

**SUPPORTING INFORMATION FOR:**  
**Sulfur Ylide Initiated Thio-Claisen Rearrangements. The Synthesis of**  
**Highly Substituted Indolines.**

Alexei V. Novikov, Abigail R. Kennedy, and Jon D. Rainier\*

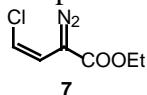
Department of Chemistry, The University of Arizona, Tucson, AZ 85721

Department of Chemistry, University of Utah, 315 South 1400 East, Salt Lake City UT,  
84112

Experimental protocols and spectroscopic data for all new compounds.

**General Information**

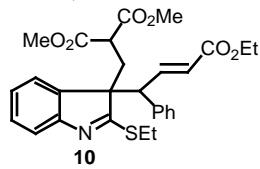
Ether and THF were distilled from sodium/benzophenone. Benzene, toluene,  $\text{CH}_2\text{Cl}_2$ ,  $\text{CHCl}_3$ , DMF,  $\text{CH}_3\text{OH}$ ,  $i\text{-Pr}_2\text{NEt}$ ,  $\text{Et}_3\text{N}$ , and  $\text{Et}_2\text{NH}$  were distilled from  $\text{CaH}_2$ .  $\text{CH}_3\text{CN}$  was distilled from  $\text{K}_2\text{CO}_3$ . All other reagents were used without purification. Unless otherwise stated, all reactions were run under an atmosphere of argon in flame-dried glassware.



7

**General procedure for the preparation of vinyl diazoacetates:**

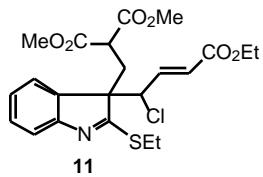
4-Chloro-2-diazo-but-3-enoic acid ethyl ester 7. To a solution of 4-acetamidobenzenesulfonyl azide (ABSA) (0.125 g, 0.52 mmol), 4-chloro-but-2-enoic acid ethyl ester (0.076 g, 0.51 mmol), and  $\text{CH}_3\text{CN}$  (3 mL) at 0°C was added DBU (0.10 mL, 0.67 mmol) dropwise. The reaction mixture was allowed to warm to rt. Upon completion (by TLC analysis), the reaction mixture was poured into a mixture of  $\text{NH}_4\text{Cl}$  (aq., sat., 2 mL) and ethyl acetate:hexanes (1:20, 20 mL). Following separation, the organic phase was passed through a short plug of silica gel (eluted with ethyl acetate:hexanes, 1:20). The resulting yellow solution was concentrated to provide 80 mg (90%) of vinyl diazoacetate 7 as a yellow oil. The diazoester was used without further purification.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 6.02 (d,  $J = 7.8\text{Hz}$ , 1 H), 5.87 (d,  $J = 7.8\text{ Hz}$ , 1 H), 4.25 (q,  $J = 7.0\text{ Hz}$ , 2 H), 1.28 (t,  $J = 7.0\text{ Hz}$ , 3H); IR (neat) 2091, 1700, 1457  $\text{cm}^{-1}$ .



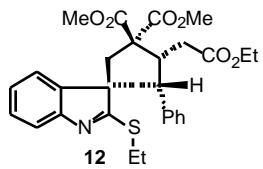
**General procedure for the coupling of vinyl diazoacetates with 3-alkyl-2-thioindoles:**

2-[3-(1-Ethoxycarbonyl-1-phenyl-allyl)-2-ethylsulfanyl-3*H*-indol-3-ylmethyl]-malonic acid dimethyl ester 10. A solution of vinyl diazoacetate 6 (0.030 g, 0.014 mmol) and  $\text{CH}_2\text{Cl}_2$  (0.8 mL) was added over 3h via syringe pump to a solution of thioindole 1 (0.030 g, 0.093 mmol),  $\text{Rh}_2(\text{OAc})_4$  (2 mg, 0.004 mmol) and  $\text{CH}_2\text{Cl}_2$  (1 mL) at rt. Following the completion of the reaction as monitored by TLC the solvent was removed and the residue was purified by flash chromatography to give 46 mg (96%) of indoline 10 as a 1:1 mixture of diastereomers as a pale yellow oil. One of the diastereomers could be separated by chromatography: diastereomer 10a:  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.40-7.24 (m, 5 H),

7.18 (dt,  $J = 7.3, 1.6$  Hz, 1 H), 7.02-6.99 (m, 1 H), 6.92 (t,  $J = 7.7$  Hz, 1 H), 6.53 (d,  $J = 7.9$  Hz, 2 H), 5.99 (d,  $J = 15.9$  Hz, 1 H), 4.20 (q,  $J = 6.8$  Hz, 2 H), 3.76 (d,  $J = 9.9$  Hz, 1 H), 3.65 (s, 3 H), 3.13 (s, 3 H), 3.11-3.07 (m, 1 H), 3.01-2.94 (m, 2 H), 2.72 (dd,  $J = 10.1, 2.5$  Hz, 1 H), 2.48 (dd,  $J = 14.5, 2.6$  Hz, 1 H), 1.29 (t,  $J = 6.8$  Hz, 3 H), 1.20 (t,  $J = 7.8$  Hz, 3 H);  $^{13}\text{C}$  NMR (75 MHz) 182.6, 169.3, 169.0, 165.9, 156.5, 145.2, 136.6, 136.1, 129.1, 128.0, 127.7, 127.6, 124.7, 124.7, 123.7, 118.9, 65.2, 60.6, 56.8, 52.8, 52.3, 47.7, 34.2, 25.1, 14.2, 14.0. Mixture of diastereomers (**10a** + **10b**):  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.43-6.89 (m, 8 H), 6.75 (d,  $J = 7.4$  Hz, 0.5 H), 6.59 (partially obs. dd,  $J = 10.3, 5.4$  Hz, 0.5 H), 6.53 (d,  $J = 7.8$  Hz, 1 H), 5.98 (d,  $J = 15.8$  Hz, 0.5 H), 5.88 (d,  $J = 15.8$  Hz, 0.5 H), 4.20 (q,  $J = 7.2$  Hz, 1 H), 4.07 (q,  $J = 7.2$  Hz, 1 H), 3.82 (d,  $J = 10.0$  Hz, 0.5 H), 3.75 (d,  $J = 9.8$  Hz, 0.5 H), 3.64 (s, 1.5 H), 3.62 (s, 1.5 H), 3.40-3.33 (m, 0.5 H), 3.19-2.93 (m, 2.5 H), 3.12 (s, 1.5 H), 3.07 (s, 1.5 H), 2.72 (dd,  $J = 7.8, 2.3$  Hz, 0.5 H), 2.61-2.55 (m, 1 H), 2.48 (dd,  $J = 12.0, 2.4$  Hz, 0.5 H), 1.43-1.16 (m, 6 H); IR (neat) 1733, 1652, 1507  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{28}\text{H}_{32}\text{O}_6\text{NS} (\text{MH}^+)$  510.1950, found 510.1943.

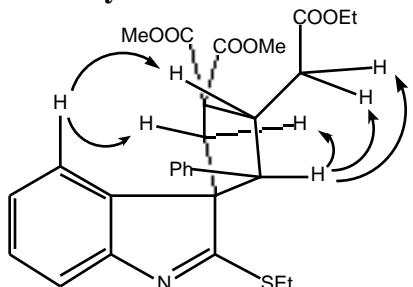


**2-[3-(1-Chloro-3-ethoxycarbonyl-allyl)-2-ethylsulfanyl-3H-indol-3-ylmethyl]-malonic acid dimethyl ester **11**.** Prepared according to the procedure for the formation of **10** using thioindole **1** (0.030 g, 0.093 mmol),  $\text{Rh}_2(\text{OAc})_4$  (2 mg, 0.004 mmol), and vinyl diazo acetate **7** (0.025 g, 0.144 mmol) to provide 43 mg (98%) of **11** as an inseparable 2:1 mixture of diastereomers and as a pale yellow oil. Characterized as a mixture of diastereomers:  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.48 (d,  $J = 7.7$  Hz, 0.66 H), 7.42 (d,  $J = 8.8$  Hz, 0.66 H), 7.34-7.29 (m, 1 H), 7.13-7.08 (m, 1.66 H), 6.83 (dd,  $J = 15.7, 8.8$  Hz, 0.33 H), 6.05-5.89 (m, 1.66 H), 4.69 (d,  $J = 7.3$  Hz, 0.66 H), 4.63 (d,  $J = 8.8$  Hz, 0.33 H), 4.19 (q,  $J = 7.2$  Hz, 0.66 H), 4.04 (q,  $J = 6.9$  Hz, 1.32 H), 3.64 (s, 3 H), 3.38-3.13 (m, 3 H), 3.16 (s, 2 H), 3.14 (s, 1 H), 2.71-2.66 (m, 1 H), 2.55-2.51 (m, 0.33 H), 2.47 (dd,  $J = 14.5, 2.8$  Hz, 0.66), 1.45-1.35 (m, 3 H), 1.27 (t,  $J = 7.3$  Hz, 1 H), 1.15 (t,  $J = 7.1$  Hz, 2 H); IR (neat) 1733, 1652, 1506  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{22}\text{H}_{27}\text{O}_6\text{NCIS} (\text{MH}^+)$  468.1248, found 468.1253.

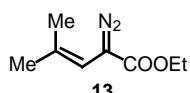


To the solution of **10** (0.020 g, 0.040 mmol) in  $\text{CH}_2\text{Cl}_2$  (0.5 mL) DBU (0.005 mL, 0.033 mmol) and the reaction mixture was stirred at rt for 18 h after which the reaction was quenched by the addition of  $\text{NH}_4\text{Cl}$  (sat., aq.). The aqueous phase was extracted with  $\text{CH}_2\text{Cl}_2$  (10 mL), the organic layer was washed with brine, dried over  $\text{Na}_2\text{SO}_4$  and concentrated. Chromatography (hexanes to 1:4 ethyl acetate:hexanes) afforded 18 mg (90%) of **12** as a pale yellow oil.  $^1\text{H}$  NMR (300 MHz,  $\text{C}_6\text{D}_6$ ) 7.77-7.73 (m, 1 H), 7.29-7.25 (m, 1 H), 7.17-7.10 (m, 1 H), 6.95-6.71 (m, 6 H), 4.55-4.45 (m, 1 H), 4.17 (d,  $J = 13.7$  Hz, 1 H), 3.82-3.65 (m, 2 H), 3.49 (d,  $J = 15.1$  Hz, 1 H), 3.40 (s, 6 H), 3.26-2.99 (m, 2 H), 2.91 (dd,  $J = 16.1, 6.8$  Hz, 1 H), 2.78 (d,  $J = 15.1$  Hz, 1 H), 2.57 (dd,  $J = 16.1, 4.9$  Hz, 1 H), 1.22 (t,  $J = 7.3$  Hz, 3 H), 0.83 (t,  $J = 7.3$  Hz, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{C}_6\text{D}_6$ ) 184.2, 171.9, 171.8, 171.6, 154.4, 142.4, 142.0, 133.7, 133.7, 128.5, 128.0, 127.4, 127.2, 123.8, 123.2, 118.4, 68.0, 60.9, 60.4, 59.6, 52.9, 45.5, 42.8, 34.5, 25.1, 14.3, 14.0; IR (neat) 1739, 1507, 1456  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{28}\text{H}_{32}\text{O}_6\text{NS} (\text{MH}^+)$  510.1950, found 510.1951.

### Summary of NOESY data for 12

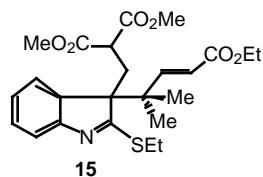


**12**



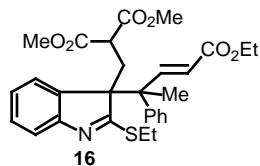
**13**

2-Diazo-4-methyl-pent-3-enoic acid ethyl ester **13**. Prepared according to the procedure used for the formation of **7** using ABSA (1.1 mmol), 4-methyl-pent-3-enoic acid ethyl ester (0.123 g, 0.866 mmol), DMF instead of CH<sub>3</sub>CN (4.5 mL), and DBU (0.16 mL, 1.2 mmol) to provide 56 mg (93%) of vinyl diazoacetate **13** as a yellow oil. The diazoester was used without any further purification. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) 5.39 (br. s, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 1.84 (s, 3H), 1.65 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H); IR (neat) 2081, 1704, 1456 cm<sup>-1</sup>.



**15**

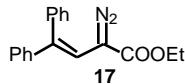
2-[3-[3-Ethoxycarbonyl-1,1-dimethyl-allyl-2-ethylsulfanyl-3H-indol-3-ylmethyl]-malonic acid dimethyl ester **15**. Prepared according to the general procedure described for the synthesis **10** using vinyl diazoacetate **13** (0.027 g, 0.16 mmol), thioindole **1** (0.030 g, 0.093 mmol), and Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mg, 0.004 mmol) to give 37 mg (85%) of indoline **15** as a colorless oil. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) 7.39 (d, *J* = 7.8 Hz, 1 H), 7.26-7.20 (m, 2 H), 7.17 (partially obscured d, *J* = 16.3 Hz, 1 H), 7.08-6.97 (m, 2 H), 5.73 (d, *J* = 15.5 Hz, 1 H), 4.18 (q, *J* = 7.4 Hz, 2 H), 3.60 (s, 3 H), 3.25 (partially obscured sep, *J* = 7.3 Hz, 2 H), 3.17 (s, 3 H), 2.81 (dd, *J* = 14.1, 9.3 Hz, 1 H), 2.51 (d, *J* = 14.2 Hz, 1 H), 2.43 (d, *J* = 9.3 Hz, 1 H), 1.39 (t, *J* = 7.2 Hz, 3 H), 1.29 (t, *J* = 7.0 Hz, 3 H), 1.11 (s, 3 H), 0.99 (s, 3 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 183.2, 169.5, 169.2, 166.5, 155.7, 153.1, 137.5, 128.7, 125.8, 123.1, 120.8, 118.7, 68.5, 60.4, 52.7, 52.4, 47.7, 41.0, 30.8, 26.2, 22.6, 22.5, 14.2, 14.0; IR (neat) 1739, 1646, 1506 cm<sup>-1</sup>; HRMS calc'd for C<sub>24</sub>H<sub>32</sub>O<sub>6</sub>NS (MH<sup>+</sup>) 462.1950, found 462.1954.



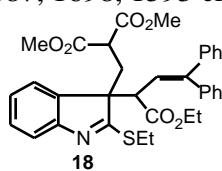
**16**

2-[3-(1-Ethoxycarbonyl-1-methyl-1-phenyl-allyl)-2-ethylsulfanyl-3H-indol-3-ylmethyl]-malonic acid dimethyl ester **16**. Prepared according to the procedure for the formation of **10** using thioindole **1** (0.030 g, 0.093 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mg, 0.004 mmol), and vinyl diazo acetate **14** (0.032 g, 0.014 mmol) to provide 47 mg (96%) of **16** as a 1.5:1 mixture of inseparable diastereomers as a pale yellow oil. Characterized as a mixture of

diastereomers:  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 8.01 (d,  $J = 15.5$  Hz, 0.6 H), 7.57 (d,  $J = 15.5$  Hz, 0.4 H), 7.29-6.86 (m, 9 H), 6.60-6.29 (m, 1 H), 5.84 (d,  $J = 15.6$  Hz, 0.4 H), 5.70 (d,  $J = 15.5$  Hz, 0.6 H), 4.24-4.15 (m, 2 H), 3.63 (s, 1.8 H), 3.62 (s, 1.2 H), 3.28-2.97 (m, 2 H), 3.12 (s, 3 H), 2.78 (dd,  $J = 14.0, 2.4$  Hz, 0.6 H), 2.69 (dd,  $J = 14.0, 2.3$  Hz, 0.4 H), 2.44 (d,  $J = 9.1$  Hz, 1 H), 1.74 (s, 1.2 H), 1.49 (s, 1.8 H), 1.36-1.17 (m, 6 H); IR (neat) 1754, 1643, 1508  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{29}\text{H}_{34}\text{O}_6\text{NS} (\text{MH}^+)$  524.2107, found 524.2112.

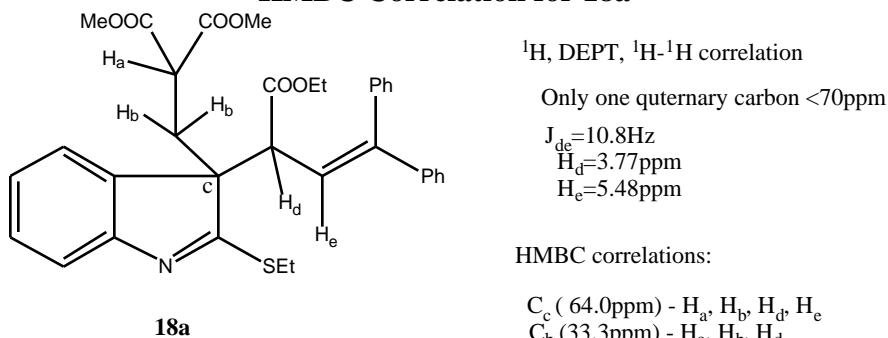


**2-Diazo-4,4-diphenyl-but-3-enoic acid ethyl ester 17.** Prepared according to the procedure used for the formation of **7** using ABSA (0.055 g, 0.23 mmol), 4,4-diphenyl-but-2-enoic acid ethyl ester (0.055 mg, 0.23 mmol),  $\text{CH}_3\text{CN}$  instead of DMF (1 mL), and DBU (0.40 mL, 0.27 mmol) to provide 56 mg (93%) of vinyl diazoacetate **17** as a yellow oil:  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.43-7.21 (m, 10 H), 6.30 (s, 1 H), 4.28 (q,  $J = 6.9$  Hz, 2 H), 1.30 (t,  $J = 7.1$  Hz, 3 H); IR (neat) 2087, 1698, 1593  $\text{cm}^{-1}$ .



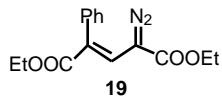
**2-[3-(1-Ethoxycarbonyl-3,3-diphenyl-allyl)-2-ethylsulfanyl-3H-indol-3-ylmethyl]-malonic acid dimethyl ester 18.** Prepared according to the procedure for the formation of **10** using thioindole **1** (0.030 g, 0.093 mmol),  $\text{Rh}_2(\text{OAc})_4$  (2 mg, 0.004 mmol), and vinyl diazo acetate **17** (0.037 g, 0.13 mmol) to provide 20 mg (36%) of **18a** (diastereomer 1) and 19 mg (35%) of **18b** (diastereomer 2) as pale yellow oils. **18a:**  $^1\text{H}$  NMR (300MHz,  $\text{CDCl}_3$ ) 7.51 (d,  $J = 8.0$  Hz, 1 H), 7.39-7.09 (m, 11 H), 6.93-6.92 (m, 2 H), 5.48 (d,  $J = 10.8$  Hz, 1 H), 4.17 (q,  $J = 7.0$  Hz, 2 H), 3.77 (d,  $J = 10.8$  Hz, 1 H), 3.62 (s, 3 H), 3.15 (s, 3 H), 3.22-3.15 (m, 2 H), 2.78 (dd,  $J = 14.3, 9.7$  Hz, 1 H), 2.63 (d,  $J = 9.7$  Hz, 1 H), 2.51 (d,  $J = 14.2$  Hz, 1 H), 1.35 (t,  $J = 7.1$  Hz, 3 H), 1.24 (t,  $J = 7.0$  Hz, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 183.0 (C), 170.6 (C), 169.1 (C), 168.9 (C), 155.9 (C), 146.5 (C), 142.0 (C), 139.0 (C), 136.4 (C), 130.0 (CH), 129.0 (CH), 128.1 (CH), 128.0 (CH), 127.7 (CH), 127.6 (CH), 127.5 (CH), 125.3 (CH), 123.7 (CH), 120.8 (CH), 118.5 (CH), 64.0 (C), 61.1 ( $\text{CH}_2$ ), 52.6 ( $\text{CH}_3$ ), 52.3 (CH), 52.2 ( $\text{CH}_3$ ), 47.4 (CH), 33.3 ( $\text{CH}_2$ ), 25.7 (CH<sub>2</sub>), 14.1 ( $\text{CH}_3$ ), 13.8 ( $\text{CH}_3$ ); IR (neat) 1750, 1506, 1456  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{34}\text{H}_{36}\text{O}_6\text{NS} (\text{MH}^+)$  586.2263, found 586.2275.

### HMBC Correlation for 18a

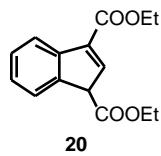


**18b:**  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.44-7.11 (m, 13 H), 7.04 (t,  $J = 7.4$  Hz, 1 H), 6.21 (d,  $J = 11.2$  Hz, 1 H), 3.94-3.86 (m, 2 H), 3.70 (d,  $J = 11.1$  Hz, 1 H), 3.60 (s, 3 H), 3.27-3.15 (m, 2 H), 3.15 (s, 3 H), 2.91 (dd,  $J = 14.7, 9.8$  Hz, 1 H), 2.54 (dd,  $J = 9.8, 2.5$  Hz, 1 H), 2.26 (dd,  $J = 14.7, 2.5$  Hz, 1 H), 1.37 (t,  $J = 7.3$  Hz, 3 H), 0.99 (t,  $J = 7.1$  Hz, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 183.2 (C), 169.7 (C), 169.3 (C), 168.9 (C), 155.5 (C), 147.3 (C), 141.7 (C), 138.6 (C), 137.4 (C), 129.9 (CH), 128.7 (CH), 128.4 (CH), 128.2 (CH), 127.8

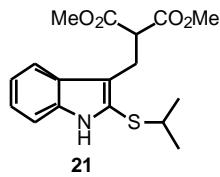
(CH), 127.6 (CH), 127.5 (CH), 124.3 (CH), 123.7 (CH), 120.9 (CH), 118.7 (CH), 63.8 (C), 60.8 (CH<sub>2</sub>), 52.7 (CH<sub>3</sub>), 52.5 (CH), 52.3 (CH<sub>3</sub>), 47.1 (CH), 33.8 (CH<sub>2</sub>), 25.5 (CH<sub>2</sub>), 14.1 (CH<sub>3</sub>), 13.8 (CH<sub>3</sub>); IR (neat) 1733, 1512, 1456 cm<sup>-1</sup>; HRMS calc'd for C<sub>34</sub>H<sub>36</sub>O<sub>6</sub>NS (MH<sup>+</sup>) 586.2263, found 586.2261.



**4-Diazo-2-phenyl-pent-2-enedioic acid diethyl ester 19:** Et<sub>3</sub>N (0.30 mL, 2.1 mmol) was added to a solution of ABSA (0.12 g, 0.50 mmol), 2-phenyl-pent-2-enedioic acid diethyl ester (0.105 g, 0.429 mmol) and CH<sub>3</sub>CN (2 mL). After stirring for 24 h, the resulting yellow solution was diluted with a mixture of ethyl acetate:hexanes (1:20, 20 mL) and passed through a short silica gel plug (eluted with 1:20 ethyl acetate:hexanes). The filtrate was concentrated to give 106 mg (91%) of diazoacetate **19** as a pale yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 7.38-7.17 (m, 6 H), 4.26 (q, J = 7.3 Hz, 2 H), 4.20 (q, J = 7.2 Hz, 2 H), 1.27 (t, J = 7.3 Hz, 3 H), 1.24 (t, J = 7.0 Hz, 3 H); IR (neat) 2095, 1700, 1623 cm<sup>-1</sup>.

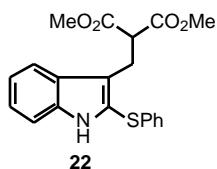


**1H-Indene-1,3-dicarboxylic acid diethyl ester 20.** Rh<sub>2</sub>(OAc)<sub>4</sub> (1 mg, 0.002 mmol) was added to a solution of vinyl diazoacetate **19** (0.030 g, 0.11 mmol) and CH<sub>2</sub>Cl<sub>2</sub> (2 ml). After stirring at rt for 24 h, the reaction mixture was concentrated. Flash chromatography (hexanes to 1:4 ethyl acetate:hexanes) gave 24 mg (89%) of indene **20** as a colorless oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 7.99 (d, J = 7.7 Hz, 1 H), 7.64 (d, J = 7.5 Hz, 1 H), 7.40-7.24 (m, 3 H), 4.51 (br. s, 1 H), 4.36 (q, J = 7.4 Hz, 2 H), 4.23-4.16 (m, 2 H), 1.40 (t, J = 6.9 Hz, 3 H), 1.27 (t, J = 7.2 Hz, 3 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 168.7, 163.7, 141.5, 140.5, 140.1, 137.4, 127.9, 126.4, 124.3, 122.7, 61.7, 60.7, 54.6, 14.3, 14.1; IR (neat) 1736, 1596, 1572 cm<sup>-1</sup>; HRMS calc'd for C<sub>15</sub>H<sub>17</sub>O<sub>4</sub> (MH<sup>+</sup>) 261.1127, found 261.1127.

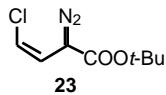


**2-Isopropylsulfanyl-3-[isopropylsulfanyl-(trimethyl-silanyl)-methyl]-1H-indole:** A solution of (2-isocyano-phenylethynyl)-trimethyl-silane isonitrile (0.200 g, 1.00 mmol), 2-propanethiol (0.48 mL, 5.2 mmol), AIBN (0.025 g, 0.16 mmol), and benzene (25 mL) was heated at reflux for 4h and then cooled to rt. After removal of the solvent the resulting residue was purified by flash chromatography (toluene to 3% EtOAc-toluene) to yield 198 mg (57%) of the corresponding bis-isopropyl thioindole as a white solid. m.p. 110-111°C <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 8.08 (d, J = 8.2 Hz, 1 H), 7.80 (s, 1 H), 7.26 (d, J = 9.9 Hz, 1 H), 7.16 (t, J = 6.8 Hz, 1 H), 7.04 (t, J = 7.6, 1 H), 3.99 (s, 1 H), 3.22 (sep, J = 6.7 Hz, 1 H), 2.56 (sep, J = 6.7 Hz, 1 H), 1.32 (d, J = 6.2 Hz, 3 H), 1.27 (d, J = 7.0 Hz, 3 H), 1.25 (d, J = 7.0 Hz, 3 H), 1.04 (d, J = 6.8 Hz, 3 H), 0.07 (s, 9 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 137.0, 126.9, 124.4, 122.7, 122.4, 121.4, 118.8, 110.3, 40.4, 34.4, 29.3, 23.7, 23.6, 23.5, 22.8, -1.4; IR (KBr) 3360, 1652, 1558 cm<sup>-1</sup>; HRMS calc'd for C<sub>18</sub>H<sub>29</sub>NSiS<sub>2</sub> (MH<sup>+</sup>) 351.1511, found 351.1514.

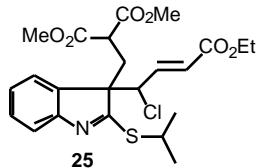
2-(2-Isopropylsulfanyl-1*H*-indol-3-ylmethyl)-malonic acid dimethyl ester **21**. A solution of bis-thioindole (0.110 g, 0.313 mmol), dimethylmalonate (0.36 mL, 3.15 mmol), KF (0.020 g, 0.34 mmol), 18-crown-6 (0.091 g, 0.34 mmol), and acetonitrile (2 mL) was heated at reflux for 8h. Removal of the solvent and flash chromatography (10% EtOAc:hexanes) provided 80 mg (76%) of **21** as a pale yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 8.11 (br. s, 1 H), 7.54 (d, *J* = 8.8 Hz, 1 H), 7.26 (d, *J* = 7.8 Hz, 1 H), 7.17 (t, *J* = 6.8 Hz, 1 H), 7.07 (dd, *J* = 8.4, 6.9 Hz, 1 H), 3.83 (t, *J* = 7.6 Hz, 1 H), 3.63 (s, 6 H), 3.49 (d, *J* = 7.8 Hz, 2 H), 3.20 (sep, *J* = 6.6 Hz, 1 H), 1.24 (d, *J* = 6.8 Hz, 6 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 169.6, 136.4, 127.5, 125.9, 123.0, 119.7, 119.0, 118.1, 110.6, 52.6, 52.5, 40.5, 24.5, 23.5; IR (neat) 3382, 1737, 1439 cm<sup>-1</sup>; HRMS calc'd for C<sub>17</sub>H<sub>21</sub>O<sub>4</sub>NS (M<sup>+</sup>) 335.1191, found 335.1183.



2-(2-Phenylsulfanyl-1*H*-indol-3-ylmethyl)-malonic acid dimethyl ester **22**. Prepared according to the procedure used for the preparation of **21** using 2-phenylsulfanyl-3-[phenylsulfanyl-(trimethyl-silanyl)-methyl]-1*H*-indole (0.120 g, 0.286 mmol), dimethyl malonate (0.330 mL, 2.89 mmol), KF (0.018 g, 0.31 mmol), 18-C-6 (0.083 g, 0.31 mmol), and acetonitrile (7 mL) to give 85 mg (80%) of thioindole **22** as a colorless oil. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) 8.24 (br s, 1 H), 7.60 (d, *J* = 7.7 Hz, 1 H), 7.27-7.02 (m, 8 H), 3.79 (t, *J* = 7.8 Hz, 1 H), 3.60 (s, 6 H), 3.51 (d, *J* = 7.8 Hz, 2 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 169.4, 136.9, 136.8, 129.1, 127.3, 126.8, 125.9, 123.4, 122.9, 119.9, 119.2, 118.8, 111.0, 52.5, 24.3; IR (neat) 3371, 1733, 1581 cm<sup>-1</sup>; HRMS calc'd for C<sub>20</sub>H<sub>19</sub>O<sub>4</sub>NS (M<sup>+</sup>) 369.1035, found 369.1037.

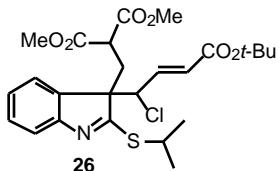


4-Chloro-2-diazo-but-3-enoic acid *tert*-butyl ester **23**. Prepared according to the procedure used for the formation of **7** using ABSA (0.333 g, 1.39 mmol), 4-chloro-but-2-enoic acid *tert*-butyl ester (0.222 g, 1.26 mmol), CH<sub>3</sub>CN instead of DMF (6.3 mL), and DBU (0.226 mL, 1.51 mmol) to provide 230 mg (90%) of vinyl diazoacetate **23** as a yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 6.01 (d, *J* = 7.8 Hz, 1 H), 5.90 (d, *J* = 7.4 Hz, 1 H), 1.47 (s, 9 H); IR (neat) 2991, 1700, 1457 cm<sup>-1</sup>.

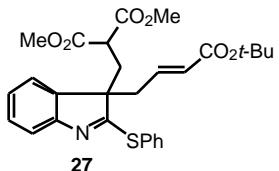


2-[3-(1-Chloro-3-ethoxycarbonyl-allyl)-2-isopropylsulfanyl-3*H*-indol-3-ylmethyl]-malonic acid dimethyl ester **25**. Prepared according to the procedure for the formation of **10** using thioindole **21** (0.030 g, 0.090 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mg, 0.04 mmol), and vinyl diazo acetate **7** (0.0250 g, 0.114 mmol) to provide 35 mg (81%) of **25** as a pale yellow oil. Characterized as a 3.4:1 mixture of diastereomers; major diastereomer crystallized out of the mixture: <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) 7.50-7.25 (m, 3 H), 7.13-7.08 (m, 1 H), 6.86 (dd, *J* = 15.6, 8.8 Hz, 0.23 H), 6.06-5.89 (m, 1.77 H), 4.67 (dd, *J* = 6.0, 1.7 Hz, 0.77 H), 4.61 (d, *J* = 8.8 Hz, 0.23 H), 4.24-4.01 (m, 3 H), 3.65 (s, 3 H), 3.27 (dd, *J* = 14.3, 9.9 Hz, 0.77 H), 3.16 (s, 2.3 H) 3.14 (s, 0.7 H), 2.73-2.68 (m, 1 H), 2.51-2.41 (m, 1 H), 1.51-1.13 (m, 9 H); IR (neat) 1731, 1510, 1439 cm<sup>-1</sup>; HRMS calc'd for C<sub>23</sub>H<sub>29</sub>O<sub>6</sub>NCIS (MH<sup>+</sup>) 482.1404, found 482.1405.

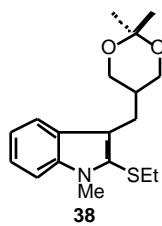
**25a** (major diastereomer): mp 99–101°C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.48 (d, *J* = 8.3 Hz, 1 H), 7.42 (d, *J* = 7.8 Hz, 1 H), 7.32 (t, *J* = 7.8 Hz, 1 H), 7.11 (t, *J* = 7.3 Hz, 1 H) 6.01–5.89 (m, 2 H), 4.67 (dd, *J* = 6.4, 2.0 Hz, 1 H), 4.24–4.01 (m, 2.23 H), 3.65 (s, 3 H), 3.28 (dd, *J* = 14.3, 10.1 Hz, 1 H), 3.16 (s, 3 H), 2.71 (dd, *J* = 10.2, 2.9 Hz, 1 H), 2.44 (dd, *J* = 14.3, 2.9 Hz, 1 H), 1.44 (d, *J* = 6.8 Hz, 3 H), 1.39 (d, *J* = 6.8 Hz, 3 H), 1.15 (t, *J* = 7.1 Hz, 3 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 179.7, 169.0, 168.8, 165.0, 156.1, 140.0, 134.8, 129.6, 125.5, 125.3, 124.1, 119.1, 65.5, 65.2, 60.6, 52.8, 52.3, 47.3, 37.0, 33.7, 23.0, 22.6, 14.0. (Also see X-ray structure on p. S10)



2-[3-(3-*tert*-Butoxycarbonyl-1-chloro-allyl)-2-isopropylsulfanyl-3*H*-indol-3-ylmethyl]-malonic acid dimethyl ester **26**. Prepared according to the procedure for the formation of **10** using thioindole **21** (0.015 g, 0.045 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (1 mg, 0.002 mmol), and vinyl diazo acetate **23** to provide 18 mg (79%) of **26** as an inseparable 3.6:1 mixture of diastereomers and as a pale yellow oil. Characterized as a mixture of diastereomers: <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.49–7.41 (m, 2 H), 7.34–7.29 (m, 1 H), 7.14–7.07 (m, 1 H), 6.79 (dd, *J* = 15.1, 8.8 Hz, 0.23 H), 5.97 (d, *J* = 15.1 Hz, 0.23 H), 5.89–5.77 (m, 1.77 H), 4.63 (d, *J* = 6.8, 1.5 Hz, 0.77 H), 4.58 (d, *J* = 8.8 Hz, 0.23 H), 4.17–4.04 (m, 1 H), 3.64 (s, 3 H), 3.31–3.17 (m, 1 H), 3.15 (s, 2.31 H), 3.13 (s, 0.69 H), 2.74–2.67 (m, 1 H), 2.48–2.40 (m, 1 H), 1.51–1.32 (m, 15 H); IR (neat) 1737, 1656, 1509 cm<sup>−1</sup>; HRMS calc'd for C<sub>25</sub>H<sub>33</sub>O<sub>6</sub>NCIS (MH<sup>+</sup>) 509.1639, found 509.1643.

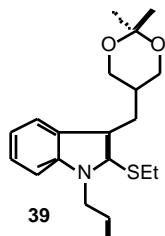


2-[3-(3-*tert*-Butoxycarbonyl-allyl)-2-phenylsulfanyl-3*H*-indol-3-ylmethyl]-malonic acid dimethyl ester **27**. Prepared according to the procedure for the formation of **10** using thioindole **22** (0.029 g, 0.079 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mg, 0.004 mmol), and vinyl diazo acetate **24** to provide 31 mg (80%) of **27** as a pale yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.64–7.61 (m, 2 H), 7.43–7.35 (m, 4 H), 7.25–7.06 (m, 3 H), 6.20 (dt, *J* = 14.2, 8.2 Hz, 1 H), 5.75 (d, *J* = 15.7 Hz, 1 H), 3.66 (s, 3 H), 3.18 (s, 3 H), 2.87–2.56 (m, 5 H), 1.38 (s, 9 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 182.1, 169.2, 169.0, 165.0, 155.2, 139.8, 138.2, 134.4, 129.3, 128.7, 127.4, 127.0, 124.3, 123.0, 119.8, 80.3, 61.7, 52.8, 52.4, 47.4, 41.0, 35.2, 28.0; IR (neat) 1739, 1652, 1516 cm<sup>−1</sup>; HRMS calc'd for C<sub>28</sub>H<sub>32</sub>O<sub>6</sub>NS (MH<sup>+</sup>) 510.1950, found 510.1956.

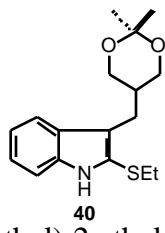


3-(2,2-Dimethyl-[1,3]dioxan-5-ylmethyl)-2-ethylsulfanyl-1-methyl-1*H*indole **38**. KOH (0.1 g, 1.35 mmol) and MeI (0.1 mL, 1.6 mmol) were added to a solution of indole **40** (0.057 g, 0.19 mmol) and DMSO (2 mL). After stirring at rt for 24 h, the reaction mixture was quenched with water (10 mL). The resulting mixture was extracted with hexanes and

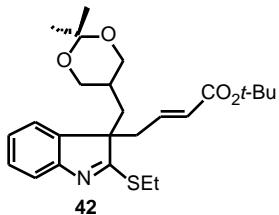
ethyl acetate (1:1, 20 mL). The extract was washed with brine (10 mL), dried ( $\text{Na}_2\text{SO}_4$ ) and concentrated. Purification by flash chromatography (hexanes to 8% ethyl acetate:hexanes) yielded 51 mg (85%) of indole **38** as a colorless oil.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.58 (d,  $J = 8.0$  Hz, 1 H), 7.29-7.21 (m, 2 H), 7.10 (t,  $J = 7.4$  Hz, 1 H), 3.84 (partially obs. dd,  $J = 11.7, 4.5$  Hz, 2 H), 3.82 (s, 3 H), 3.70 (dd,  $J = 11.7, 8.3$  Hz, 2 H), 2.89 (d,  $J = 8.0$  Hz, 2 H), 2.66 (q,  $J = 7.5$  Hz, 2 H), 2.23-2.16 (m, 1 H), 1.48 (s, 3 H), 1.38 (s, 3 H), 1.18 (t,  $J = 7.4$  Hz, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 137.7, 128.3, 126.9, 122.7, 119.3, 119.3, 119.2, 109.5, 97.8, 64.7, 35.7, 31.0, 30.1, 26.2, 24.8, 21.9, 14.7; IR (neat) 3053, 2934, 2860, 1457  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{18}\text{H}_{25}\text{O}_2\text{NS} (\text{M}^+)$  319.1606, found 319.1600.



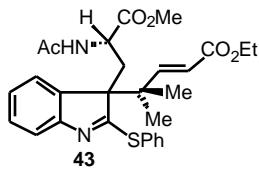
**3-(2,2-Dimethyl-[1,3]dioxan-5-ylmethyl)-2-ethylsulfanyl-1*H*indole **39**.** Prepared according to the procedure for **38** using KOH (0.100 g, 1.35 mmol), DMSO (2 mL), Allyl bromide (0.1 mL, 1.16 mmol) instead of MeI, and indole **40** (0.060 g, 0.20 mmol). Isolated 55 mg (81%) of **39** as a pale yellow oil.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.58 (d,  $J = 7.8$  Hz, 1 H), 7.26-7.17 (m, 2 H), 7.09 (td,  $J = 7.5, 1.5$  Hz 1 H), 5.99-5.86 (m, 1H), 5.09 (dd,  $J = 10.5, 1.0$  Hz, 1.3 H), 4.96-4.93 (m, 2H), 4.81 (dd,  $J = 17.1, 1.5$  Hz, 1 H), 3.82 (dd,  $J = 11.9, 4.6$  Hz, 2 H), 3.70 (dd,  $J = 11.8, 8.8$  Hz, 2 H), 2.89 (d,  $J = 7.3$  Hz, 2 H), 2.66 (q,  $J = 7.3$  Hz, 2 H), 2.29-2.15 (m, 1 H), 1.47 (s, 3 H), 1.38 (s, 3 H), 1.17 (t,  $J = 7.3$  Hz, 3 H). ( $^{13}\text{C}$ , 75 MHz) 137.5, 134.0, 128.2, 127.4, 123.0, 120.0, 119.6, 119.4, 116.3, 110.4, 108.5, 98.1, 65.0, 46.1, 35.8, 31.4, 26.6, 25.1, 22.0, 14.8; IR (neat) 2988, 2926, 2856, 1717  $\text{cm}^{-1}$ .



**3-(2,2-Dimethyl-[1,3]dioxan-5-ylmethyl)-2-ethylsulfanyl-1*H*indole **40**.**  $\text{LiAlH}_4$  (0.100 g, 2.64 mmol) was added in portions to a solution of malonate **1** (0.100 g, 0.31 mmol) and THF (4 mL). The reaction mixture was stirred for 5 h. Water (100  $\mu\text{L}$ ) was added, followed in 15 min by 15% NaOH (100  $\mu\text{L}$ ) and then, after an additional 15 min, another portion of water (100  $\mu\text{L}$ ). The reaction mixture was stirred for 2 h and then filtered through celite. The residue was dissolved in methylene chloride (2 mL), 2,2-dimethoxypropane (0.5 mL, 4.1 mmol) and TsOH (2 mg, 0.01 mmol) were added and the reaction mixture was kept at rt for 10 h, then washed with saturated  $\text{NaHCO}_3$  (2 mL), dried over  $\text{Na}_2\text{SO}_4$  and concentrated. The residue was purified by flash chromatography (hexanes to 10% EtOAc-hexanes) to yield 57 mg (60%) of acetonide **40** as a pale yellow oil.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) 7.99 (br s, 1 H), 7.54 (d,  $J = 8.5$  Hz, 1 H), 7.28 (d,  $J = 7.2$  Hz, 1 H), 7.18 (t,  $J = 7.6$  Hz, 1 H), 7.09 (t,  $J = 7.8$  Hz, 1 H), 3.83 (dd,  $J = 11.5, 4.3$  Hz, 2 H), 3.69 (dd,  $J = 11.6, 8.6$  Hz, 2 H), 2.82 (d,  $J = 7.4$  Hz, 2 H), 2.75 (q,  $J = 7.3$  Hz, 2 H), 2.24-2.16 (m, 1 H), 1.47 (s, 3 H), 1.38 (s, 3 H), 1.22 (t,  $J = 7.3$  Hz, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 136.4, 128.0, 125.5, 122.9, 119.7, 119.1, 119.1, 110.6, 97.8, 64.7, 35.4, 30.9, 26.3, 24.2, 21.8, 15.4; IR (neat) 3322, 1722, 1614  $\text{cm}^{-1}$ ; HRMS calc'd for  $\text{C}_{17}\text{H}_{23}\text{O}_2\text{NS} (\text{M}^+)$  305.1450, found 305.1458.



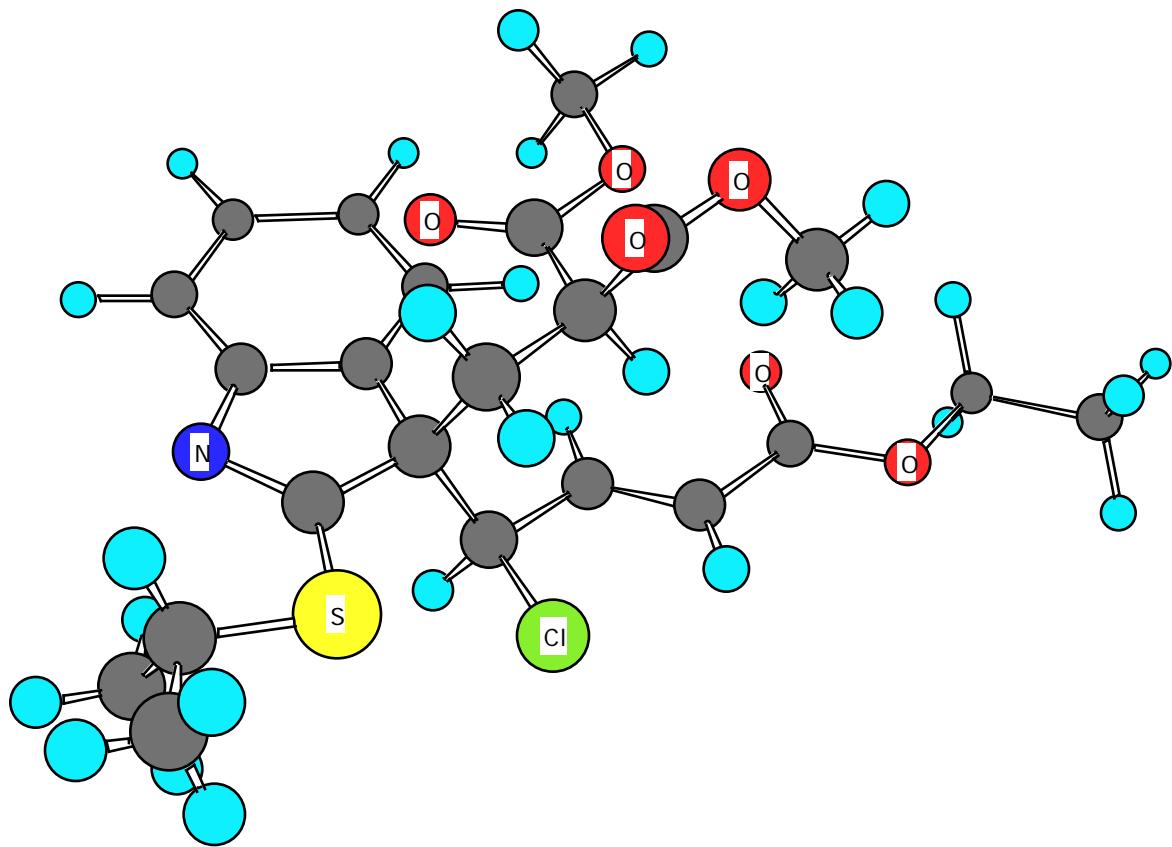
4-[3-(2,2-Dimethyl-[1,3]dioxan-5-ylmethyl)-2-ethylsulfanyl-3*H*-indol-3-yl]-but-2-enoic acid *tert*-butyl ester **42**. Prepared according to the procedure for the formation of **10** using thioindole **40** (0.030 g, 0.098 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mg, 0.004 mmol), and vinyl diazo acetate **2** to provide 33 mg (75%) of **42** as a pale yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 7.43 (d, *J* = 7.9 Hz, 1 H), 7.27 (t, *J* = 7.4 Hz, 1 H), 7.15 (d, *J* = 6.8 Hz, 1 H), 7.08 (t, *J* = 7.4 Hz, 1 H), 6.21 (dt, *J* = 15.7, 7.6 Hz, 1 H) 5.63 (d, *J* = 15.5 Hz, 1 H), 3.64 (dd, *J* = 11.3, 4.5 Hz, 1 H), 3.47 (dd, *J* = 11.1, 8.9 Hz, 1 H), 3.35-3.05 (m, 3 H), 2.97 (dd, *J* = 11.7, 5.0 Hz, 1 H), 2.63 (dd, *J* = 14.3, 7.1 Hz, 1 H), 2.42 (dd, *J* = 14.3, 7.7 Hz, 1 H), 1.88 (dd, *J* = 14.4, 7.1 Hz, 1 H), 1.67 (dd, *J* = 14.2, 4.0 Hz, 1 H), 1.54-1.37 (m, 4 H), 1.37 (s, 9 H), 1.30 (s, 3 H), 1.22 (s, 3 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 184.4, 165.1, 155.1, 140.4, 128.7, 126.6, 124.2, 121.7, 119.2, 97.4, 80.2, 65.0, 64.9, 61.7, 49.8, 41.8, 36.5, 30.7, 28.0, 26.5, 25.0, 20.9, 14.2; IR (neat) 1695, 1652, 1506 cm<sup>-1</sup>; HRMS calc'd for C<sub>25</sub>H<sub>36</sub>O<sub>4</sub>NS (MH<sup>+</sup>) 446.2365, found 446.2357.



4-[3-(2-Acetylaminocarbonyl-2-methoxycarbonyl-ethyl)-2-phenylsulfanyl-3*H*-indol-3-yl]-4-methyl-pent-2-enoic acid ethyl ester **43**. Prepared according to the procedure for the formation of **10** using thioindole **41** (0.040 g, 0.11 mmol), Rh<sub>2</sub>(OAc)<sub>4</sub> (2 mg, 0.004 mmol), and vinyl diazo acetate **13** (0.030 g, 0.18 mmol) to provide 25 mg (46%) of **43a** (major diastereomer) and 20 mg (36%) of **43b** (minor diastereomer) as pale yellow oils. **43a**: [α]<sub>D</sub><sup>26.5</sup> = -60.9 (c = 0.009, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 7.71-7.67 (m, 2 H), 7.46-7.43 (m, 3 H), 7.33 (d, *J* = 7.3 Hz, 1 H), 7.28-7.22 (m, 2 H), 7.17 (d, *J* = 9.4 Hz, 1 H), 7.10 (t, *J* = 7.3 Hz, 1 H), 5.81 (d, *J* = 16.0 Hz, 1 H), 5.59 (d, *J* = 8.9 Hz, 1 H), 4.23 (q, *J* = 7.0 Hz, 2 H), 4.11-3.96 (m, 1 H), 3.49 (s, 3 H), 2.69 (dd, *J* = 14.7, 5.1 Hz, 1 H), 2.39 (dd, *J* = 14.1, 9.3 Hz, 1 H), 1.64 (s, 3 H), 1.31 (t, *J* = 7.1 Hz, 3 H), 1.15 (s, 3 H), 1.09 (s, 3 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 181.9, 172.5, 168.9, 166.5, 155.5, 152.8, 137.4, 134.2, 129.4, 129.3, 128.8, 128.1, 124.8, 124.0, 121.2, 119.9, 67.7, 60.6, 52.5, 49.7, 41.4, 33.6, 22.8, 22.6, 22.2, 14.3; IR (neat) 3292, 1717, 1653, 1512 cm<sup>-1</sup>; HRMS calc'd for C<sub>28</sub>H<sub>33</sub>O<sub>5</sub>N<sub>2</sub>S (MH<sup>+</sup>) 509.2110, found 509.2102.

**43b**: [α]<sub>D</sub><sup>28.7</sup> = +71.7 (c = 0.008, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) 7.70-7.69 (m, 2 H), 7.47-7.40 (m, 3 H), 7.35 (d, *J* = 7.5 Hz, 1 H), 7.28-7.20 (m, 3 H), 7.09 (t, *J* = 7.5 Hz, 1 H), 5.80 (d, *J* = 15.4 Hz, 1 H), 4.84 (d, *J* = 7.3 Hz, 1 H), 4.50-4.42 (m, 1 H), 4.23 (q, *J* = 7.4 Hz, 2 H), 3.62 (s, 3 H), 2.67 (dd, *J* = 14.2, 4.4 Hz, 1 H), 2.52 (dd, *J* = 14.2, 9.4 Hz, 1 H), 1.40 (s, 3 H), 1.31 (t, *J* = 7.1 Hz, 3 H), 1.22 (s, 3 H), 1.03 (s, 3 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 182.3, 172.1, 169.1, 166.5, 155.5, 152.9, 139.8, 134.6, 129.4, 129.3, 128.7, 128.2, 123.9, 123.7, 121.2, 120.1, 67.4, 60.6, 52.5, 50.0, 41.6, 33.3, 22.5, 22.5, 14.3; IR (neat) 3308, 1741, 1713, 1669, 1512; HRMS calc'd for (MH<sup>+</sup>) C<sub>28</sub>H<sub>33</sub>O<sub>5</sub>N<sub>2</sub>S 509.2110, found 509.2109.

STRUCTURAL REPORT FOR Indoline 25.



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##### cif submission form for molecular structure report
##### (acta cryst. c) #####
##### version: 2.0.2
##### (6 july 1998) #####
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# this is an electronic "form" for submitting a structural
paper to acta cryst.
# section c as a crystallographic information file. full
details of the format
# of such files are given in the paper "the crystallographic
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# (cif): a new standard archive file for crystallography" by
s. r. hall, f. h.
# allen and i. d. brown [acta cryst. (1991), a47, 655-685].
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# the current version of the core cif dictionary is
obtainable from
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number is 2.0.1.
# a few data names below appear in the 1998 notes for authors
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# are indicated by the comment 'not in version 2.0.1'.
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# lines should not exceed 80 characters in length.
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 C35 0.0240(10) 0.0314(11) 0.0296(10) -0.0020(9) 0.0098(8) 0.0009(8)  
 C32 0.0257(10) 0.0274(10) 0.0266(10) -0.0017(8) 0.0093(8) 0.0014(8)  
 C33 0.0258(10) 0.0347(11) 0.0294(11) 0.0012(9) 0.0058(8) 0.0019(9)  
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 C34 0.0273(11) 0.0538(14) 0.0555(14) 0.0020(11) 0.0193(10) 0.0015(10)  
 C36 0.0783(18) 0.0329(13) 0.0474(14) 0.0112(11) 0.0173(13) 0.0071(12)  
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0.0056(10)
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0.0094(11)
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0.0177(12)
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0.0214(14)
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0.0047(8)

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;
All esds (except the esd in the dihedral angle between two
l.s. planes)
are estimated using the full covariance matrix. The cell
esds are taken
into account individually in the estimation of esds in
distances, angles
and torsion angles; correlations between esds in cell
parameters are only
used when they are defined by crystal symmetry. An
approximate (isotropic)
treatment of cell esds is used for estimating esds involving
l.s. planes.
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