

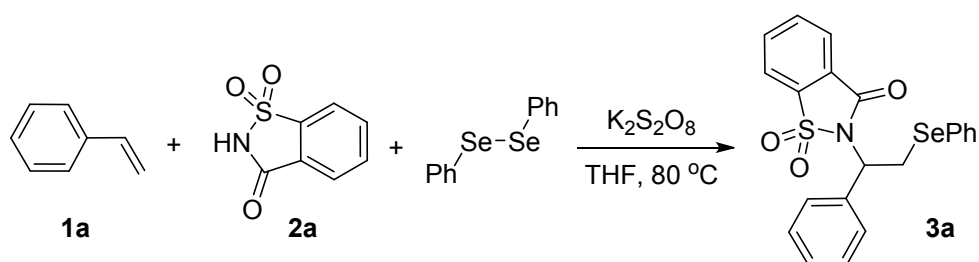
## Supporting Information

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## 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.  $^1\text{H}$  NMR spectra of compounds **3** was recorded at 25°C on a Bruker Ascend<sup>TM</sup> 400 spectrometer. Chemical shifts (in ppm) were referenced TMS in  $\text{CDCl}_3$  (0 ppm).  $^{13}\text{C}$ -NMR spectra were obtained by using the same NMR spectrometers and were calibrated with  $\text{CDCl}_3$  ( $\delta = 77.00$  ppm). HRMS data were obtained on a Waters LCT Premierxe<sup>TM</sup> (USA). IR spectra (KBr) were recorded on a Magna-560 FTIR spectrophotometer in the range of 400–4000  $\text{cm}^{-1}$ . All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 200–300 mesh silica gel at increased pressure.

## II. Synthesis procedure for compounds **3** (**3a** as an example).



Styrene **1a** (52.0 mg, 0.5 mmol), saccharin **2a** (100.7 mg, 0.55 mmol), diphenyl diselenide (156.0 mg, 0.5 mmol) and  $\text{K}_2\text{S}_2\text{O}_8$  (269.8 mg, 1.0 mmol) were added to THF (3 mL). The mixture was stirred at 80 °C for 12.0 h (monitored by TLC), quenched with water, extracted with dichloromethane (5×3 ml), and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . 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 **3a** as a white solid (394.3 mg, 89%).

## III. Crystallographic data for **3a**

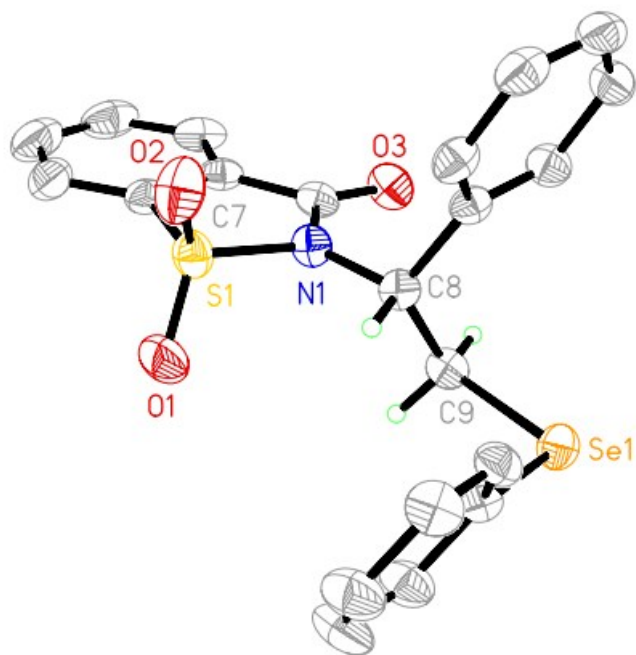
### Crystallographic Data Collection and Refinement.

The single crystal of compound **3a** was mounted on the tips of glass fibers with commercially available glue. X-ray data collection of **3a** was performed at room temperature using diffractometer equipped with a normal focus, sealed tube X-ray source with graphite monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073\text{\AA}$ ). The data were integrated using SAINT<sup>1</sup> program and the absorption corrections were made with SADABS.<sup>2</sup> The structure of **3a** was solved by SHELXS-97<sup>3</sup> using Patterson method and followed by successive Fourier and difference Fourier synthesis. Full matrix least-squares refinements were performed on  $F^2$  using SHELXL-97<sup>3</sup> with anisotropic displacement parameters for all non-hydrogen atoms. All the hydrogen atoms were fixed geometrically by HFIX command and placed in ideal positions. Data collection and structure refinement parameters along with crystallographic data of **3a** are given in Table 1.

### References

1. SMART (V 5.628), SAINT (V 6.45a), XPREP, SHELXTL, Bruker AXS Inc., Madison, WI, 2004.
2. G. M. Sheldrick, SADABS (Version 2.03), University of Göttingen, Germany, 2002.
3. G. M. Sheldrick, SHELXS-97, Acta. Crystallogr., 2008, **A64**, 112.

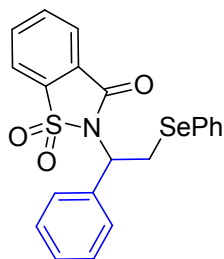
Table 1. Crystallographic and Structural Refinement Parameters of **3a**.



**Fig. 1.** Thermal ellipsoid of **3a** (30% propability)

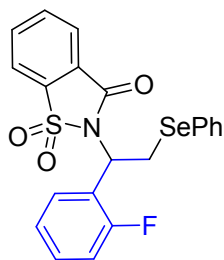
Formula	C <sub>21</sub> H <sub>17</sub> NO <sub>3</sub> SSe
Formula Weight	442.38
Crystal System	Triclinic
Space group	<i>P</i> -1
<i>a</i> /Å	9.7234(4)
<i>b</i> /Å	9.7234(4)
<i>c</i> /Å	22.0952(9)
<i>α</i> /°	102.367(3)
<i>β</i> /°	94.393(3)
<i>γ</i> /°	107.218(3)
<i>V</i> /Å <sup>3</sup>	1948.22(14)
<i>Z</i>	4
<i>D</i> <sub>c</sub> /g cm <sup>-3</sup>	1.508
<i>μ</i> /mm <sup>-1</sup>	2.055
<i>F</i> (000)	896
<i>θ</i> range/°	2.24 to 25.60
Reflections collected	21294
Unique reflections	7204
Reflections <i>I</i> > 2σ( <i>I</i> )	5259
<i>R</i> <sup>int</sup>	0.0271
Goodness-of-fit ( <i>F</i> <sup>2</sup> )	1.014
<i>R</i> <sub>1</sub> ( <i>I</i> > 2σ( <i>I</i> ))	<i>R</i> <sub>1</sub> = 0.0331
<i>wR</i> <sub>2</sub> ( <i>I</i> > 2σ( <i>I</i> ))	<i>wR</i> <sub>2</sub> = 0.0846

#### IV. Analytical data of products obtained in this study



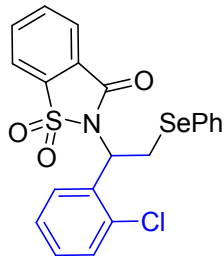
##### 2-(1-phenyl-2-(phenylselanyl)ethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide **3a**

**3a** was purified by a short column chromatography (PE/EA = 4:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.86 (q, *J* = 7.6 Hz, 1H), 4.15 (q, *J* = 8.4 Hz, 1H), 5.45 (d, *J* = 8.4 Hz, 1H), 7.28-7.39 (m, 6H), 7.60-7.63 (m, 4H), 7.72-7.77 (m, 3H), 7.84 (t, *J* = 7.2 Hz, 1H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 29.1, 57.8, 120.7, 125.1, 127.0, 127.6, 128.6, 128.8, 129.1, 129.2, 133.7, 134.2, 134.7, 136.7, 137.3, 158.7. HRMS (ESI-TOF) Calcd for C<sub>21</sub>H<sub>18</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 444.0171; Found 444.0176.



##### 2-(1-(2-fluorophenyl)-2-(phenylselanyl)ethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide **3b**

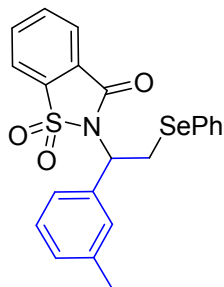
**3b** was purified by a short column chromatography (PE/EA = 5:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.79 (q, *J* = 8.0 Hz, 1H), 4.40 (q, *J* = 8.0 Hz, 1H), 5.86 (d, *J* = 8.4 Hz, 1H), 7.08-7.34 (m, 6H), 7.57-7.85 (m, 6H), 8.02 (d, *J* = 7.2 Hz, 1H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 28.8, 50.5, 115.5, 115.7, 120.7, 124.3, 125.2, 126.9, 127.7, 129.1, 129.3, 129.4, 130.5, 133.8, 134.2, 134.8, 137.5, 158.8, 161.8. HRMS (ESI-TOF) Calcd for C<sub>21</sub>H<sub>17</sub>FNO<sub>3</sub>SSe, [M+H]<sup>+</sup> 426.0078; Found 426.0073. IR (film) 739, 1462, 1580, 1715, 2927, 3074 cm<sup>-1</sup>.



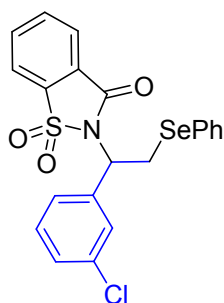
##### 2-(1-(2-chlorophenyl)-2-(phenylselanyl)ethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide **3c**

**3c** was purified by a short column chromatography (PE/EA = 5:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.76 (q, *J* = 8.0 Hz, 1H), 4.01 (q, *J* = 8.0 Hz, 1H), 6.02 (t, *J* = 8.4 Hz, 1H), 7.27-7.31 (m, 5H), 7.40 (d, *J* = 6.4 Hz, 1H), 7.62 (d, *J* =

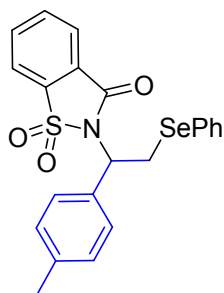
3.6 Hz, 2H), 7.63-8.06 (m, 5H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta$  = 29.0, 54.1, 120.6, 125.3, 126.8, 127.2, 127.7, 128.8, 129.1, 129.2, 129.9, 130.1, 133.8, 134.0, 134.3, 134.9, 137.5, 158.9. HRMS (ESI-TOF) Calcd for  $\text{C}_{21}\text{H}_{17}\text{ClNO}_3\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  477.9784; Found 477.9778. IR (film) 750, 1485, 1580, 1715, 2927, 3074  $\text{cm}^{-1}$ .



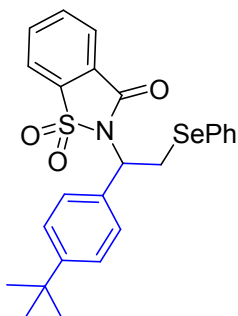
**2-(2-(phenylselanyl)-1-(*m*-tolyl)ethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3d**  
**3d** was purified by a short column chromatography (PE/EA = 4:1,  $R_f$  = 0.4) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta$  = 3.82 (q,  $J$  = 8.4 Hz, 1H), 4.09 (q,  $J$  = 8.0 Hz, 1H), 5.39 (t,  $J$  = 8.0 Hz, 1H), 7.13-7.27 (m, 5H), 7.38 (d,  $J$  = 9.2 Hz, 2H), 7.57 (q,  $J$  = 3.6 Hz, 2H), 7.78-7.85 (m, 3H), 7.99 (d,  $J$  = 7.6 Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta$  = 21.4, 29.1, 57.8, 120.7, 125.1, 125.5, 127.1, 127.6, 128.4, 129.1, 129.2, 129.5, 133.7, 134.2, 134.6, 136.6, 137.4, 138.2, 158.7. HRMS (ESI-TOF) Calcd for  $\text{C}_{22}\text{H}_{20}\text{NO}_3\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  458.0325; Found 458.0329. IR (film) 739, 1450, 1580, 1721, 2921  $\text{cm}^{-1}$ .



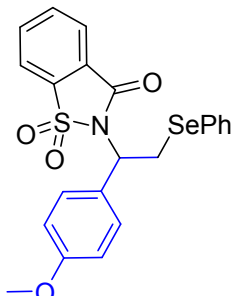
**2-(1-(3-chlorophenyl)-2-(phenylselanyl)ethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3e**  
**3e** was purified by a short column chromatography (PE/EA = 5:1,  $R_f$  = 0.4) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta$  = 3.79 (t,  $J$  = 8.0 Hz, 1H), 4.04 (t,  $J$  = 8.4 Hz, 1H), 5.33 (t,  $J$  = 8.4 Hz, 1H), 7.26-7.29 (m, 5H), 7.45 (d,  $J$  = 4.0 Hz, 1H), 7.55 (q,  $J$  = 3.6 Hz, 3H), 7.80-7.99 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta$  = 28.7, 57.2, 120.8, 125.2, 126.8, 126.9, 127.8, 128.6, 128.9, 129.2, 133.8, 134.3, 134.4, 134.8, 137.3, 138.6, 158.7. HRMS (ESI-TOF) Calcd for  $\text{C}_{21}\text{H}_{17}\text{ClNO}_3\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  477.9784; Found 477.9789. IR (film) 744, 1568, 1715, 2927, 3057  $\text{cm}^{-1}$ .



**2-(2-(phenylselanyl)-1-(*p*-tolyl)ethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide **3f****  
**3f** was purified by a short column chromatography (PE/EA = 4:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 2.34 (s, 3H), 3.82 (q, *J* = 8.0 Hz, 1H), 4.07 (q, *J* = 8.4 Hz, 1H), 5.38 (t, *J* = 8.4 Hz, 1H), 7.15-7.27 (m, 5H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.55 (t, *J* = 3.6 Hz, 3H), 7.78-7.98 (m, 4H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 21.1, 30.3, 57.6, 120.7, 125.1, 127.1, 127.5, 128.5, 129.1, 129.2, 133.5, 133.6, 134.1, 134.6, 137.4, 138.6, 158.7. HRMS (ESI-TOF) Calcd for C<sub>22</sub>H<sub>20</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 458.0325; Found 458.0321. IR (film) 739, 1456, 1574, 1721, 2927 cm<sup>-1</sup>.

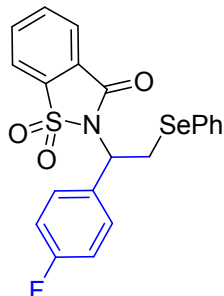


**2-(1-(4-(tert-butyl)phenyl)-2-(phenylselanyl)ethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide **3g****  
**3g** was purified by a short column chromatography (PE/EA = 4:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 1.31 (s, 9H), 3.82 (q, *J* = 8.0 Hz, 1H), 4.14 (q, *J* = 8.4 Hz, 1H), 5.40 (t, *J* = 8.4 Hz, 1H), 7.25-7.38 (m, 5H), 7.51-7.58 (m, 4H), 7.76-7.97 (m, 4H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 29.2, 31.2, 34.6, 57.7, 120.7, 125.1, 125.4, 127.1, 127.5, 128.2, 129.1, 133.7, 134.2, 134.6, 137.3, 151.6, 158.7. HRMS (ESI-TOF) Calcd for C<sub>25</sub>H<sub>26</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 500.0799; Found 500.0792.



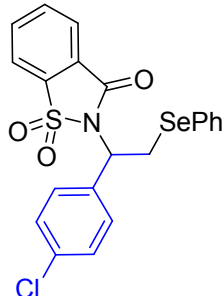
**2-(1-(4-methoxyphenyl)-2-(phenylselanyl)ethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide **3h****  
**3h** was purified by a short column chromatography (PE/EA = 4:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.78 (s, 3H), 3.85 (dd, *J*<sub>1</sub> = 2.0 Hz, *J*<sub>2</sub> = 8.4 Hz,

1H), 4.06 (dd,  $J_1 = 2.0$  Hz,  $J_2 = 8.0$  Hz, 1H), 5.40 (d,  $J = 4.4$  Hz, 1H), 6.87-7.28 (m, 5H), 7.52-7.57 (m, 4H), 7.76-7.96 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 29.2, 55.2, 57.4, 113.8, 114.1, 120.7, 125.1, 127.1, 127.5, 128.5, 129.1, 130.0, 133.6, 134.2, 134.7, 137.4, 158.7, 159.8$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{22}\text{H}_{20}\text{NO}_4\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  474.0278; Found 474.0272. IR (film) 738, 1250, 1520, 1609, 1715, 2945  $\text{cm}^{-1}$ .



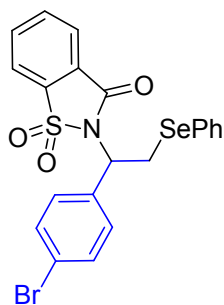
**2-(1-(4-fluorophenyl)-2-(phenylselanyl)ethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 3i**

**3i** was purified by a short column chromatography (PE/EA = 5:1,  $R_f = 0.4$ ) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta = 3.79$  (q,  $J = 8.0$  Hz, 1H), 4.04 (q,  $J = 8.0$  Hz, 1H), 5.37 (t,  $J = 8.4$  Hz, 1H), 7.02 (t,  $J = 8.0$  Hz, 5H), 7.25-7.27 (m, 3H), 7.53-7.58 (m, 4H), 7.79-7.98 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 28.9, 57.1, 115.3, 115.5, 120.7, 125.1, 127.0, 127.7, 128.8, 129.2, 129.3, 130.5, 130.6, 132.4, 133.7, 134.3, 134.8, 137.3, 138.6$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{21}\text{H}_{17}\text{FNO}_3\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  426.0078; Found 426.0071. IR (film) 744, 1514, 1609, 1727, 2921, 3068  $\text{cm}^{-1}$ .



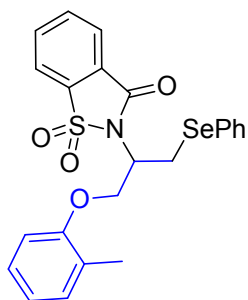
**2-(1-(4-chlorophenyl)-2-(phenylselanyl)ethyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 3j**

**3j** was purified by a short column chromatography (PE/EA = 5:1,  $R_f = 0.4$ ) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta = 3.81$  (q,  $J = 8.0$  Hz, 1H), 4.04 (q,  $J = 8.0$  Hz, 1H), 5.38 (t,  $J = 8.4$  Hz, 1H), 7.02 (t,  $J = 8.0$  Hz, 5H), 7.26-7.32 (m, 5H), 7.50-7.55 (m, 4H), 7.78-7.98 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 28.7, 57.1, 120.8, 125.1, 127.0, 128.7, 129.2, 130.1, 133.8, 134.3, 134.6, 134.8, 135.1, 137.3, 158.6$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{21}\text{H}_{17}\text{ClNO}_3\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  477.9784; Found 477.9788. IR (film) 734, 1497, 1574, 1727, 2927, 3062  $\text{cm}^{-1}$ .



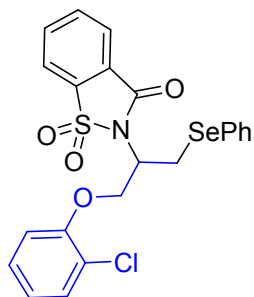
**2-(1-(4-bromophenyl)-2-(phenylselanyl)ethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3k**

**3k** was purified by a short column chromatography (PE/EA = 5:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.80 (q, *J* = 8.0 Hz, 1H), 4.04 (q, *J* = 8.0 Hz, 1H), 5.34 (t, *J* = 8.4 Hz, 1H), 7.25-7.55 (m, 9H), 7.80-7.99 (m, 4H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 28.6, 57.2, 120.8, 125.2, 127.7, 129.2, 130.3, 131.7, 133.8, 134.3, 134.8, 135.5, 158.6. HRMS (ESI-TOF) Calcd for C<sub>21</sub>H<sub>17</sub>NBrO<sub>3</sub>SSe, [M+H]<sup>+</sup> 521.9278; Found 521.9270. IR (film) 732, 1474, 1597, 1709, 2927 cm<sup>-1</sup>.



**2-(1-(phenylselanyl)-3-(*o*-tolylloxy)propan-2-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3l**

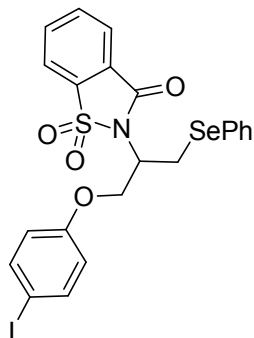
**3l** was purified by a short column chromatography (PE/EA = 4:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 2.29 (s, 3H), 4.41-4.29 (m, 2H), 4.34 (d, *J* = 4.4 Hz, 1H), 4.43 (t, *J* = 6.0 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 3.2 Hz, 3H), 7.69-8.05 (m, 6H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 16.2, 41.1, 41.3, 68.3, 111.0, 120.8, 121.0, 125.3, 126.6, 127.1, 127.7, 128.1, 129.3, 130.7, 134.4, 134.6, 134.9, 137.6, 156.3, 159.2. HRMS (ESI-TOF) Calcd for C<sub>23</sub>H<sub>22</sub>NO<sub>4</sub>SSe, [M+H]<sup>+</sup> 488.0435; Found 488.0439. IR (film) 750, 1497, 1603, 1721, 2927, 3074 cm<sup>-1</sup>.



**2-(1-(2-chlorophenoxy)-3-(phenylselanyl)propan-2-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide 3m**

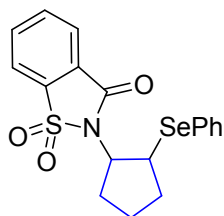


**3m** was purified by a short column chromatography (PE/EA = 5:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 4.09-4.42 (m, 5H), 6.85 (q, *J* = 7.6 Hz, 2H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.32-7.34 (m, 4H), 7.70-8.05 (m, 6H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 40.6, 41.3, 69.8, 113.7, 120.9, 121.9, 123.3, 125.3, 127.2, 127.5, 128.2, 129.3, 130.3, 134.3, 134.8, 137.6, 153.8, 159.2. HRMS (ESI-TOF) Calcd for C<sub>22</sub>H<sub>19</sub>NClO<sub>4</sub>SSe, [M+H]<sup>+</sup> 507.9889; Found 507.9886. IR (film) 738, 1580, 1727, 2933, 3068 cm<sup>-1</sup>.



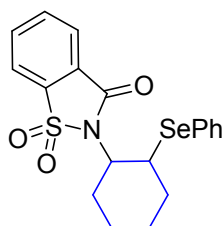
**2-(1-(4-iodophenoxy)-3-(phenylselanyl)propan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 3n**

**3n** was purified by a short column chromatography (PE/EA = 5:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 4.02-4.31 (m, 5H), 6.62 (d, *J* = 8.8 Hz, 2H), 7.33 (dd, *J*<sub>1</sub> = 2.0 Hz, *J*<sub>2</sub> = 4.6 Hz, 3H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.84-8.05 (m, 6H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 40.4, 41.1, 68.7, 117.1, 121.0, 125.3, 127.0, 127.2, 129.3, 134.3, 134.8, 134.9, 137.5, 138.1, 158.1, 159.1. HRMS (ESI-TOF) Calcd for C<sub>22</sub>H<sub>19</sub>NIO<sub>4</sub>SSe, [M+H]<sup>+</sup> 599.9241; Found 599.9246.



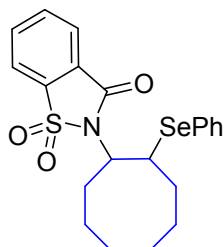
**2-(2-(phenylselanyl)cyclopentyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 3o**

**3o** was purified by a short column chromatography (PE/EA = 5:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 1.60-1.77 (m, 5H), 2.03-2.33 (m, 2H), 3.42 (s, 1H), 4.16 (d, *J* = 6.0 Hz, 1H), 4.49 (d, *J* = 8.8 Hz, 1H), 7.17-7.28 (m, 3H), 7.55-7.97 (m, 6H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 22.1, 22.6, 42.0, 49.7, 59.9, 120.6, 125.0, 127.1, 127.4, 127.5, 129.1, 129.4, 158.7. HRMS (ESI-TOF) Calcd for C<sub>18</sub>H<sub>18</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 408.0173; Found 408.0178.



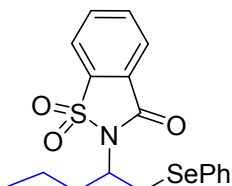
**2-(2-(phenylselanyl)cyclohexyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide 3p**

**3p** was purified by a short column chromatography (PE/EA = 5:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 1.26-1.47 (m, 4H), 1.65-1.90 (m, 3H), 2.17-2.28 (m, 3H), 4.14 (s, 2H), 7.17 (t, *J* = 7.2 Hz, 3H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.78-7.96 (m, 4H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 25.7, 26.5, 29.6, 31.8, 34.8, 58.6, 120.6, 125.1, 127.2, 127.6, 127.7, 128.6, 134.1, 134.5, 135.9, 137.3, 158.8. HRMS (ESI-TOF) Calcd for C<sub>19</sub>H<sub>20</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 422.0329; Found 422.0323. IR (film) 756, 1450, 1721, 2857, 2933 cm<sup>-1</sup>.



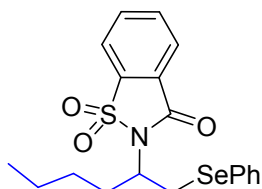
### 2-(2-(phenylselanyl)cyclooctyl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide **3q**

**3q** was purified by a short column chromatography (PE/EA = 5:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 1.54-1.94 (m, 9H), 2.13-2.43 (m, 3H), 1.21-2.28 (m, 3H), 4.45-4.55 (m, 2H), 7.12 (d, *J* = 3.2 Hz, 3H), 7.51-7.53 (m, 2H), 7.75-7.90 (m, 4H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 25.1, 25.3, 25.9, 27.4, 29.5, 33.0, 46.6, 59.1, 120.7, 125.0, 127.3, 127.4, 128.47, 129.2, 134.0, 134.5, 135.0, 137.2, 158.9. HRMS (ESI-TOF) Calcd for C<sub>21</sub>H<sub>24</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 450.0642; Found 450.0648. IR (film) 741, 1462, 1574, 1721, 2921 cm<sup>-1</sup>.



### 2-(1-(phenylselanyl)pentan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide **3r**

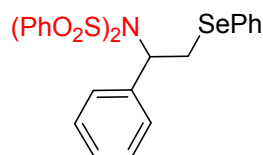
**3r** was purified by a short column chromatography (PE/EA = 5:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 0.91-0.94 (m, 4H), 1.47-1.78 (m, 3H), 3.73 (q, *J* = 3.6 Hz, 1H), 4.01 (q, *J* = 3.6 Hz, 2H), 7.30 (t, *J* = 3.2 Hz, 3H), 7.64 (d, *J* = 3.6 Hz, 2H), 7.85-8.05 (m, 4H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 13.7, 20.7, 34.1, 42.0, 44.5, 120.9, 125.2, 127.2, 127.7, 129.1, 133.3, 134.3, 134.8, 137.5, 159.1. HRMS (ESI-TOF) Calcd for C<sub>18</sub>H<sub>20</sub>NO<sub>3</sub>SSe, [M+H]<sup>+</sup> 410.0329; Found 410.0324. IR (film) 739, 1456, 1580, 2956 cm<sup>-1</sup>.



### 2-(1-(phenylselanyl)hexan-2-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide **3s**

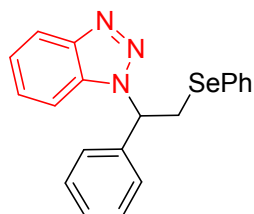
**3s** was purified by a short column chromatography (PE/EA = 5:1, Rf = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 1.27-1.36 (m, 3H), 1.44-1.81 (m, 6H), 3.72 (t, *J* = 2.8 Hz, 1H), 4.01 (q, *J* = 3.6 Hz, 2H), 7.27-7.30 (m, 3H), 7.64 (d, *J* = 3.2 Hz, 2H),

7.82-8.05 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 13.9, 22.3, 29.6, 31.7, 42.2, 44.5, 120.9, 125.2, 127.2, 127.7, 127.8, 129.2, 133.3, 134.3, 134.8, 137.6, 159.1$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{19}\text{H}_{22}\text{NO}_3\text{SSe}$ ,  $[\text{M}+\text{H}]^+$  424.0483; Found 424.0486.



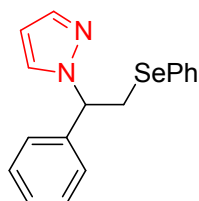
### ***N*-(1-phenyl-2-(phenylselanyl)ethyl)-*N*-(phenylsulfonyl)benzenesulfonamide 3t**

**3t** was purified by a short column chromatography (PE/EA = 2:1,  $R_f = 0.3$ ) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta = 3.60$  (dd,  $J_1 = 3.2$  Hz,  $J_2 = 15.2$  Hz, 1H), 4.92 (t,  $J = 15.2$  Hz, 1H), 5.02 (dd,  $J_1 = 3.6$  Hz,  $J_2 = 15.6$  Hz, 1H), 7.30-7.39 (m, 8H), 7.42-7.52 (m, 11H), 7.75 (d,  $J = 6.8$  Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 46.7, 52.4, 128.1, 128.5, 128.6, 128.7, 128.9, 129.1, 129.3, 129.4, 133.5, 136.0, 138.1, 138.4$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{26}\text{H}_{24}\text{NO}_4\text{S}_2\text{Se}$ ,  $[\text{M}+\text{H}]^+$  558.0313; Found 558.0318. IR (film) 744, 1450, 1479, 1580, 2904  $\text{cm}^{-1}$ .



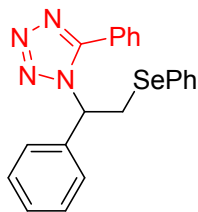
### **1-(1-phenyl-2-(phenylselanyl)ethyl)-1*H*-benzo[*d*][1,2,3]triazole 3u**

**3u** was purified by a short column chromatography (PE/EA = 4:1,  $R_f = 0.4$ ) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta = 3.82$  (q,  $J = 6.4$  Hz, 1H), 4.28 (q,  $J = 6.4$  Hz, 1H), 5.89 (q,  $J = 6.4$  Hz, 1H), 7.30-7.39 (m, 8H), 7.24-7.45 (m, 13H), 8.05 (d,  $J = 8.0$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 32.5, 63.6, 109.5, 120.0, 123.9, 126.8, 127.2, 127.7, 128.7, 128.9, 129.0, 129.2, 133.0, 133.6, 138.4, 146.1$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{20}\text{H}_{18}\text{N}_3\text{Se}$ ,  $[\text{M}+\text{H}]^+$  380.0666; Found 380.0661. IR (film) 706, 1571, 1580, 1617, 2931, 3059  $\text{cm}^{-1}$ .



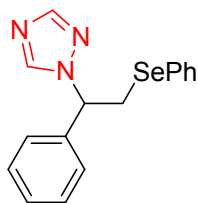
### **1-(1-phenyl-2-(phenylselanyl)ethyl)-1*H*-pyrazole 3v**

**3v** was purified by a short column chromatography (PE/EA = 5:1,  $R_f = 0.4$ ) on silica gel.  $^1\text{H}$  NMR (400 MHz;  $\text{CDCl}_3$ ):  $\delta = 3.60$  (q,  $J = 6.0$  Hz, 1H), 4.00 (q,  $J = 9.2$  Hz, 1H), 5.45 (q,  $J = 6.0$  Hz, 1H), 7.28-7.34 (m, 9H), 7.40-7.61 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{CDCl}_3$ ):  $\delta = 32.9, 65.9, 105.5, 126.8, 127.4, 128.3, 128.7, 129.2, 129.6, 133.3, 139.6, 139.8$ . HRMS (ESI-TOF) Calcd for  $\text{C}_{17}\text{H}_{17}\text{N}_2\text{Se}$ ,  $[\text{M}+\text{H}]^+$  329.0557; Found 329.0554. IR (film) 738, 1479, 1574, 2945, 3057  $\text{cm}^{-1}$ .



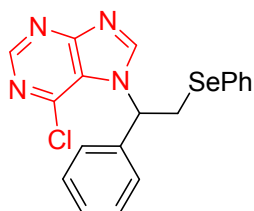
### 5-phenyl-1-(1-phenyl-2-(phenylselanyl)ethyl)-1H-tetrazole **3w**

**3w** was purified by a short column chromatography (PE/EA = 5:1, R<sub>f</sub> = 0.3) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.71 (q, *J* = 5.6 Hz, 1H), 4.03-4.09 (m, 1H), 6.09 (q, *J* = 5.2 Hz, 1H), 7.28-7.56 (m, 13H), 8.17 (t, *J* = 4.0 Hz, 2H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 32.4, 68.4, 125.9, 127.0, 127.1, 127.5, 128.0, 128.3, 128.5, 128.8, 129.0, 129.2, 129.4, 130.3, 133.0, 134.2, 137.1, 165.1. HRMS (ESI-TOF) Calcd for C<sub>21</sub>H<sub>19</sub>N<sub>4</sub>Se, [M+H]<sup>+</sup> 407.0775; Found 407.0771. IR (film) 744, 1444, 1468, 1580, 3057 cm<sup>-1</sup>.



### 1-(1-phenyl-2-(phenylselanyl)ethyl)-1H-1,2,4-triazole **3x**

**3x** was purified by a short column chromatography (PE/EA = 5:1, R<sub>f</sub> = 0.4) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.57 (q, *J* = 4.8 Hz, 1H), 3.91 (t, *J* = 10.0 Hz, 1H), 5.80 (q, *J* = 4.2 Hz, 1H), 7.21-7.45 (m, 10H), 7.98 (s, 1H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 33.0, 63.7, 127.0, 127.5, 128.3, 128.5, 128.7, 129.2, 129.5, 132.8, 133.4, 144.4, 152.6. HRMS (ESI-TOF) Calcd for C<sub>16</sub>H<sub>16</sub>N<sub>3</sub>Se, [M+H]<sup>+</sup> 330.0509; Found 330.0503. IR (film) 685, 738, 1474, 1586, 2927, 3062 cm<sup>-1</sup>.



### 6-chloro-7-(1-phenyl-2-(phenylselanyl)ethyl)-7H-purine **3y**

**3y** was purified by a short column chromatography (PE/EA = 4:1, R<sub>f</sub> = 0.3) on silica gel. <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>): δ = 3.71 (q, *J* = 4.2 Hz, 1H), 4.19 (q, *J* = 14.4 Hz, 1H), 5.79 (q, *J* = 4.2 Hz, 1H), 7.13-7.41 (m, 10H), 8.06 (s, 1H), 8.65 (s, 1H). <sup>13</sup>C NMR (100 MHz; CDCl<sub>3</sub>): δ = 30.8, 61.6, 127.0, 127.4, 127.9, 129.0, 129.2, 131.8, 133.7, 137.6, 144.3, 150.9, 151.6. HRMS (ESI-TOF) Calcd for C<sub>19</sub>H<sub>16</sub>ClN<sub>4</sub>Se, [M+H]<sup>+</sup> 415.0229; Found 415.0223. IR (film) 738, 1485, 1556, 2939, 3062 cm<sup>-1</sup>.

V.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra copies of compounds 3 and H

