9, 129.3, 129.0, 127.6, 126.9, 122.6, 116.5, 109.2, 77.4, 77.1, 76.8, 61.2, 55.8. HPLC: Chiracel AD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 85/15, flow = 0.7 mL/min, retention time 36.7 min and 42.5(maj) min.

#### (S)-3-(3-(((tert-butyldimethylsilyl)oxy)methyl)phenyl)-2-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide(S4):



97% yield, 89% ee(*S*), unknown compound, white solid, m.p.= 149.1-152.2°C,  $[\alpha]^{20}_{D}$ = +105.9 (c 0.57, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.63–7.47 (m, 2H), 7.45–7.33 (m, 2H), 7.29 (t, J = 2.0 Hz, 1H), 7.23 (tt, J = 5.2, 3.0 Hz, 1H), 7.09–7.01 (m, 1H), 5.21 (s, 1H), 4.76 (s, 2H), 2.78 (s, 3H), 0.93 (s, 9H), 0.10 (d, J = 3.6 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  142.7, 138.4, 136.6, 133.0, 129.3, 129.1, 126.8, 126.8, 125.7, 125.1, 121.1, 67.0, 64.6, 27.4, 25.9, 18.4, -5.2. HRMS Calculated for C<sub>21</sub>H<sub>30</sub>NO<sub>3</sub>SSi [M+H]<sup>+</sup> 404.1716, found: 404.1703. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 80/20, flow = 0.8 mL/min, retention time 6.8 min (maj) and 8.5 min.

(*S*)-3-(3-(hydroxymethyl)phenyl)-2-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (3): 87% yield, 88% ee(*S*), known compound<sup>4b</sup>, white solid,  $[\alpha]^{20}_{D}$ = +134.4 (c 0.17, CHCl<sub>3</sub>). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.95– 7.75 (m, 1H), 7.60–7.45 (m, 2H), 7.39 (d, J = 5.6 Hz, 2H), 7.33 (s, 1H), 7.26 (m, J = 5.8, 2.6, 2.2 Hz, 1H), 7.13 – 6.98 (m, 1H), 5.21 (s, 1H), 4.68 (s, 2H), 2.76 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$ 142.2, 138.3, 136.9, 133.9, 133.1, 129.4, 129.4, 127.7, 127.3, 126.3, 125.1, 121.1, 77.4, 77.1, 76.8, 67.0, 64.6, 27.5. HPLC: Chiracel OD column, 220 nm, 30 °C, *n*-hexane/*i*-propanol = 70/30, flow = 0.8 mL/min, retention time 6.8 min (maj) and 8.5 min.

## 8. References

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## 9. Copy of NMR and HPLC for the Compounds



100 90 f1 (ppm) 















210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

















<sup>1</sup>H NMR(400 HMz, CDCl<sub>3</sub>)



30 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 2 f1 (ppm)

-1.79 HDO





f1 (ppm)













Data file:	YL-3-29-V-2022-07-12 20-39-32+08-00.dx				
Sequence Name:	SingleSample Project Name: 1260				
Sample name:	YL-3-29 Operator:		SYSTEM		
Instrument:	lc1260	2022-07-12 20:40:20+08:00			
Acq. method:	YL-1-57.amx Type: Sample				
Processing method:	GC_LC Area Percent_DefaultMethod.pmx				
Sample Info:	OJ, Hexane/i-PrOH = 70/30, 0,7 mL/min, 30 oC, 220 nm				





Signal:	VWD1A,Wavelength=2	20 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
20,559	2,397	6333,43	134,39	98,29	
22.521	1.703	109.99	2.48	1.71	
	Sum	6443.42			



Data file:	YL-4-84-V-2023-04-12 08-01-12+08-00.dx				
Sequence Name:	SingleSample Project Name: 1260				
Sample name:	YL-4-84 Operator:		SYSTEM		
Instrument:	lc1260	2023-04-12 08:11:49+08:00			
Acq. method:	YL-1-57.amx Type: Sample				
Processing method:	GC_LC Area Percent_DefaultMethod,pmx				
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,8 mL/min, 30 oC, 220 nm				





Signal:	VWD1A,Wavelength=220 nm					
RT [min]	Peak Width Base	Area	Height	Area%		
7,363	1,690	7540,80	502,23	95,41		
8.979	0.287	362.37	19.10	4.59		
	Sum	7903.17				



Data file:	YL-3-71-V-2022-11-11 18-44-11+08-00.dx					
Sequence Name:	SingleSample Project Name: 1260					
Sample name:	YL-3-71	SYSTEM				
Instrument:	lc1260 Injection date: 2022-11-11 18:45:24+0					
Acq. method:	YL-1-57.amx Type: Sample					
Processing method:	GC_LC Area Percent_DefaultMethod.pmx					
Sample Info:	AD, Hexane/i-PrOH = 80/20, 1 mL/min, 30 oC, 220 nm					



Signal:	VWD1A,Wavelength	=220 nm			O S S
RT [min]	Peak Width Base	Area	Height	Area%	↓ NH
10,835	0,333	13704 72	634,53	50,06	~ I
12.112	0.371	13673.82	568.12	49.94	
	Sum	27378,54			Me
					rac- <b>1c</b>
Data file:	YL-3	-71-V-2022-11-	11 19-03-30	+08–00.dx	
Sequence N	lame: Singl	eSample		Project Name	: 1260
Sample nan	ne: YL-3-	-71		Operator:	SYSTEM
Instrument:	lc126	0		Injection date	: 2022-11-11 19:04:16+08:00
Acq. metho	d: YL-1-	-57.amx		Туре:	Sample
Processing	method: GC_I	LC Area Percer	nt_DefaultMe	thod.pmx	
Sample Info	:	AD, Hexan	e/i-PrOH = 8	0/20, 1 mL/min, 30 o	C, 220 nm



Signal:	VWD1A,Wavelength=	220 nm		
RT [min]	Peak Width Base	Area	Height	Area%
10,785	1,117	485,07	22,92	3,87
12.026	0.370	12040.99	500.00	96.13
	Sum	12526.05		



Data file:	YL-3-62-V-2022-07-22 14-40-27+08-00.dx					
Sequence Name:	SingleSample Project Name: 1260					
Sample name:	YL-3-62	Operator:	SYSTEM			
Instrument:	lc1260 Injection date:		2022-07-22 14:40:52+08:00			
Acq. method:	YL-1-57.amx	Sample				
Processing method:	GC_LC Area Percent_DefaultMethod.pmx					
Sample Info:	OD Hexane/i-PrOH = $70/30$ 0.7 ml/min 30 oC 220 nm					





Signal:	VWD1A,Wavelength=220 nm					
RT [min]	Peak Width Base	Area	Height	Area%		
20,206	2,210	721,15	18,51	3,86		
22.765	4.170	17967.40	415.34	96.14		
	Sum	18688.55				

0 NH (S) Me (S)-1d

Data file:	YL-3-138 1-V-2022-10-15 15-08-50+08-00.dx		
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-3-138 1	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2022-10-15 15:09:36+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod.pmx		
Sample Info:	AD, Hexane/i-PrOH = 80/20, 0,6 mL/min, 30 oC, 220 nm		









Data file:	YL-3-130 3-V-2022-10-14 18-10-38+08-00.dx				
Sequence Name:	SingleSample Project Name: 1260				
Sample name:	YL-3-130 3	Operator:	SYSTEM		
Instrument:	lc1260	Injection date:	2022-10-14 18:10:51+08:00		
Acq. method:	YL-1-57.amx	Туре:	Sample		
Processing method:	GC_LC Area Percent_DefaultMethod,pmx				
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,7 mL/min, 30 oC, 220 nm				





Signal:	VWD1A,Wavelength=	220 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
14,950	3,483	757,76	24,59	3,53	
21.448	5.057	20718.05	458.18	96.47	
	Sum	21475.81			



Data file:	YL-3-160-V-2022-11-07 17-04-02+08-00.dx				
Sequence Name:	SingleSample Project Name: 1260				
Sample name:	YL-3-160	Operator:	SYSTEM		
Instrument:	lc1260	Injection date:	2022-11-07 17:28:24+08:00		
Acq. method:	YL-1-57.amx	Туре:	Sample		
Processing method:	GC_LC Area Percent_DefaultMethod.pmx				
Sample Info:	OD, Hexane/i-PrOH = 80/20, 0.6 mL/min, 30 oC, 220 nm				



OD, Hexane/i-PrOH = 80/20, 0,6 mL/min, 30 oC, 220 nm



Signal:	VWD1A,Wavelength=2	20 nm		
RT [min]	Peak Width Base	Area	Height	Area%
42,413	5,093	8225,70	99,96	97,46
48.284	4.660	214.40	2.28	2.54
	Sum	8440.10		



Data file:	YL-3-67-V-2022-07-22 19-50-40+08-00.dx		
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-3-67	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2022-07-22 19:51:09+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod,pmx		
Sample Info:	AD. Hexane/i-PrOH = 80/20, 0.6 mL/min, 30 oC, 220 nm		





Signal:	VWD1A,Wavelength=2	220 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
12,774	1,809	20239,24	911,15	99,59	
14.948	0.607	83.67	1.90	0.41	
	Sum	20322.92			



Data file:	YL-3-154-V-2022-10-28 15-58-42+08-00.dx				
Sequence Name:	SingleSample Project Name: 1260				
Sample name:	YL-3-154	Operator:	SYSTEM		
Instrument:	lc1260 Injection date: 2022-10-28 16:01:47+08:0				
Acq. method:	YL-1-57.amx	Туре:	Sample		
Processing method:	GC_LC Area Percent_DefaultMethod.pmx				
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,8 mL/min, 30 oC, 220 nm				





Signal:	VWD1A,Wavelength=2	220 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
14,112	0,442	9630,80	334,42	84,34	
21.193	0.692	1788.51	39.84	15.66	
	Sum	11419.31			



Data file:	YL-3-146-V-2022-10-29 14-50-38+08-00.dx				
Sequence Name:	SingleSample Project Name: 1260				
Sample name:	YL-3-146	Operator:	SYSTEM		
Instrument:	lc1260	Injection date:	2022-10-29 15:01:06+08:00		
Acq. method:	YL-1-57.amx	Туре:	Sample		
Processing method:	GC_LC Area Percent_DefaultMethod.pmx				
Sample Info:	AD. Hexane/i-PrOH = 90/10, 0.7 mL/min, 30 oC, 220 nm				





Signal:	VWD1A,Wavelength=2	20 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
11,085	1,674	832,20	40,32	18,86	
12.519	2.987	3579.95	154.08	81.14	
	Sum	4412.15			



Data file:	YL-3-100 1-V-2022-09-12 20-18-44+08-00.dx		
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-3-100 1	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2022-09-12 20:19:31+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod.pmx		
Sample Info:	AD, Hexane/i-PrOH = 80/20, 0,7 mL/min, 30 oC, 220 nm		





Signal:	VWD1A,Wavelength=2	20 nm		
RT [min]	Peak Width Base	Area	Height	Area%
22,084	0,586	470,64	12,28	9,46
30.509	0.850	4503.60	82.39	90.54
	Sum	4974,23		



Data file:	YL-3-154-V-2022-10-27 20-07-44+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-154	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-10-27 20:08:15+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod,pmx			
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,8 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=2	20 nm		
RT [min]	Peak Width Base	Area	Height	Area%
24,892	0,829	3032,34	55,61	94,29
38.242	1.177	183.76	1.82	5.71
	Sum	3216.10		



Data file:	YL-3-130 3-V-2022-10-14 15-58-40+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-130 3	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-10-14 15:59:25+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod.pmx			
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,7 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=	220 nm		
RT [min]	Peak Width Base	Area	Height	Area%
26,278	4,130	9528,35	194,10	94,38
30.811	3.202	567.11	7.96	5.62
	Sum	10095.47		



Data file:	YL-3-146-V-2022-10-31 14-16-57+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-146	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-10-31 14:18:08+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod.pmx			
Sample Info:	AD, Hexane/i-PrOH = 80/20, 0,6 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=2	20 nm		
RT [min]	Peak Width Base	Area	Height	Area%
23,545	2,047	374,78	8,94	4,33
31.337	3.917	8276.09	141.36	95.67
	Sum	8650,88		





Data file:	YL-3-64-V-2022-07-22 15-51-31+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-64	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-07-22 15:52:06+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod.pmx			
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,7 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=2	20 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
12,769	2,973	8658,93	375,74	96,05	
19.317	2.457	355.83	9.67	3.95	
	Sum	9014.76			



Data file:	YL-3-65-V-2022-07-22 17-04-17+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-65	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-07-22 17:04:28+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod.pmx			
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,7 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=2	220 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
16,113	2,995	9847,51	322,07	97,59	
20.639	2.500	242.71	6.08	2.41	
	Sum	10090.21			



Data file:	YL-3-65-V-2022-07-22 11-07-45+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-65	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-07-22 11:08:34+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod.pmx			
Sample Info:	O.I. Hexane/i-PrOH = 70/30, 0.7 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=2	20 nm			
RT [min]	Peak Width Base	Area	Height	Area%	
25,011	4,713	4575,66	67,88	94,02	
29.659	3.498	290.86	3.18	5.98	
	Sum	4866.53			



Data file:	YL-3-160-V-2022-10-31 16-45-04+08	-00.dx	
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-3-160	Operator:	SYSTEM
Instrument:	lc1260	njection date:	2022-10-31 16:45:58+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod	.pmx	
Sample Info:	AD, Hexane/i-PrOH = 80/20,	0,6 mL/min, 30 oC, 22	0 nm





38.369

3.078

Sum

342.05

8690.05

4.85

3.94

Data file:	YL-3-130-V-2022-10-10 19-47-45+08	-00.dx	
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-3-130	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2022-10-10 19:49:26+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod	l,pmx	
Sample Info:	AD, Hexane/i-PrOH = 80/20, 0,7	mL/min, 30 oC, 220 nm	





Signal:	VWD1A,Wavelength=	220 nm		
RT [min]	Peak Width Base	Area	Height	Area%
30,430	1,723	247,45	4,90	2,05
38.693	5.449	11822.36	154.51	97.95
	Sum	12069.81		



Data file:	YL-3-174-V-2022-11-22 16-31-36+0	8-00.dx	
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-3-174	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2022-11-22 16:34:25+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMetho	d.pmx	
Sample Info:	OD. Hexane/i-PrOH = 70	)/30. 0.8 mL/min. 30 o(	C. 220 nm





Signal:	VWD1A,Wavelength=2	20 nm		
RT [min]	Peak Width Base	Area	Height	Area%
38,042	6,650	5153,09	58,45	94,20
49.921	1.317	317.11	2.82	5.80
	Sum	5470.20		



Data file:	YL-5-9-V-2023-06-28 17-35-54+08-0	0.dx	
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-5-9	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2023-06-28 17:36:32+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod	,pmx	
Sample Info:	AD, Hexane/i-PrOH = 85	i/15, 0,5 mL/min, 30 oC,	220 nm



Signal:	VWD1A,Wavele	ength=2	20 nm				O S NH
RT [min]	Peak Width E	Base	Area	Height	Area%		Me
37,480	C	,940	13904,39	224,30	48,91		
39.876	1	.026	14526.94	214.72	51.09		
		Sum	28431.33				rac-2a
Data file:		YL-5-9-\	V-2023-06-28	16-45-40+0	8-00.dx		
Sequence N	ame:	SingleS	ample		Project Nam	ie:	1260
Sample nam	ne:	YL-5-9			Operator:		SYSTEM
Instrument:	I	c1260			Injection dat	te:	2023-06-28 16:46:16+08:00
Acq. metho	d:	YL-1-57	amx		Type:		Sample
Processing	method:	GC_LC	Area Percent	t_DefaultMet	hod.pmx		
Sample Info	:		AD, Hex	ane/i-PrOH	= 85/15, 0,5 mL/mi	in, 30 oC, 2	20 nm



	-					
Ti	m	e	[r	ni	in]	

Signal:	VWD1A,Wavelength=;	220 nm		
RT [min]	Peak Width Base	Area	Height	Area%
37,325	2,503	586,82	9,57	3,82
39.644	5.419	14756.18	215.79	96.18
	Sum	15343.00		



Data file:	YL-5-10-V-2023-06-29 13-17-45+08-	00.dx	
Sequence Name:	SingleSample	Project Name:	1260
Sample name:	YL-5-10	Operator:	SYSTEM
Instrument:	lc1260	Injection date:	2023-06-29 13:30:35+08:00
Acq. method:	YL-1-57.amx	Туре:	Sample
Processing method:	GC_LC Area Percent_DefaultMethod	l.pmx	
Sample Info:	AD, Hexane/i-PrOH = 8	5/15, 0,7 mL/min, 30 o	C, 220 nm





Signal:	Signal: VWD1A,Wavelength=220 nm				
RT [min]	Peak Width Base	Area	Height	Area%	
36,733	3,578	1137,23	16,74	7,54	
42.542	4.836	13938.38	178.81	92.46	
	Sum	15075.61			



ΝH

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Data file:	YL-3-29-V-2022-11-12 16-34-28+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-3-29	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2022-11-12 16:36:30+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod,pmx			
Sample Info:	OD, Hexane/i-PrOH = 80/20, 0,8 mL/min, 30 oC, 220 nm			



Signal:	VWD1A,Wavelength=	220 nm			
RT [min]	Peak Width Base	Area	Height	Area%	> .(R)
27,565	2,855	410,97	7,57	1,56	
32.872	1.030	25910.82	382.78	98.44	
	Sum	26321.79			( <i>R</i> )-1a
Data file:	YL-3-29	-V-2022-11-11	21-05-00+0	8–00.dx	
Sequence Na	me: SingleSa	ample		Project Name:	1260
Sample name	: YL-3-29			Operator:	SYSTEM
Instrument:	lc1260			Injection date:	2022-11-11 21:05:27+08:00
Acq. method:	YL-1-57.	amx		Туре:	Sample
Processing m	Processing method: GC_LC Area Percent_DefaultMethod.pmx				
Sample Info: OD, Hexane/i-PrOH = 80/20, 0,8 mL/min, 30 oC, 220 nm					



Signal:	VWD1A,Wavelength=220 nm				
RT [min]	Peak Width Base	Area	Height	Area%	
26,244	3,772	9032,54	176,38	92,94	
31.897	4.153	686.50	11.09	7.06	
	Sum	9719.04			



Data file:	YL-4-88-V-2023-04-19 08-18-18+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-4-88	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2023-04-19 08:24:49+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod.pmx			
Sample Info:	OD, Hexane/i-PrOH = 80/20, 0,8 mL/min, 30 oC, 220 nm			





Sum

6286.11

(S)-**2** 

Data file:	YL-4-127-V-2023-05-03 17-00-47+08-00.dx			
Sequence Name:	SingleSample	Project Name:	1260	
Sample name:	YL-4-127	Operator:	SYSTEM	
Instrument:	lc1260	Injection date:	2023-05-03 17:02:43+08:00	
Acq. method:	YL-1-57.amx	Туре:	Sample	
Processing method:	GC_LC Area Percent_DefaultMethod,pmx			
Sample Info:	OD, Hexane/i-PrOH = 70/30, 0,8 mL/min, 30 oC, 220 nm			





Signal:	VWD1A,Wavelength=220 nm				
RT [min]	Peak Width Base	Area	Height	Area%	
10,486	0,394	16649 56	646,16	94,14	
13.403	0.507	1035.93	31.16	5.86	
	Sum	17685.50			

