Supporting Information

***N*-Methoxy-3-methyl-2-butenamide (6b):** 1.9 g (yield 46%) from 3,3-dimethylacryloyl chloride (4 g); colorless oil; IR ($CHCl_3$) 3394 (NH), 1655 (CON) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.34 (1H, br s), 5.65 (1H, br s), 3.76 (3H, s), 2.18 and 1.88 (each 3H, br s); HRMS (EI, *m/z*) calcd for $C_6H_{11}NO_2$ (M^+) 129.0789, found 129.0797.

(*E*)-3-Phenyl-*N*-phenylmethoxy-2-propenamide (6c): 2.5 g (yield 49%) from cinnamoyl chloride (3.3 g); colorless crystals: mp 101-102 °C (hexane/$CHCl_3$); IR ($CHCl_3$) 3395 (NH), 1634 (CON) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 8.20 (1H, br s), 7.75 (1H, d, *J*=15.5 Hz), 7.60-7.25 (10H, m), 6.40 (1H, d, *J*=15.5 Hz), 4.95 (2H, s); HRMS (EI, *m/z*) calcd for $C_{16}H_{15}NO_2$ (M^+) 253.1102, found 253.1110. Anal. Calcd for $C_{16}H_{15}NO_2$: C, 75.87; H, 5.97; N, 5.53. Found : C, 75.73; H, 5.99; N, 5.46.

Ethyl (*E*)-3-[*N*-(Phenylmethoxy)carbamoyl]-2-propenoate (6d): 685 mg (yield 92%) from (*E*)-3-methoxycarbonyl-2-propenoyl chloride (488 mg) ; colorless oil; IR ($CHCl_3$) 3519 (NH), 1713 (COO), 1641 (CON) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 8.70 (1H, br s), 7.48-7.31 (5H, br s), 6.90 (1H, br s), 6.49 (1H, br s), 4.95 (2H, br s), 4.23 (2H, q, *J*=7 Hz), 1.30 (3H, t, *J*=7 Hz); HRMS (EI, *m/z*) calcd for $C_{13}H_{15}NO_4$ (M^+) 249.1000, found 249.1018.

***N*-Methoxy-2-methyl-2-butenamide (6e):** 145 mg (yield 63%) from methacryloyl chloride (209 mg); colorless oil; IR ($CHCl_3$) 3394 (NH), 1655 (CON)

cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 8.58 (1H, br s), 5.67 (1H, dq, *J*=1, 0.5 Hz), 5.37 (1H, dq, *J*=1, 0.5 Hz) 3.81 (3H, s), 1.96 (3H, br s). After being characterized by ^{1}H NMR spectrum, unstable hydroxamate **6e** was immediately subjected to the following allylation.

2-Propenyl (*Z*)-*N*-Methoxy-3-methyl-2-butenimidate (8b): 56 mg (yield 11%) from **6b** (400 mg); colorless oil; IR ($CHCl_3$) 1623 (C=N) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.41 (1H, br s), 5.93 (1H, ddt, *J*=17, 10, 5 Hz), 5.32 (1H, dq, *J*=17, 1.5 Hz), 5.24 (1H, dq, *J*=10, 1.5 Hz), 4.53 (2H, dt, *J*=5, 1.5 Hz), 3.85 (3H, s), 2.17 and 1.90 (each 3H, br s); HRMS (EI, *m/z*) calcd for $C_9H_{15}NO_2$ (M^+) 169.1102, found 169.1095. After being characterized by ^{1}H NMR spectrum, unstable hydroxamate **8b** was immediately subjected to the following allylation.

2-Propenyl (*Z,E*)-3-Phenyl-*N*-phenylmethoxy-2-propenimidate (8c): 340 mg (yield 58%) from **6c** (507 mg); colorless oil; IR ($CHCl_3$) 1634 (C=N) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48-7.23 (10H, m), 7.12 (1H, d, *J*=15.5 Hz), 6.51 (1H, d, *J*=15.5 Hz), 6.03 (1H, ddt, *J*=17, 10, 6 Hz), 5.34 (1H, dq, *J*=17, 1.5 Hz), 5.14 (1H, dq, *J*=10, 1.5 Hz), 5.09 (2H, s), 4.78 (2H, dt, *J*=6, 1.5 Hz); ^{13}H NMR ($CDCl_3$) δ 155.5, 137.8, 136.1, 135.3, 133.6, 128.9, 128.8, 128.6, 128.4, 128.2, 127.3, 119.5, 118.6, 77.9, 72.8; HRMS (EI, *m/z*) calcd for $C_{19}H_{19}NO_2$ (M^+) 293.1415, found 293.1433.

Ethyl (*E,Z*)-4-[(Phenylmethoxy)imino]-4-(2-propenyloxy)-2-butenoate (8d): 112 mg (yield 57%) from **6d** (169 mg); colorless oil; IR ($CHCl_3$)

1713 (COO), 1641 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.42-7.29 (5H, m), 6.95 (1H, d, *J*=16 Hz), 6.38 (1H, d, *J*=16 Hz), 5.93 (1H, ddt, *J*=17, 10, 6 Hz), 5.29 (1H, dq, *J*=17, 1.5 Hz), 5.21 (1H, dq, *J*=10, 1.5 Hz), 5.10 (2H, s), 4.75 (2H, dt, *J*=6, 1.5 Hz), 4.22 (2H, q, *J*=7 Hz), 1.29 (3H, t, *J*=7 Hz); HRMS (EI, *m/z*) calcd for $C_{16}H_{19}NO_4$ (M^+) 289.1313, found 289.1312.

3-Phenyl-2-propenyl [*E*(*Z*)]-*N*-Methoxy-2-methyl-2-propenimidate (20a): 381 mg (yield 33%) from **6e** (576 mg); yellow oil; IR ($CHCl_3$) 1632 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.60-7.20 (5H, m), 6.66 (1H, br d, *J*=16 Hz), 6.35 (1H, dt, *J*=16, 6 Hz), 5.65 (1H, br s), 5.24 (1H, br s), 4.78 (2H, dd, *J*=6, 1.5 Hz), 3.88 (3H, br s), 1.91 (3H, br s); HRMS (EI, *m/z*) calcd for $C_{14}H_{17}NO_2$ (M^+) 231.1260, found 231.1266. After being characterized by ^1H NMR spectrum, unstable hydroximate **20a** was immediately subjected to the following radical cyclization.

2-Butenyl [*E*(*Z*)]-*N*-methoxy-2-methyl-2-propenimidate (20b): 397 mg (yield 47%) from **6e** (576 mg); yellow oil; IR ($CHCl_3$) 1678 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 5.86-5.65 (2H, m), 5.59 (1H, br s), 5.21 (1H, br quint., *J*=1.5 Hz), 4.53 (2H, d, br d, *J*=5 Hz), 3.85 (3H, s), 1.89 (3H, br s), 1.73 (3H, br d, *J*=5 Hz); HRMS (EI, *m/z*) calcd for $C_9H_{15}NO_2$ (M^+) 169.1104, found 169.1100. After being characterized by ^1H NMR spectrum, unstable hydroximate **20b** was immediately subjected to the following radical cyclization.

3-Methyl-2-butenyl (*Z*)-*N*-Methoxy-2-methyl-2-propenimidate (20c):

82 mg (yield 10%) from **6e** (518 mg); yellow oil; ^{1}H NMR (200 MHz, $CDCl_3$) δ 5.59 (1H, br s), 5.43 (1H, m), 5.21 (1H, br quint., *J*=1.5 Hz), 4.62 (2H, br d, *J*=7 Hz), 3.86 (3H, s), 1.89 (3H, br s), 1.76 and 1.70 (each 3H, br s). After being characterized by ^{1}H NMR spectrum, unstable hydroximate **20c** was immediately subjected to the following radical cyclization.

Ethyl [*E*(*Z*)]-4-(1-Methoxyimino-2-methyl-2-propenyloxy)-2-butenoate (20d): 300 mg (yield 44%) from **6e** (345 mg); colorless oil; IR ($CHCl_3$) 1718 (COO), 1631 (C=N) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.90 (1H, dt, *J*=15.5, 4.5 Hz), 6.15 (1H, dt, *J*=15.5, 1.5 Hz), 5.61 (1H, br s), 5.24 (1H, br quint., *J*=1.5 Hz), 4.80 (2H, dd, *J*=4.5, 1.5 Hz), 4.22 (2H, q, *J*=7 Hz), 3.85 (3H, s), 1.91 (3H, br d, *J*=2 Hz), 1.30 (3H, t, *J*=7 Hz); HRMS (EI, *m/z*) calcd for $C_{11}H_{17}NO_4$ (M^+) 227.1156, found 227.1162. After being characterized by ^{1}H NMR spectrum, unstable hydroximate **20d** was immediately subjected to the following radical cyclization.

2-Propenyl (*Z*)-*N*-Methoxy-2-methyl-2-propenimidate (20e): 287 mg (yield 37%) from **6e** (576 mg); colorless oil; ^{1}H NMR (200 MHz, $CDCl_3$) δ 5.97 (1H, ddt, *J*=17, 10, 6 Hz), 5.61 (1H, br s), 5.32(1H, dm, *J*=17 Hz), 5.26 (1H, dm, *J*=10 Hz), 5.22 (1H, br s), 4.62 (2H, ddd, *J*=6, 2.5, 1 Hz), 3.85 (3H, s), 1.90 (3H, br s). After being characterized by ^{1}H NMR spectrum, unstable hydroximate **20e** was immediately subjected to the following radical cyclization.

3-Butenyl (*Z, E*)-*N*-Methoxy-3-phenyl-2-propenimidate (23a): 85 mg (yield 37%) from **6a** (177 mg); colorless oil; IR ($CHCl_3$) 1642 (C=N) cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.50-7.25 (5H, m), 7.14 (1H, d, *J*=16 Hz), 6.48 (1H, d,

J=16 Hz), 5.89 (1H, ddt, *J*=17, 10, 6.5 Hz), 5.19 (1H, dq, *J*=17, 1.5 Hz), 5.12 (1H, dq, *J*=10, 1.5 Hz), 4.31 (2H, t, *J*=6.5 Hz), 3.88 (3H, s), 2.51 (2H, qt, *J*=6.5, 1.5 Hz); HRMS (EI, *m/z*) calcd for $C_{14}H_{17}NO_2$ (M^+) 231.1258, found 231.1255.

4-Pentenyl (*Z, E*)-*N*-Methoxy-3-phenyl-2-propenimidate (23b): 459 mg (yield 62%) from **6a** (532 mg); colorless oil; IR ($CHCl_3$) 1639 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.48-7.26 (5H, m), 7.12 (1H, d, *J*=16 Hz), 6.49 (1H, d, *J*=16 Hz), 5.85 (1H, ddt, *J*=16.5, 10, 6.5 Hz), 5.08 (1H, dq, *J*=16.5, 1.5 Hz), 5.01 (1H, dq, *J*=10, 1.5 Hz), 4.26 (2H, t, *J*=6.5 Hz), 3.87 (3H, s), 2.23 (2H, br q, *J*=7 Hz), 1.85 (2H, tt, *J*=8, 7 Hz); HRMS (EI, *m/z*) calcd for $C_{15}H_{19}NO_2$ (M^+) 245.1414, found 245.1418.

5-Hexenyl (*Z, E*)-*N*-Methoxy-3-phenyl-2-propenimidate (23c): 433 mg (yield 56%) from **6a** (532 mg); colorless oil; IR ($CHCl_3$) 1639 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.51-7.22 (5H, m), 7.11 (1H, d, *J*=16 Hz), 6.49 (1H, d, *J*=16 Hz), 5.83 (1H, ddt, *J*=17, 10, 6.5 Hz), 5.03 (1H, dq, *J*=17, 1.5 Hz), 4.98 (1H, dq, *J*=10, 1.5 Hz), 4.25 (2H, t, *J*=6.5 Hz), 3.87 (3H, s), 2.13 (2H, br dt, *J*=8, 6.5 Hz), 1.87 and 1.56 (each 2H, tt, *J*=8, 6.5 Hz); HRMS (EI, *m/z*) calcd for $C_{16}H_{21}NO_2$ (M^+) 259.1571, found 259.1577.

[*Z*(*cis*)]-*N*-[Tetrahydro-3-(1-methylethyl)-4-(phenylsulfanyl)-methylfuran-2-ylidene]-*O*-methylhydroxyamine (13b): 70 mg (yield 50%) from **8b** (85 mg); colorless oil; IR ($CHCl_3$) 1667 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.45-7.15 (5H, m), 4.33 (1H, dd, *J*=9, 4 Hz), 4.21 (1H, ddd, *J*=9, 4.5, 1 Hz), 3.81 (3H, s), 3.16 (1H, ddd, *J*=12.5, 3, 1 Hz), 2.78 (1H, dd, *J*=12.5, 11 Hz),

2.82-2.51 (2H, m), 1.95 (1H, m), 1.12 and 0.99 (each 3H, d, *J*=6.5 Hz); ^{13}H NMR ($CDCl_3$) δ 158.8, 137.7, 130.5, 129.0, 126.9, 73.2, 62.2, 50.0, 40.0, 31.6, 26.0, 21.9, 20.6; HRMS (EI, *m/z*) calcd for $C_{15}H_{21}NO_2S$ (M^+) 279.1292, found 279.1289.

[*Z*(*trans*)]-*N*-[Tetrahydro-3-(1-methylethyl)-4-(phenylsulfanyl)-methylfuran-2-ylidene]-*O*-methylhydroxyamine (14b): 42 mg (yield 30%) from **8b** (85 mg); colorless oil; IR ($CHCl_3$) 1667 (C=N) cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.45-7.15 (5H, m), 4.37 (1H, dd, *J*=9.5, 6.5 Hz), 4.19 (1H, dd, *J*=9.5, 4.5 Hz), 3.81 (3H, s), 3.07 (1H, dd, *J*=13, 6.5 Hz), 2.93 (1H, dd, *J*=13, 8.5 Hz), 2.56 (1H, dd, *J*=5.5, 3.5 Hz), 2.45 (1H, m), 1.97 (1H, m), 0.99 and 0.94 (each 3H, d, *J*=7 Hz); ^{13}H NMR ($CDCl_3$) δ 159.8, 134.8, 130.0, 129.0, 126.6, 74.8, 62.1, 50.9, 38.7, 37.8, 30.2, 19.9, 19.2; HRMS (EI, *m/z*) calcd for $C_{15}H_{21}NO_2S$ (M^+) 279.1292, found 279.1294.

[*Z*(*cis*)]-*N*-[Tetrahydro-3-phenylmethyl-4-(phenylsulfanyl)-methylfuran-2-ylidene]-*O*-phenylmethylhydroxyamine (13c): 123 mg (yield 61%) from **8c** (147 mg); colorless crystals: mp 127-128 °C (Et_2O); IR ($CHCl_3$) 1673 (C=N) cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.46-6.84 (15H, m), 5.00 (2H, s), 4.48 (1H, dd, *J*=9.5, 1.5 Hz), 4.15 (1H, ddd, *J*=9.5, 5, 1.5 Hz), 3.37 (1H, ddd, *J*=11, 6, 5 Hz), 3.25 (1H, dd, *J*=15, 6 Hz), 3.17 (1H, ddd, *J*=13, 3, 1.5 Hz), 2.69 (1H, dd, *J*=15, 11 Hz), 2.59 (1H, t, *J*=13 Hz), 2.46 (1H, m); ^{13}H NMR ($CDCl_3$) δ 159.1, 138.2, 137.6, 134.5, 128.8, 128.6, 128.4, 128.1, 127.6, 126.5, 125.8, 76.3, 73.0, 43.2, 38.5, 31.5, 30.0; HRMS (EI, *m/z*) calcd for $C_{25}H_{25}NO_2S$ (M^+) 403.1604, found 403.1598. Anal. Calcd for $C_{25}H_{25}NO_2S$: C, 74.41; H, 6.25; N, 3.47; S, 7.95. Found:

C, 74.19; H, 6.20; N, 3.47; S, 8.15.

[*Z*(*trans*)]-*N*-[Tetrahydro-3-phenylmethyl-4-(phenylsulfanyl)-methylfuran-2-ylidene]-*O*-phenylmethylhydroxyamine (14c): 66 mg (yield 33%) from **8c** (147 mg); colorless crystals: mp 89-91 °C (Et_2O); IR ($CHCl_3$) 1671 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.45-7.00 (15H, m), 5.02 (2H, s), 4.29 (1H, dd, *J*=9, 6.5 Hz), 4.03 (1H, dd, *J*=9, 6 Hz), 3.07 (1H, dd, *J*=13.5, 4.5 Hz), 2.85 (1H, m), 2.75 (2H, m), 2.60 (1H, dd, *J*=13.5, 9 Hz), 2.37 (1H, m); ^{13}H NMR ($CDCl_3$) δ 160.3, 137.8, 134.5, 130.1, 129.1, 128.9, 128.5, 128.4, 128.2, 127.7, 126.6, 76.3, 74.4, 45.6, 40.8, 37.4, 36.4; HRMS (EI, *m/z*) calcd for $C_{25}H_{25}NO_2S$ (M^+) 403.1604, found 403.1605.

Ethyl [*cis*(*Z*)]-Tetrahydro-2-[(phenylmethoxy)imino]-4-(phenylsulfanyl)methyl-3-furanacetate (13d): 70 mg (yield 35%) from **8d** (145 mg); colorless oil; IR ($CHCl_3$) 1730 (COO), 1676 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.43-7.28 (10H, m), 4.96 (2H, s), 4.49 (1H, dd, *J*=9, 1.5 Hz), 4.24 (1H, ddd, *J*=9, 5, 1 Hz), 4.14 (2H, q, *J*=7 Hz), 3.39 (1H, ddd, *J*=10, 6.5, 5 Hz), 3.06 (1H, ddd, *J*=12, 3, 1 Hz), 2.75 (1H, m), 2.79 (1H, dd, *J*=17, 5 Hz), 2.59 (1H, dd, *J*=12, 11 Hz), 2.46 (1H, dd, *J*=17, 10 Hz), 1.24 (3H, t, *J*=7 Hz); ^{13}H NMR ($CDCl_3$) δ 171.1, 158.2, 137.6, 134.7, 129.7, 129.0, 128.3, 128.1, 127.6, 126.6, 76.3, 73.5, 60.8, 39.1, 38.8, 31.6, 31.2, 14.0; HRMS (EI, *m/z*) calcd for $C_{22}H_{25}NO_4S$ (M^+) 399.1503, found 399.1511.

Ethyl [*trans*(*Z*)]-Tetrahydro-2-[(phenylmethoxy)imino]-4-(phenylsulfanyl)methyl-3-furanacetate (14d): 86 mg (yield 43%) from

8d (145 mg); colorless oil; IR ($CHCl_3$) 1731 (COO), 1676 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.43-7.15 (10H, m), 4.95 (2H, s), 4.45 (1H, dd, *J*=9, 7 Hz), 4.11 (2H, q, *J*=7 Hz), 4.09 (1H, dd, *J*=9, 7 Hz), 3.22 (1H, dd, *J*=13.5, 5 Hz), 3.07 (1H, m), 2.87 (1H, dd, *J*=13.5, 9.5 Hz), 2.72 (1H, dd, *J*=16.5, 5 Hz), 2.48 (1H, dd, *J*=16.5, 8.5 Hz), 2.47 (1H, m), 1.23 (3H, t, *J*=7 Hz); ^{13}H NMR ($CDCl_3$) δ 170.8, 159.1, 137.5, 134.7, 129.6, 128.9, 128.2, 128.0, 127.5, 126.5, 76.2, 74.1, 60.6, 42.2, 40.8, 35.7, 35.4, 13.9; HRMS (EI, *m/z*) calcd for $C_{22}H_{25}NO_4S$ (M^+) 399.1503, found 399.1510.

[*Z*(*cis*)]-*N*-[Tetrahydro-3-methyl-4-phenylmethyl-3-(phenylsulfanyl)methylfuran-2-ylidene]-*O*-methylhydroxyamine (21a): 84 mg (yield 49%) from **20a** (116 mg); colorless oil; IR ($CHCl_3$) 1668 (C=N) cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.46-7.16 (10H, m), 4.18 (2H, d, *J*=5.5 Hz), 3.76 (3H, s), 3.33 and 3.18 (2H, ABq, *J*=13 Hz), 3.07 (1H, m), 2.50 (2H, m), 1.43 (3H, s). NOE was observed between the methyl group (δ 1.43) and 4-H (δ 3.07), and 1'-H (δ 3.33 and 3.18) and 1"-H (δ 2.50) in NOESY spectroscopy. ^{13}H NMR ($CDCl_3$) δ 161.8, 138.7, 136.3, 129.8, 128.8, 128.6, 128.5, 126.4, 126.3, 72.6, 62.0, 48.5, 46.3, 39.7, 33.1, 24.1; HRMS (EI, *m/z*) calcd for $C_{20}H_{23}NO_2S$ (M^+) 341.1432, found 341.1441.

[*Z*(*trans*)]-*N*-[Tetrahydro-3-methyl-4-phenylmethyl-3-(phenylsulfanyl)methylfuran-2-ylidene]-*O*-methylhydroxyamine (22a): 49 mg (yield 29%) from **20a** (116 mg); colorless oil; IR ($CHCl_3$) 1670 (C=N) cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.45-6.88 (10H, m), 4.13 (1H, dd, *J*=9, 7 Hz), 3.92 (1H, t, *J*=9 Hz), 3.75 (3H, s), 3.36 and 3.15 (2H, ABq, *J*=13.5 Hz), 2.94

(1H, m), 2.87 (1H, dd, *J*=13.5, 4.5 Hz), 2.43 (1H, dd, *J*=13.5, 10.5 Hz), 1.33 (3H, s). NOE was observed between the methyl group (δ 1.33) and 1"-H (δ 2.87 and 2.43), and 1'-H (δ 3.36 and 3.15) and 4-H (δ 2.94) in NOESY spectroscopy. ^{13}H NMR ($CDCl_3$) δ 162.2, 138.5, 137.0, 129.9, 128.9, 128.5, 128.2, 126.4, 126.3, 73.3, 62.1, 46.6, 44.6, 42.2, 33.3, 19.9; HRMS (EI, *m/z*) calcd for $C_{20}H_{23}NO_2S$ (M^+) 341.1432, found 341.1433.

[*Z*(*cis/trans*)]-*N*-[4-Ethyltetrahydro-3-methyl-3-(phenylsulfanyl)methylfuran-2-ylidene]-*O*-methylhydroxyamine (21b) and (22b). 78 mg(yield 56%) from **20b** (85 mg); The diastereoisomers **21b** and **22b** couldn't be separated by repeated medium-pressure column chromatography. The ratio of **21b** and **22b** was determined by 200 MHz ^{1}H NMR. Pale yellow oil; IR ($CHCl_3$) 1669 (C=N) cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.48-7.12 (5H, m), 4.44 (2/3H, dd, *J*=8.5, 7 Hz), 4.41 (1/3H, dd, *J*=9.5, 7 Hz), 4.19 (2/3H, dd, *J*=8.5, 7 Hz), 3.87 (1/3H, dd, *J*=9.5, 8.5 Hz), 3.75 (1H, s), 3.72 (2H, s), 3.31 and 3.05 (4/3H, ABq, *J*=13 Hz), 3.20 and 3.14 (2/3H, ABq, *J*=12.5 Hz), 2.52 (1/3H, m), 2.11 (2/3H, m), 1.69-1.20 (2H, m), 1.38 (2H, s), 1.20 (1H, s), 0.96 (2H, t, *J*=7 Hz), 0.79 (1H, t, *J*=7 Hz); HRMS (EI, *m/z*) calcd for $C_{15}H_{21}NO_2S$ (M^+) 279.1294, found 279.1280.

[*Z*(*cis*)]-*N*-[Tetrahydro-3-methyl-4-(1-methylethyl)-3-(phenylsulfanyl)methylfuran-2-ylidene]-*O*-methylhydroxyamine (21c): 44 mg (yield 30%) from **20c** (92 mg); colorless oil; IR ($CHCl_3$) 1668 (C=N) cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.45-7.15 (5H, m), 4.37 (1H, dd, *J*=9, 7.5 Hz), 4.24 (1H, dd, *J*=9, 7.5 Hz), 3.70 (3H, s), 3.31 and 3.11 (2H, ABq, *J*=12.5 Hz), 2.10-

1.95 (2H, m), 1.43 (3H, s), 1.02 and 0.88 (each 3H, d, *J*=6 Hz); ^{13}H NMR ($CDCl_3$) δ 162.6, 136.7, 129.9, 128.8, 126.3, 72.3, 62.0, 53.3, 46.1, 39.9, 26.8, 26.0, 22.2, 20.0; HRMS (EI, *m/z*) calcd for $C_{16}H_{23}NO_2S$ (M^+) 293.1448, found 293.1440.

[*Z*(*trans*)]-*N*-[Tetrahydro-3-methyl-4-(1-methylethyl)-3-(phenylsulfanyl)methylfuran-2-ylidene]-*O*-methylhydroxyamine (22c): 41 mg (yield 28%) from **20c** (92 mg); colorless oil; IR ($CHCl_3$) 1670 (C=N) cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.50-7.15 (5H, m), 4.39 (1H, dd, *J*=9, 8 Hz), 3.94 (1H, t, *J*=9 Hz), 3.70 (3H, s), 3.41 and 3.14 (2H, ABq, *J*=12.5 Hz), 2.52 (1H, br q, *J*=9 Hz), 1.74 (1H, m), 1.27 (3H, s), 0.86 and 0.83 (each 3H, d, *J*=7 Hz); ^{13}H NMR ($CDCl_3$) δ 162.5, 137.0, 130.8, 128.7, 126.4, 72.4, 62.0, 47.8, 46.7, 43.8, 26.8, 21.2, 20.5, 20.0; HRMS (EI, *m/z*) calcd for $C_{16}H_{23}NO_2S$ (M^+) 293.1448, found 293.1444.

Ethyl [*cis*(*Z*)]-Tetrahydro-5-(methoxyimino)-4-methyl-4-(phenylsulfanyl)methyl-3-furanacetate (21d): 47 mg (yield 28%) from **20d** (114 mg); colorless oil; IR ($CHCl_3$) 1729 (COO), 1670 (C=N) cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.18 (5H, m), 4.54 (1H, dd, *J*=9, 6 Hz), 4.20 (1H, dd, *J*=9, 6 Hz), 4.15 (2H, q, *J*=7 Hz), 3.74 (3H, s), 3.21 and 3.03 (2H, ABq, *J*=13 Hz), 2.70 (1H, m), 2.69 (1H, dd, *J*=16.5, 12.5 Hz), 2.44 (1H, dd, *J*=16.5, 12.5 Hz), 1.41 (3H, s), 1.26 (3H, t, *J*=7 Hz). NOE was observed between 1'-H (δ 3.21 and 3.03) and 1"-H (δ 2.44) in NOESY spectroscopy. ^{13}H NMR ($CDCl_3$) δ 171.5, 161.3, 136.0, 129.9, 128.9, 126.4, 73.6, 62.1, 60.8, 45.7, 43.1, 40.0, 32.2, 24.1, 14.0; HRMS (EI, *m/z*) calcd for $C_{17}H_{23}NO_4S$ (M^+) 337.1346, found 337.1360.

Ethyl [*trans*(*Z*)]-Tetrahydro-5-(methoxyimino)-4-methyl-4-(phenylsulfanyl)methyl-3-furanacetate (22d): 35 mg (yield 21%) from **20d** (114 mg); colorless oil; IR ($CHCl_3$) 1730 (COO), 1670 (C=N) cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.43-7.17 (5H, m), 4.60 (1H, dd, *J*=9, 7.5 Hz), 4.10 (2H, q, *J*=7Hz), 3.92 (1H, t, *J*=9 Hz), 3.74 (3H, s), 3.30 and 3.18 (2H, ABq, *J*=13.5 Hz), 3.02 (1H, m), 2.63 (1H, dd, *J*=16.5, 4 Hz), 2.24 (1H, dd, *J*=16.5, 11.5 Hz), 1.24 (3H, t, *J*=7 Hz), 1.22 (3H, s). NOE was observed between the methyl group (δ 1.22) and 1''-H (δ 2.63 and 2.24), and 1'-H (δ 3.30) and 4-H (δ 3.02) in NOESY spectroscopy. ^{13}H NMR ($CDCl_3$) δ 171.2, 161.6, 136.5, 130.0, 128.8, 126.4, 73.5, 62.7, 60.7, 46.0, 42.8, 39.9, 32.6, 19.6, 14.0; HRMS (EI, *m/z*) calcd for $C_{17}H_{23}NO_4S$ (M^+) 337.1346, found 337.1348.

[*Z*(*cis/trans*)]-*N*-[Tetrahydro-3,4-dimethyl-3-(phenylsulfanyl)methylfuran-2-ylidene]-*O*-methylhydroxyamine (21e) and (22e). 41 mg (yield 31%) from **20e** (78 mg); The diastereoisomers **21e** and **22e** could not be separated by repeated medium-pressure column chromatography. The ratio of **21e** and **22e** was determined by 200 MHz ^1H NMR. Pale yellow oil; IR ($CHCl_3$) 1667 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.45-7.13 (5H, m), 4.42 (3/5H, dd, *J*=8.5, 6 Hz), 4.38 (2/5H, dd, *J*=8.5, 6 Hz), 4.05 (3/5H, dd, *J*=8.5, 6 Hz), 3.81 (2/5H, dd, *J*=8.5, 6 Hz), 3.75 (3H, s), 3.29 and 3.06 (6/5H, ABq, *J*=12.5 Hz), 3.21 and 3.15 (4/5H, ABq, *J*=12.5 Hz), 2.70 (2/5H, m), 2.35 (3/5H, m), 1.37 (9/5H, s), 1.21 (6/5H, s), 1.11 (9/5H, d, *J*=7 Hz), 0.98 (6/5H, s); HRMS (EI, *m/z*) calcd for $C_{14}H_{19}NO_2S$ (M^+) 265.1137, found 265.1120.

3-Butenyl (*E,E*)-*N*-Methoxy-3-phenyl-2-propenimidate (24a): 28 mg (yield 24%) from **23a** (116 mg); colorless oil; IR ($CHCl_3$) 1637 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.56-7.28 (5H, m), 7.22 (1H, d, *J*=16 Hz), 7.07 (1H, d, *J*=16 Hz), 5.90 (1H, ddt, *J*=17, 10, 6.5 Hz), 5.17 (1H, dq, *J*=17, 1.5 Hz), 5.10 (1H, dq, *J*=10, 1.5 Hz), 4.14 (2H, t, *J*=6.5 Hz), 3.82 (3H, s), 2.52 (2H, qt, *J*=6.5, 1.5 Hz); HRMS (EI, *m/z*) calcd for $C_{14}H_{17}NO_2$ (M^+) 231.1258, found 231.1257.

4-Pentenyl (*E,E*)-*N*-Methoxy-3-phenyl-2-propenimidate (24b): 45 mg (yield 37%) from **23b** (123 mg); colorless oil; IR ($CHCl_3$) 1638 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.57-7.29 (5H, m), 7.23 (1H, d, *J*=16 Hz), 7.08 (1H, d, *J*=16 Hz), 5.88 (1H, ddt, *J*=16.5, 10, 6.5 Hz), 5.08 (1H, dq, *J*=16.5, 1.5 Hz), 5.01 (1H, dq, *J*=10, 1.5 Hz), 4.10 (2H, t, *J*=6.5 Hz), 3.81 (3H, s), 2.22 (2H, br q, *J*=7 Hz), 1.89 (2H, tt, *J*=8, 6.5 Hz); HRMS (EI, *m/z*) calcd for $C_{15}H_{19}NO_2$ (M^+) 245.1414, found 245.1397.

5-Hexenyl (*E,E*)-*N*-Methoxy-3-phenyl-2-propenimidate (24c): 20 mg (yield 15%) from **23c** (130 mg); colorless oil; IR ($CHCl_3$) 1637 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.72-7.29 (5H, m), 7.22 (1H, d, *J*=16 Hz), 7.08 (1H, d, *J*=16 Hz), 5.85 (1H, ddt, *J*=17, 10, 6.5 Hz), 5.05 (1H, dq, *J*=17, 1.5 Hz), 4.98 (1H, dq, *J*=10, 1.5 Hz), 4.09 (2H, t, *J*=6.5 Hz), 3.81 (3H, s), 2.41 (2H, br dt, *J*=8, 6.5 Hz), 1.98 and 1.76 (each 2H, tt, *J*=8, 6.5 Hz); HRMS (EI, *m/z*) calcd for $C_{16}H_{21}NO_2$ (M^+) 259.1571, found 259.1578.

5-(Phenylsulfanyl)pentyl (*Z,E*)-*N*-Methoxy-3-phenyl-2-propenimidate (25b): 4 mg (yield 3%) from **23b** (123 mg); colorless oil; IR

($CHCl_3$) 1634 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.49-7.17 (10H, m), 7.11 (1H, d, *J*=16 Hz), 6.48 (1H, d, *J*=16 Hz), 4.24 (2H, t, *J*=6.5 Hz), 3.86 (3H, s), 2.95 (2H, t, *J*=7 Hz), 1.84-1.52 (6H, m); HRMS (EI, *m/z*) calcd for $C_{21}H_{25}NO_2S$ (M^+) 355.1604, found 355.1596.

6-(Phenylsulfanyl)hexyl (*Z,E*)-*N*-Methoxy-3-phenyl-2-propenimidate (25c): 3 mg (yield 5%) from **23c** (130 mg); colorless oil; IR ($CHCl_3$) 1639 (C=N) cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.50-7.15 (10H, m), 7.10 (1H, d, *J*=16 Hz), 6.50 (1H, d, *J*=16 Hz), 4.23 (2H, t, *J*=6.5 Hz), 3.87 (3H, s), 2.93 (2H, t, *J*=6.5 Hz), 1.85-1.23 (8H, m); HRMS (EI, *m/z*) calcd for $C_{22}H_{27}NO_2S$ (M^+) 369.1761, found 369.1769.

Compound **13**

Stereoscopic View of

C19H21NO2S Pbca(z=16) Prof. Naito

Compound **13**

Parallel View of
C19H21NO2S Pbca(z=16) Prof. Naito

Compound **13**

C19H21NO2S Pbca(z=16) Proof. Naito

Parallel View of

Crystal Data

Compound Compound 13 C19H21NO2S Pbca(z=16) Prof. Naito
Molecular Formular C19H21NO2S
Molecular Weight 327.442

Crystal Class : Orthorhombic
Space Group : P b c a
Lattice Constants
a = 18.131(3) b = 26.611(2) c = 14.575(1) A
alpha = 90.000(0) beta = 90.000(0) gamma = 90.000(0) Deg.
U = 7032.4(1.5) A**3
Cell Parameters were Refined from 25 Reflections (85 < 2_Theta < 90 deg.s)
Z = 16 (No. of Molecules in Unit Cell)
Density = 1.237 Mg m**-3

Xray : Cu K-alpha (1.5418A, Graphite Monochomatized)
Recrystalized from ether-hexane
Crystal Shape : Prism
Crystal Colour : Colorless
Crystal Size : 0.5 * 0.5 * 0.3 mm**3
Linear Absorption Coefficient = 17.003 mm**-1
Temperature : 291 K

Data Collection

Diffractometer : Rigaku_AFC5R_diffractometer
Scan Method : 2Theta/Omega Scan
3 Standard Reflections Measured at every 200 reflections
Intensity Variation of Standard Reflections : 2.0%
Absorption Correction : None (T_min = 1.0, T_max = 0.95)
Total Reflections Measured : 5974
Observed Independent Reflections : 4133(|Fo| > 2.667*sigma(Fo))
2Theta Max. : <130Deg.
h_min -> h_max : 0 -> 21
k_min -> k_max : 0 -> 31
l_min -> l_max : 0 -> 16

Structure Analysis & Refine

Method of Structure Determination : SHELXS-86
Refinement : Full Matrix Leastsquare Method
Refinement on : w(|Fo|**2 - |Fc|**2)
Final R Value : 0.060
Final wR Value : 0.044
Goodness of Fit : 2.452
No. of Reflections : 5980 (Without |Fo|=0) 4144
No. of Parameters : 583
Temperature Factors
All Hydrogens Refined
Weighting Scheme :
1/w=sigma(Fo)**2
Atomic Scattering Factors : International_Tables Vol. IV

Final atomic coordinates and
equivalent thermal factors
with e.s.d. in parentheses

Atom	X	Y	Z	Beq
S 1A	0.5968(0)	0.4532(0)	0.2197(0)	5.56(1)
O 2A	0.4969(1)	0.4401(1)	0.4828(1)	4.84(2)
C 3A	0.5263(2)	0.3964(1)	0.5121(2)	4.17(3)
C 4A	0.5329(2)	0.3589(1)	0.4362(2)	4.12(3)
C 5A	0.5287(2)	0.3929(1)	0.3510(2)	4.29(3)
C 6A	0.4804(2)	0.4359(1)	0.3847(2)	5.18(4)
N 7A	0.5449(1)	0.3885(1)	0.5958(2)	4.51(2)
O 8A	0.5281(1)	0.4315(0)	0.6502(1)	5.05(2)
C 9A	0.5536(5)	0.4233(2)	0.7404(4)	8.56(8)
C 10A	0.5978(2)	0.3229(1)	0.4467(2)	4.53(3)
C 11A	0.6052(2)	0.2856(1)	0.3695(2)	3.96(2)
C 12A	0.6735(2)	0.2766(1)	0.3291(2)	4.61(3)
C 13A	0.6817(2)	0.2417(1)	0.2603(2)	5.17(4)
C 14A	0.6222(3)	0.2150(1)	0.2295(2)	5.89(4)
C 15A	0.5542(3)	0.2240(1)	0.2688(4)	6.75(5)
C 16A	0.5454(2)	0.2587(1)	0.3376(3)	5.45(3)
C 17A	0.6035(2)	0.4117(1)	0.3182(2)	4.39(3)
C 18A	0.5631(2)	0.4137(1)	0.1320(2)	4.82(3)
C 19A	0.5810(2)	0.3635(1)	0.1233(3)	5.91(4)
C 20A	0.5557(2)	0.3353(2)	0.0505(3)	7.29(5)
C 21A	0.5125(3)	0.3583(2)	-0.0159(3)	8.13(6)
C 22A	0.4944(3)	0.4080(2)	-0.0082(3)	7.91(5)
C 23A	0.5195(2)	0.4354(2)	0.0656(3)	6.42(4)
S 1B	0.7589(0)	0.2993(0)	0.0528(0)	5.61(1)
O 2B	0.8689(1)	0.3081(0)	-0.2062(1)	4.42(2)
C 3B	0.8453(2)	0.3535(1)	-0.2346(2)	3.97(3)
C 4B	0.8413(2)	0.3907(1)	-0.1580(2)	3.83(2)
C 5B	0.8384(2)	0.3556(1)	-0.0738(2)	3.92(3)
C 6B	0.8821(2)	0.3107(1)	-0.1073(2)	4.63(3)
N 7B	0.8279(1)	0.3639(1)	-0.3175(2)	4.96(2)
O 8B	0.8390(1)	0.3211(1)	-0.3748(1)	5.99(2)
C 9B	0.8101(5)	0.3330(2)	-0.4630(3)	7.65(7)
C 10B	0.7810(2)	0.4299(1)	-0.1698(2)	4.44(3)
C 11B	0.7716(2)	0.4647(1)	-0.0894(2)	3.94(3)
C 12B	0.8312(2)	0.4832(1)	-0.0404(2)	4.33(3)
C 13B	0.8217(2)	0.5157(1)	0.0319(2)	5.39(4)
C 14B	0.7527(3)	0.5304(1)	0.0590(3)	6.25(4)
C 15B	0.6931(3)	0.5119(2)	0.0112(4)	7.61(5)
C 16B	0.7017(2)	0.4796(1)	-0.0619(3)	6.33(4)
C 17B	0.7606(2)	0.3414(1)	-0.0447(2)	4.59(3)
C 18B	0.7957(2)	0.3362(1)	0.1424(2)	4.71(3)
C 19B	0.7742(2)	0.3854(1)	0.1588(2)	5.32(3)
C 20B	0.8001(2)	0.4110(2)	0.2346(3)	6.70(5)
C 21B	0.8471(3)	0.3872(3)	0.2947(3)	8.25(7)
C 22B	0.8688(3)	0.3386(2)	0.2788(4)	7.80(6)
C 23B	0.8435(2)	0.3124(2)	0.2029(3)	6.27(4)

Final atomic coordinates and
equivalent thermal factors
with e.s.d. in parentheses

H 1	0.486 (1)	0.338 (1)	0.440 (2)	2.6(8)
H 2	0.504 (1)	0.376 (1)	0.302 (2)	2.2(8)
H 3	0.434 (1)	0.429 (1)	0.382 (2)	2.7(9)
H 4	0.491 (1)	0.475 (1)	0.356 (2)	3.3(9)
H 5	0.540 (2)	0.459 (1)	0.774 (2)	6.3(13)
H 6	0.532 (2)	0.396 (1)	0.758 (3)	6.0(19)
H 7	0.605 (2)	0.419 (2)	0.740 (3)	9.1(23)
H 8	0.640 (1)	0.342 (1)	0.452 (2)	1.8(8)
H 9	0.594 (1)	0.301 (1)	0.510 (2)	4.0(10)
H 10	0.713 (1)	0.297 (1)	0.345 (2)	2.1(8)
H 11	0.732 (1)	0.238 (1)	0.235 (2)	3.5(10)
H 12	0.627 (2)	0.190 (1)	0.179 (2)	3.9(10)
H 13	0.515 (2)	0.208 (1)	0.258 (3)	5.2(13)
H 14	0.495 (2)	0.261 (1)	0.373 (2)	4.8(11)
H 15	0.627 (1)	0.439 (1)	0.369 (2)	4.5(9)
H 16	0.636 (1)	0.383 (1)	0.303 (2)	2.9(9)
H 17	0.612 (2)	0.345 (1)	0.168 (2)	4.9(12)
H 18	0.562 (2)	0.291 (2)	0.049 (3)	10.7(17)
H 19	0.494 (2)	0.337 (1)	-0.057 (2)	4.8(12)
H 20	0.457 (2)	0.423 (1)	-0.063 (3)	11.6(18)
H 21	0.506 (2)	0.473 (1)	0.074 (2)	4.1(10)
H 22	0.887 (1)	0.408 (1)	-0.159 (2)	1.7(7)
H 23	0.864 (1)	0.372 (1)	-0.020 (1)	0.8(6)
H 24	0.867 (1)	0.276 (1)	-0.081 (2)	1.7(7)
H 25	0.936 (1)	0.313 (1)	-0.099 (2)	3.5(10)
H 26	0.823 (2)	0.297 (1)	-0.488 (3)	9.5(17)
H 27	0.759 (2)	0.335 (2)	-0.455 (3)	8.1(23)
H 28	0.829 (2)	0.360 (1)	-0.484 (2)	4.4(14)
H 29	0.793 (1)	0.453 (1)	-0.228 (2)	3.8(9)
H 30	0.739 (1)	0.413 (1)	-0.185 (2)	2.0(8)
H 31	0.881 (1)	0.476 (1)	-0.063 (2)	2.6(8)
H 32	0.862 (2)	0.528 (1)	0.071 (2)	4.7(11)
H 33	0.744 (2)	0.554 (1)	0.110 (2)	7.3(13)
H 34	0.645 (2)	0.518 (1)	0.024 (3)	6.0(15)
H 35	0.658 (2)	0.465 (1)	-0.097 (2)	6.5(14)
H 36	0.734 (1)	0.370 (1)	-0.029 (2)	1.9(8)
H 37	0.736 (1)	0.322 (1)	-0.100 (2)	2.4(8)
H 38	0.742 (2)	0.403 (1)	0.117 (2)	4.2(12)
H 39	0.789 (2)	0.451 (1)	0.243 (2)	4.8(11)
H 40	0.862 (2)	0.405 (1)	0.341 (3)	5.6(14)
H 41	0.903 (2)	0.317 (1)	0.318 (3)	8.8(18)
H 42	0.860 (2)	0.273 (1)	0.184 (2)	6.0(13)

Atom	B11	B22	B33	B12	B13	B23
S 1A	0.0060(0)	0.0015(0)	0.0052(0)	-0.0001(0)	0.0008(0)	0.0003(0)
O 2A	0.0039(1)	0.0019(0)	0.0046(1)	0.0007(0)	0.0001(1)	-0.0001(0)
C 3A	0.0031(1)	0.0015(0)	0.0049(2)	-0.0001(0)	0.0005(1)	0.0000(1)
C 4A	0.0034(1)	0.0016(0)	0.0041(2)	-0.0001(0)	0.0001(1)	0.0001(1)
C 5A	0.0033(1)	0.0018(0)	0.0040(2)	0.0002(0)	-0.0003(1)	0.0001(1)
C 6A	0.0037(2)	0.0024(1)	0.0048(2)	0.0007(1)	-0.0002(1)	0.0000(1)
N 7A	0.0042(1)	0.0016(0)	0.0040(1)	0.0000(0)	0.0002(1)	0.0000(0)
O 8A	0.0048(1)	0.0019(0)	0.0041(1)	0.0001(0)	0.0001(1)	-0.0004(0)
C 9A	0.0101(5)	0.0029(1)	0.0050(3)	0.0009(2)	-0.0021(3)	-0.0006(1)
C 10A	0.0036(1)	0.0016(0)	0.0051(2)	0.0002(0)	-0.0004(1)	-0.0001(1)
C 11A	0.0035(1)	0.0014(0)	0.0038(1)	0.0000(0)	-0.0004(1)	0.0003(0)
C 12A	0.0037(1)	0.0015(0)	0.0056(2)	-0.0002(0)	-0.0003(1)	-0.0001(1)
C 13A	0.0045(2)	0.0016(0)	0.0059(2)	0.0002(1)	0.0008(2)	0.0002(1)
C 14A	0.0066(2)	0.0017(0)	0.0050(2)	0.0001(1)	-0.0003(2)	-0.0005(1)
C 15A	0.0048(2)	0.0021(1)	0.0094(3)	-0.0007(1)	-0.0017(2)	-0.0008(1)
C 16A	0.0037(1)	0.0018(0)	0.0075(2)	-0.0003(1)	-0.0002(2)	-0.0006(1)
C 17A	0.0037(1)	0.0015(0)	0.0047(2)	-0.0001(0)	0.0004(1)	0.0001(1)
C 18A	0.0039(1)	0.0019(0)	0.0046(2)	0.0003(1)	0.0013(1)	0.0003(1)
C 19A	0.0050(2)	0.0022(0)	0.0059(2)	0.0006(1)	-0.0008(2)	-0.0003(1)
C 20A	0.0058(2)	0.0029(1)	0.0070(3)	0.0004(1)	-0.0007(2)	-0.0011(1)
C 21A	0.0063(2)	0.0040(1)	0.0057(3)	0.0003(1)	-0.0005(2)	-0.0015(2)
C 22A	0.0064(2)	0.0037(1)	0.0057(3)	0.0010(1)	-0.0003(2)	0.0001(1)
C 23A	0.0057(2)	0.0026(1)	0.0054(2)	0.0010(1)	0.0007(2)	0.0005(1)
S 1B	0.0063(0)	0.0014(0)	0.0053(0)	-0.0001(0)	0.0012(0)	0.0003(0)
O 2B	0.0039(1)	0.0016(0)	0.0043(1)	0.0003(0)	-0.0003(1)	-0.0005(0)
C 3B	0.0033(1)	0.0014(0)	0.0042(2)	-0.0003(0)	0.0002(1)	-0.0002(1)
C 4B	0.0034(1)	0.0013(0)	0.0041(2)	0.0000(0)	0.0000(1)	-0.0001(0)
C 5B	0.0033(1)	0.0015(0)	0.0038(2)	0.0000(0)	-0.0006(1)	-0.0001(0)
C 6B	0.0040(1)	0.0018(0)	0.0043(2)	0.0005(1)	-0.0003(1)	-0.0002(1)
N 7B	0.0053(1)	0.0016(0)	0.0039(1)	-0.0001(0)	0.0001(1)	-0.0003(0)
O 8B	0.0070(1)	0.0019(0)	0.0041(1)	0.0000(0)	-0.0004(1)	-0.0006(0)
C 9B	0.0096(4)	0.0023(1)	0.0044(2)	-0.0011(2)	-0.0014(2)	0.0000(1)
C 10B	0.0040(1)	0.0015(0)	0.0045(2)	0.0002(0)	-0.0009(1)	0.0000(1)
C 11B	0.0037(1)	0.0013(0)	0.0039(1)	0.0003(0)	-0.0001(1)	0.0002(0)
C 12B	0.0036(1)	0.0013(0)	0.0052(2)	-0.0001(0)	0.0003(1)	-0.0003(1)
C 13B	0.0056(2)	0.0014(0)	0.0055(2)	-0.0003(1)	-0.0004(2)	-0.0003(1)
C 14B	0.0067(2)	0.0018(0)	0.0057(2)	0.0004(1)	0.0016(2)	-0.0004(1)
C 15B	0.0047(2)	0.0030(1)	0.0096(4)	0.0011(1)	0.0015(2)	-0.0009(1)
C 16B	0.0038(2)	0.0024(1)	0.0083(3)	0.0006(1)	-0.0007(2)	-0.0008(1)
C 17B	0.0041(1)	0.0016(0)	0.0046(2)	0.0000(1)	0.0001(1)	0.0001(1)
C 18B	0.0038(1)	0.0019(0)	0.0045(2)	-0.0001(0)	0.0009(1)	0.0007(1)
C 19B	0.0041(1)	0.0022(0)	0.0052(2)	-0.0002(1)	0.0005(1)	-0.0001(1)
C 20B	0.0051(2)	0.0029(1)	0.0060(3)	-0.0007(1)	0.0012(2)	-0.0006(1)
C 21B	0.0057(2)	0.0047(2)	0.0044(3)	-0.0022(2)	0.0007(2)	-0.0005(2)
C 22B	0.0042(2)	0.0042(1)	0.0070(3)	-0.0007(1)	0.0001(2)	0.0019(2)
C 23B	0.0039(1)	0.0029(1)	0.0064(2)	-0.0001(1)	0.0012(2)	0.0013(1)

Bond lengths with e.s.d in parentheses(Mol A).

S 1A	-	C 17A	1.814(4)
S 1A	-	C 18A	1.765(4)
O 2A	-	C 3A	1.349(5)
O 2A	-	C 6A	1.465(5)
C 3A	-	C 4A	1.495(5)
C 3A	-	N 7A	1.284(5)
C 4A	-	C 5A	1.539(5)
C 4A	-	C 10A	1.526(6)
C 5A	-	C 6A	1.523(6)
C 5A	-	C 17A	1.522(6)
N 7A	-	O 8A	1.426(4)
O 8A	-	C 9A	1.411(7)
C 10A	-	C 11A	1.506(5)
C 11A	-	C 12A	1.393(6)
C 11A	-	C 16A	1.380(6)
C 12A	-	C 13A	1.375(6)
C 13A	-	C 14A	1.368(7)
C 14A	-	C 15A	1.380(8)
C 15A	-	C 16A	1.372(7)
C 18A	-	C 19A	1.378(6)
C 18A	-	C 23A	1.377(6)
C 19A	-	C 20A	1.380(7)
C 20A	-	C 21A	1.386(8)
C 21A	-	C 22A	1.369(10)
C 22A	-	C 23A	1.376(8)

Bond lengths with e.s.d in parentheses(Mol B).

S 1B	-	C 17B	1.810(4)
S 1B	-	C 18B	1.765(4)
O 2B	-	C 3B	1.347(4)
O 2B	-	C 6B	1.463(5)
C 3B	-	C 4B	1.493(5)
C 3B	-	N 7B	1.278(5)
C 4B	-	C 5B	1.544(5)
C 4B	-	C 10B	1.522(6)
C 5B	-	C 6B	1.513(6)
C 5B	-	C 17B	1.521(6)
N 7B	-	O 8B	1.426(4)
O 8B	-	C 9B	1.423(7)
C 10B	-	C 11B	1.503(5)
C 11B	-	C 12B	1.385(6)
C 11B	-	C 16B	1.386(6)
C 12B	-	C 13B	1.375(6)
C 13B	-	C 14B	1.369(8)
C 14B	-	C 15B	1.376(8)
C 15B	-	C 16B	1.378(8)
C 18B	-	C 19B	1.386(6)
C 18B	-	C 23B	1.389(6)
C 19B	-	C 20B	1.381(7)
C 20B	-	C 21B	1.376(8)
C 21B	-	C 22B	1.373(11)
C 22B	-	C 23B	1.386(8)

Bond angles with e.s.d in parentheses(Mol B).

C 17B	-	S 1B	-	C 18B	103.3(2)
C 3B	-	O 2B	-	C 6B	108.1(3)
O 2B	-	C 3B	-	C 4B	112.4(3)
O 2B	-	C 3B	-	N 7B	124.2(3)
C 4B	-	C 3B	-	N 7B	123.4(3)
C 3B	-	C 4B	-	C 5B	101.3(3)
C 3B	-	C 4B	-	C 10B	113.9(3)
C 5B	-	C 4B	-	C 10B	118.8(3)
C 4B	-	C 5B	-	C 6B	101.7(3)
C 4B	-	C 5B	-	C 17B	113.7(3)
C 6B	-	C 5B	-	C 17B	112.4(3)
O 2B	-	C 6B	-	C 5B	105.7(3)
C 3B	-	N 7B	-	O 8B	110.3(3)
N 7B	-	O 8B	-	C 9B	107.4(4)
C 4B	-	C 10B	-	C 11B	114.6(3)
C 10B	-	C 11B	-	C 12B	122.1(4)
C 10B	-	C 11B	-	C 16B	120.3(4)
C 12B	-	C 11B	-	C 16B	117.6(4)
C 11B	-	C 12B	-	C 13B	121.3(4)
C 12B	-	C 13B	-	C 14B	121.0(5)
C 13B	-	C 14B	-	C 15B	118.0(5)
C 14B	-	C 15B	-	C 16B	121.7(5)
C 11B	-	C 16B	-	C 15B	120.3(5)
S 1B	-	C 17B	-	C 5B	112.8(3)
S 1B	-	C 18B	-	C 19B	123.1(3)
S 1B	-	C 18B	-	C 23B	116.8(4)
C 19B	-	C 18B	-	C 23B	119.8(4)
C 18B	-	C 19B	-	C 20B	120.5(4)
C 19B	-	C 20B	-	C 21B	119.6(5)
C 20B	-	C 21B	-	C 22B	120.3(6)
C 21B	-	C 22B	-	C 23B	120.9(6)
C 18B	-	C 23B	-	C 22B	118.9(5)

Bond angles with e.s.d in parentheses(Mol A).

C 17A	-	S 1A	-	C 18A	103.5(2)
C 3A	-	O 2A	-	C 6A	108.8(3)
O 2A	-	C 3A	-	C 4A	112.0(3)
O 2A	-	C 3A	-	N 7A	123.1(3)
C 4A	-	C 3A	-	N 7A	124.9(3)
C 3A	-	C 4A	-	C 5A	101.5(3)
C 3A	-	C 4A	-	C 10A	114.1(3)
C 5A	-	C 4A	-	C 10A	119.2(3)
C 4A	-	C 5A	-	C 6A	102.1(3)
C 4A	-	C 5A	-	C 17A	113.8(3)
C 6A	-	C 5A	-	C 17A	111.5(3)
O 2A	-	C 6A	-	C 5A	104.8(3)
C 3A	-	N 7A	-	O 8A	109.9(3)
N 7A	-	O 8A	-	C 9A	108.8(4)
C 4A	-	C 10A	-	C 11A	114.0(3)
C 10A	-	C 11A	-	C 12A	120.5(4)
C 10A	-	C 11A	-	C 16A	121.6(4)
C 12A	-	C 11A	-	C 16A	117.9(3)
C 11A	-	C 12A	-	C 13A	121.4(4)
C 12A	-	C 13A	-	C 14A	120.3(4)
C 13A	-	C 14A	-	C 15A	118.6(4)
C 14A	-	C 15A	-	C 16A	121.6(5)
C 11A	-	C 16A	-	C 15A	120.2(4)
S 1A	-	C 17A	-	C 5A	112.9(3)
S 1A	-	C 18A	-	C 19A	124.1(3)
S 1A	-	C 18A	-	C 23A	117.2(3)
C 19A	-	C 18A	-	C 23A	118.5(4)
C 18A	-	C 19A	-	C 20A	121.3(4)
C 19A	-	C 20A	-	C 21A	118.9(6)
C 20A	-	C 21A	-	C 22A	120.4(6)
C 21A	-	C 22A	-	C 23A	119.7(5)
C 18A	-	C 23A	-	C 22A	121.1(5)