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Synthesis and antifungal activity of novel pyrazolines and isoxazolines derived from cuminaldehyde

Tao ZHANG, Mengya DONG, Jianjiang ZHAO,

Xiaofang ZHANG and Xiangdong MEI

Pesticide Science Society of Japan

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3-(2-methylphenyl)-5-(4-isopropylphenyl)isoxazoline (2a)

Yield 57%; white powder; mp: 124-125°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.69-7.28(m, 8H), 4.32-4.35 (dd, *J*=8.66 Hz, 1H), 3.60-3.67 (dd, *J*=21.37 Hz, 1H), 3.02-3.08 (dd, *J*=19.03 Hz, 1H), 2.86-3.00 (m, 1H), 2.32 (s, 3H), 1.16-1.18 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.22, 24.09, 30.61, 33.27, 63.60, 125.04, 125.94, 126.26, 129.11, 129.85, 131.17, 136.10, 139.99, 146.36, 155.21; HRMS *m/z* (M⁺): Calcd. for C₁₉H₂₁NO: 280.1623, found: 280.1631.

3-(2-bromophenyl)-5-(4-isopropylphenyl)isoxazoline (2b)

Yield 49%; brown powder; mp: 152-153°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.13-7.42 (m, 8H), 4.30-4.34 (dd, *J*=13.7 Hz, 1H), 3.47-3.54 (q, *J*=21.7 Hz, 1H), 3.01-3.07 (dd, *J*=19.3 Hz, 1H), 2.96-2.98 (m, 1H), 1.15-1.17 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 23.96, 30.87, 42.36, 62.30, 123.20, 125.92, 126.88, 129.13, 131.65, 133.70, 137.48, 138.46, 146.51, 153.02; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈BrNO: 344.0572, found: 344.0576.

3-(2-chlorophenyl)-5-(4-isopropylphenyl)isoxazoline (2c)

Yield 53%; white powder; mp: 138-139°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.10-7.40 (m, 8H), 4.14-4.17 (dd, *J*=8.62 Hz, 1H), 3.15-3.22 (dd, *J*=22.42 Hz, 1H), 2.90-2.96 (dd, *J*=18.91 Hz, 1H), 2.80-2.86 (m, 1H), 1.15-1.17 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 24.07, 30.92, 33.27, 63.46, 125.08, 126.14, 127.09, 128.13, 129.85, 130.46, 133.03, 138.66, 139.28, 147.36, 155.21; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈ClNO: 300.1077, found: 300.1072.

3-(2-fluorophenyl)-5-(4-isopropylphenyl)isoxazoline (2d)

Yield 50%; buff crystal; mp: 143-144°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.13-7.30 (m, 8H), 4.33-4.37 (dd, *J*=13.7 Hz, 1H), 3.58-3.65 (dd, *J*=22.6 Hz, 1H), 2.98-3.03 (dd, *J*=18.8 Hz, 1H), 2.85-2.88 (m, 1H), 1.16-1.18 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 24.20, 30.40, 33.33, 62.99, 114.62, 120.25, 122.32, 125.73, 129.10, 133.79, 138.83, 149.81, 153.43, 159.21, 161.64; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈FNO: 364.0634, found: 364.0638.

3-(3-methylphenyl)-5-(4-isopropylphenyl)isoxazoline (2e)

Yield 60%; white powder; mp: 114-115°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.13-7.30 (m, 8H), 4.29-4.34 (dd, *J*=13.95 Hz, 1H), 3.59-3.67 (dd, *J*=22.53 Hz, 1H), 2.96-3.02 (dd, *J*=18.51 Hz, 1H), 2.85-2.90 (m, 1H), 2.31 (s, 3H), 1.21-1.24 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.20, 24.08, 30.82, 33.26, 63.50, 123.41, 125.79, 126.90, 127.52, 128.08, 129.04, 136.64, 137.19, 139.99, 146.95, 155.02; HRMS *m/z* (M⁺): Calcd. for C₁₉H₂₁NO: 279.1623, found: 279.1617.

3-(3-bromophenyl)-5-(4-isopropylphenyl)isoxazoline (2f)

Yield 65%; gray powder; mp: 143-144°C ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.15-7.63 (m, 8H), 4.28-4.33 (dd, *J*=13.78 Hz, 1H), 3.48-3.55 (dd, *J*=21.63 Hz, 1H), 3.01-3.03 (dd, *J*=19.30 Hz, 1H), 2.95-2.98 (m, 1H), 1.21-1.24 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 24.07, 30.80, 33.25, 56.88, 122.10, 123.23, 124.67, 129.30, 137.17, 142.95, 151.65, 152.4; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈BrNO: 344.0572, found: 344.0576.

3-(3-chlorophenyl)-5-(4-isopropylphenyl)isoxazoline (2g)

Yield 62%; white powder; mp: 134-135°C, ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.06-7.42 (m, 8H), 4.08-4.12 (dd, *J*=13.7 Hz, 1H), 3.14-3.21 (dd, *J*=21.71 Hz, 1H), 2.87-2.93 (dd, *J*=19.32 Hz, 1H), 2.78-2.86 (m, 1H), 1.14-1.16 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 24.06, 30.86, 33.27, 63.34, 124.84, 125.79, 127.49, 128.13, 129.97, 133.03, 138.92, 139.66, 147.07, 154.09; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈ClNO: 300.1077, found: 300.1072.

3-(3-fluorophenyl)-5-(4-isopropylphenyl)isoxazoline (2h)

Yield 61%; yellow crystal; mp: 156-157°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.14-7.27 (m, 8H), 4.31-4.36 (dd, *J*=13.80 Hz, 1H), 3.57-3.66 (dd, *J*=22.09 Hz, 1H), 2.95-3.02 (dd, *J*=19.23 Hz, 1H), 2.84-2.89 (m, 1H), 1.20-1.23 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 23.99, 29.53, 33.28, 62.82, 112.96, 115.65, 122.32, 125.87, 128.11, 130.49, 138.93, 149.17, 153.06, 160.51, 163.73; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈FNO: 284.1372, found: 284.1377.

3-(4-methylphenyl)-5-(4-isopropylphenyl)isoxazoline (2i)

Yield 67%; white crystal; mp: 115-116°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.09-7.38 (m, 8H), 4.08-4.12 (dd, *J*=13.74 Hz, 1H), 3.08-3.16 (q, *J*=22.56 Hz, 1H), 2.95-3.01 (dd, *J*=18.73 Hz, 1H), 2.79-2.81 (m, 1H), 2.28 (s, 3H), 1.14-1.17 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 20.91, 22.02, 23.81, 24.09, 30.51, 63.59, 126.16, 128.36, 133.39, 138.20, 146.98, 149.01, 153.13, 154.79; HRMS *m/z* (M⁺): Calcd. for C₁₉H₂₁NO: 280.1623, found: 280.1631.

3-(4-bromophenyl)-5-(4-isopropylphenyl)isoxazoline (2j)

Yield 57%; gray crystal; mp: 125-126°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.05-7.47 (m, 8H), 4.21-4.24 (dd, *J*=13.64 Hz, 1H), 3.42-3.47 (dd, *J*=21.57 Hz, 1H), 3.16-3.22 (dd, *J*=19.13 Hz, 1H), 2.78-2.80 (m, 1H), 1.17-1.19 (d, *J*=6.6 Hz, 6H); ¹³C-NMR (DMSO-d₆): 24.08, 30.51, 33.25, 63.42, 121.72, 125.78, 126.21, 127.52, 128.26, 130.93, 131.19, 135.93, 139.54, 147.07, 154.24; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈BrNO: 344.0572, found: 344.0576.

3-(4-chlorophenyl)-5-(4-isopropylphenyl)isoxazoline (2k)

Yield 60%; white crystal; mp: 130-131°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 7.05-7.50(m, 8H), 4.08-4.13 (dd, *J*=14.07 Hz, 1H), 3.12-3.19 (dd, *J*=19.86 Hz, 1H), 2.90-2.97 (dd, *J*=19.30 Hz, 1H), 2.76-2.85 (m, 1H), 1.14-1.16 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 24.07, 30.72, 33.26, 63.46, 115.25, 125.79, 127.54, 128.09, 128.39, 130.57, 133.31, 139.61, 147.06, 154.18, 160.88, 164.14; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈ClNO: 300.1077, found: 300.1072.

3-(4-fluorophenyl)-5-(4-isopropylphenyl)isoxazoline (2l)

Yield 55%; white powder; mp: 132-133°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 6.95-7.49(m, 8H) 4.29-4.33 (dd, *J*=13.83 Hz, 1H), 3.55-3.62 (dd, *J*=22.08 Hz, 1H), 2.97-3.03 (dd, *J*=19.02 Hz, 1H), 2.85-2.90 (m, 1H), 1.21-1.23 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 23.95, 30.22, 33.39, 64.47, 115.54, 126.93, 128.15, 128.49, 130.92, 133.81, 142.00, 148.40, 153.96, 160.97, 164.22 ; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₈FNO: 284.1372, found: 284.1377.

3-phenyl-5-(4-isopropylphenyl)isoxazoline (2-U)

Yield 66%; white powder; mp: 117-118°C; ¹H-NMR (300 MHz, DMSO-d₆) δ: 6.98-7.44(m, 9H) 4.10-4.14 (dd, *J*=11.1 Hz, 1H), 3.10-3.17 (dd, *J*=13.56 Hz, 1H), 2.98-3.05 (dd, *J*=21.63 Hz, 1H), 2.78-2.81 (m, 1H), 1.16-1.19 (d, *J*=7.8 Hz, 6H); ¹³C-NMR (DMSO-d₆): 22.45, 24.37, 24.78, 31.33, 63.59, 127.24, 129.13, 133.39, 138.94, 147.88, 149.82, 154.02, 155.61; HRMS *m/z* (M⁺): Calcd. for C₁₈H₁₉NO: 265.3496, found: 265.3502.

1-acetyl-3-(2-methylphenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3a)

Yield 70%; white powder; mp: 103-104°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.37-7.16 (m, 8H), 5.49-5.54 (dd, *J*=16.08 Hz, 1H), 3.75-3.84 (dd, *J*=29.13 Hz, 1H), 3.19-3.26 (dd, *J*=21.93 Hz, 1H), 2.84-2.89 (m, 1H), 2.67 (s, 3H), 2.40 (s, 3H), 1.20-1.22 (d, *J*=6.93 Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.89, 23.04, 23.96, 33.22, 44.37, 58.40, 125.57, 126.20, 126.65, 129.50, 130.06, 131.67, 137.37, 140.04, 147.36, 154.87, 167.58; HRMS *m/z* (M⁺): Calcd. for C₂₁H₂₄N₂O: 320.4281, found: 320.4285.

1-acetyl-3-(2-bromophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3b)

Yield 77%; brown powder; mp: 123-124°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.65-7.18 (m, 8H), 5.56-5.61 (dd, *J*=16.7 Hz, 1H), 3.64-3.73 (dd, *J*=27.63 Hz, 1H), 3.21-3.28 (dd, *J*=21.4, 1H), 2.84-2.88 (m, 1H), 2.40(s, 3H), 1.19-1.21 (d, *J*=6.9 Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.87, 23.94,

33.21, 44.82, 59.44, 125.1, 126.62, 129.99, 130.21, 131.32, 131.80, 139.77, 147.40, 152.70, 167.68; HRMS m/z (M⁺): Calcd. for C₂₀H₂₁BrN₂O: 385.2976, found: 385.2981.

1-acetyl-3-(2-chlorophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3c)

Yield 74%; white powder; mp: 110-111°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.77- 7.25 (m, 8H), 5.55-5.60 (dd, $J=16.2$ Hz, 1H), 3.87-3.97 (dd, $J=29.9$ Hz, 1H), 3.29-3.37 (dd, $J=22.5$ Hz, 1H), 2.84-2.89 (m, 1H), 2.41 (s, 3H), 1.20-1.22 (d, $J=6.9$ Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.83, 23.94, 33.21, 44.89, 59.35, 125.57, 126.66, 127.53, 130.24, 130.91, 131.84, 139.75, 147.46, 152.93, 167.77; HRMS m/z (M⁺): Calcd. for C₂₀H₂₁ClN₂O: 340.8467, found: 340.8470.

1-acetyl-3-(2-fluorophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3d)

Yield 66%; white powder; mp: 81-82°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.23-7.95 (m, 8H), 5.54-5.59 (dd, $J=16.44$ Hz, 1H), 3.79-3.88 (dd, $J=27.66$ Hz, 1H), 3.24-3.32 (dd, $J=22.92$, 1H), 2.82-2.91 (m, 1H), 2.42 (s, 3H), 1.20-1.22 (d, $J=6.9$ Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.88, 23.97, 33.23, 42.31, 59.60, 114.61, 117.80, 124.87, 125.93, 126.69, 130.40, 135.80, 139.94, 147.56, 152.72, 164.15, 167.73; HRMS m/z (M⁺): Calcd. for C₂₀H₂₁FN₂O: 324.3919, found: 324.3925.

1-acetyl-3-(3-methylphenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3e)

Yield 60%; white powder; mp: 115-116°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.12-7.50 (m, 8H), 5.55-5.60 (dd, $J=16.13$ Hz, 1H), 3.66-3.76 (dd, $J=29.37$ Hz, 1H), 3.12-3.20 (dd, $J=22.06$ Hz, 1H), 2.84-2.88 (m, 1H), 2.43 (s, 3H), 2.40 (s, 3H), 1.20-1.22 (d, $J=6.93$ Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.02, 21.85, 23.97, 33.23, 42.26, 59.25, 123.99, 125.50, 126.65, 127.17, 128.77, 131.22, 138.15, 140.03, 147.38, 154.37, 167.41; HRMS m/z (M⁺): Calcd. for C₂₁H₂₄N₂O: 320.4281, found: 320.4286.

1-acetyl-3-(3-bromophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3f)

Yield 71%; yellow crystal; mp: 125-126°C ¹H-NMR (300 MHz, CDCl₃) δ: 7.11-7.90(m, 1H), 5.56-5.61 (dd, $J=16.4$ Hz, 1H), 3.64-3.74 (dd, $J=29.5$ Hz, 1H), 3.09-3.16 (dd, $J=22.2$ Hz, 1H), 2.84-2.88 (m, 1H), 2.42 (s, 3H), 1.20-1.22 (d, $J=6.9$ Hz, 6H); ¹³C-NMR (DMSO-d₆): 21.87, 23.98, 33.22, 42.00, 59.58, 122.26, 125.59, 126.66, 129.07, 131.06, 132.98, 133.66, 139.83, 147.46, 153.07, 167.66; HRMS m/z (M⁺): Calcd. for C₂₀H₂₁BrN₂O: 385.2976, found: 385.2982.

1-acetyl-3-(3-chlorophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3g)

Yield 63%; white powder; mp: 137-138°C; ¹H-NMR (300 MHz, CDCl₃) δ: 7.18-7.75 (m, 8H), 5.56-5.61 (dd, $J=16.3$ Hz, 1H), 3.65-3.75 (dd, $J=29.5$ Hz, 1H), 3.09-3.17 (dd, $J=22.2$ Hz, 1H),

2.82-2.90 (m, 1H), 2.42 (s, 3H), 1.20-1.22 (d, $J=6.9$ Hz, 6H); ^{13}C -NMR (DMSO- d_6): 21.82, 23.96, 33.23, 42.10, 59.57, 122.30, 125.51, 126.34, 128.99, 131.97, 133.68, 133.90, 139.89, 147.43, 153.10, 167.65; HRMS m/z (M^+): Calcd. for $\text{C}_{20}\text{H}_{21}\text{ClN}_2\text{O}$: 340.8467, found: 340.8470.

1-acetyl-3-(3-fluorophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3h)

Yield 69%; buff crystal; mp: 109-110°C; ^1H -NMR (300 MHz, CDCl_3) δ : 7.12-7.50 (m, 8H), 5.56-5.62 (dd, $J=16.45$ Hz, 1H), 3.66-3.76 (dd, $J=29.48$ Hz, 1H), 3.10-3.18 (dd, $J=22.20$ Hz, 1H), 2.84-2.89 (m, 1H), 2.42 (s, 3H) 1.20-1.22 (d, $J=6.9$ Hz, 6H); ^{13}C -NMR (DMSO- d_6): 21.81, 23.95, 33.23, 42.14, 59.58, 113.41, 117.26, 122.94, 125.57, 126.66, 131.04, 133.73, 139.87, 147.45, 153.29, 160.78, 164.02, 167.64; HRMS m/z (M^+): Calcd. for $\text{C}_{20}\text{H}_{21}\text{FN}_2\text{O}$: 324.3919, found: 324.3924.

1-acetyl-3-(4-methylphenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3i)

Yield 80%; white powder; mp: 97-98°C; ^1H -NMR (300 MHz, CDCl_3) δ : 7.12-7.64 (m, 8H), 5.54-5.59 (dd, $J=16.17$ Hz, 1H), 3.65-3.75 (dd, $J=29.31$ Hz, 1H), 3.11-3.19 (dd, $J=22.02$ Hz, 1H), 2.81-2.90 (m, 1H), 2.42 (s, 3H), 2.39(s, 3H) 1.19-1.22 (d, $J=6.9$ Hz, 6H); ^{13}C -NMR (DMSO- d_6): 21.13, 21.83, 23.96, 42.24, 59.22, 125.52, 126.71, 128.55, 129.45, 140.22, 147.35, 154.27, 167.33; HRMS m/z (M^+): Calcd. for $\text{C}_{21}\text{H}_{24}\text{N}_2\text{O}$: 320.4281, found: 320.4287.

1-acetyl-3-(4-bromophenyl)-5-(4-isopropylphenyl)-2-pyrazoline-1 (3j)

Yield 66%; brown powder; mp: 126-127°C; ^1H -NMR (300 MHz, CDCl_3) δ : 7.14-7.65 (m, 8H), 5.56-5.61 (dd, $J=16.30$ Hz, 1H), 3.65-3.74 (dd, $J=29.43$ Hz, 1H), 3.09-3.16 (dd, $J=22.20$ Hz, 1H), 2.81-2.90 (m, 1H), 2.41 (s, 3H), 1.19-1.22 (d, $J=6.9$ Hz, 6H); ^{13}C -NMR (DMSO- d_6): 21.84, 23.96, 33.22, 42.05, 59.54, 123.75, 125.55, 126.66, 128.67, 130.52, 131.88, 139.88, 147.43, 153.38, 167.54; HRMS m/z (M^+): Calcd. for $\text{C}_{20}\text{H}_{21}\text{BrN}_2\text{O}$: 385.2976, found: 385.2981.

1-acetyl-3-(4-chlorophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3k)

Yield 77%; white powder; mp: 118-119°C; ^1H -NMR (300 MHz, CDCl_3) δ : 7.13-7.75 (m, 8H), 5.56-5.61 (dd, $J=16.23$ Hz, 1H), 3.66-3.76 (dd, $J=29.4$ Hz, 1H), 3.10-3.18 (dd, $J=22.11$ Hz, 1H), 2.82-2.90 (m, 1H), 2.41 (s, 3H), 1.20-1.22 (d, $J=6.9$ Hz, 6H); ^{13}C -NMR (DMSO- d_6): 21.79, 23.92, 33.19, 42.25, 59.44, 116.06, 125.53, 126.62, 127.88, 129.12, 139.93, 147.39, 153.36, 161.70, 164.99, 167.43; HRMS m/z (M^+): Calcd. for $\text{C}_{20}\text{H}_{21}\text{ClN}_2\text{O}$: 340.8467, found: 340.8472.

1-acetyl-3-(4-fluorophenyl)-5-(4-isopropylphenyl)-2-pyrazoline (3l)

Yield 63%; white powder; mp: 106-107°C; ^1H -NMR (300 MHz, CDCl_3) δ : 7.15-7.77 (m, 8H),

5.56-5.61 (t, $J=16.23$ Hz, 1H), 3.66-3.76 (dd, $J=29.3$ Hz, 1H), 3.10-3.18 (dd, $J=22.2$ Hz, 1H), 2.84-2.92 (m, 1H), 2.41 (s, 3H), 1.20-1.22 (d, $J=6.9$ Hz, 6H); $^{13}\text{C-NMR}$ (DMSO- d_6): 21.82, 23.96, 33.23, 42.28, 59.45, 115.80, 116.09, 125.55, 126.65, 127.94, 129.04, 139.96, 147.41, 153.39, 167.45; HRMS m/z (M^+): Calcd. for $\text{C}_{20}\text{H}_{21}\text{FN}_2\text{O}$: 324.3919, found: 324.3925.

1-acetyl-3-phenyl-5-(4-isopropylphenyl)-2-pyrazoline (3-U)

Yield 78%; white powder; mp: 91-92°C; $^1\text{H-NMR}$ (300 MHz, CDCl_3) δ : 7.16-7.69 (m, 9H), 5.57-5.65 (dd, $J=15.84$ Hz, 1H), 3.69-3.79 (dd, $J=29.30$ Hz, 1H), 3.16-3.24 (dd, $J=24.36$ Hz, 1H), 2.85-2.95 (m, 1H), 2.49 (s, 3H), 1.21-1.24 (d, $J=6.9$ Hz, 6H); $^{13}\text{C-NMR}$ (DMSO- d_6): 21.76, 24.22, 42.42, 59.45, 126.13, 127.08, 129.20, 130.04, 140.88, 148.01, 155.03, 167.63; HRMS m/z (M^+): Calcd. for $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}$: 306.4015, found: 306.4018.

Table S1. The structure, yield and melting point of title compounds

Compounds	Linking cycle	R	Appearance	Yield	Mp (°C)
2a	isoxazoline	<i>o</i> -CH ₃	white powder	57%	124-125
2b	isoxazoline	<i>o</i> -Br	brown powder	49%	152-153
2c	isoxazoline	<i>o</i> -Cl	white powder	53%	138-139
2d	isoxazoline	<i>o</i> -F	buff crystal	50%	143-144
2e	isoxazoline	<i>m</i> -CH ₃	white powder	60%	114-115
2f	isoxazoline	<i>m</i> -Br	gray powder	65%	143-144
2g	isoxazoline	<i>m</i> -Cl	white powder	62%	134-135
2h	isoxazoline	<i>m</i> -F	yellow crystal	61%	156-157
2i	isoxazoline	<i>p</i> -CH ₃	white crystal	67%	115-116
2j	isoxazoline	<i>p</i> -Br	gray crystal	57%	125-126
2k	isoxazoline	<i>p</i> -Cl	white crystal	60%	130-131
2l	isoxazoline	<i>p</i> -F	white powder	55%	132-133
2-U ^{a)}	isoxazoline	H	white powder	66%	117-118
3a	pyrazoline	<i>o</i> -CH ₃	white powder	70%	103-104
3b	pyrazoline	<i>o</i> -Br	brown powder	77%	123-124
3c	pyrazoline	<i>o</i> -Cl	white powder	74%	110-111
3d	pyrazoline	<i>o</i> -F	white powder	66%	81-82
3e	pyrazoline	<i>m</i> -CH ₃	white powder	60%	115-116
3f	pyrazoline	<i>m</i> -Br	yellow crystal	71%	125-126
3g	pyrazoline	<i>m</i> -Cl	white powder	63%	137-138
3h	pyrazoline	<i>m</i> -F	buff crystal	69%	109-110
3i	pyrazoline	<i>p</i> -CH ₃	white powder	80%	97-98
3j	pyrazoline	<i>p</i> -Br	brown powder	66%	126-127
3k	pyrazoline	<i>p</i> -Cl	white powder	77%	118-119
3l	pyrazoline	<i>p</i> -F	white powder	63%	106-107
3-U ^{b)}	pyrazoline	H	white powder	78%	91-92

^{a)} Unsubstituted isoxazoline derivatives

^{b)} Unsubstituted pyrazoline derivatives

Table S2 EC₅₀ values of compounds containing fluorine atom against
six fungi

Compound	EC ₅₀ ± SE (µg·mL ⁻¹)					
	<i>B. cinerea</i>	<i>C. lagenarium</i>	<i>Py. oryzae</i>	<i>Ph. piricola</i>	<i>R. solani</i>	<i>S. sclerotiorum</i>
2d	18.75 ± 1.66	53.38 ± 4.26	15.58 ± 1.27	7.25 ± 0.64	16.83 ± 1.34	34.53 ± 2.42
2h	33.36 ± 2.87	188.54 ± 15.54	55.64 ± 4.81	10.51 ± 0.84	>200	22.59 ± 1.50
2l	77.84 ± 7.15	110.23 ± 10.05	132.27 ± 11.04	13.68 ± 0.95	163.26 ± 12.21	20.80 ± 1.43
3d	14.28 ± 0.13	95.51 ± 8.57	20.87 ± 1.65	15.67 ± 1.18	84.61 ± 7.25	12.75 ± 0.88
3h	69.87 ± 6.33	153.89 ± 13.84	86.93 ± 8.03	60.08 ± 5.27	>200	20.76 ± 1.61
3l	82.41 ± 7.38	133.67 ± 11.36	147.43 ± 12.24	47.36 ± 4.05	170.63 ± 14.30	22.80 ± 1.60
Cuminaldehyde	66.94 ± 5.80	>200	128.95 ± 9.46	25.50 ± 1.83	96.75 ± 8.84	63.62 ± 5.45
Thiabendazole	18.85 ± 1.62	47.35 ± 3.69	73.21 ± 6.53	21.84 ± 1.73	10.56 ± 0.75	44.57 ± 3.36
Azoxystrobin	54.52 ± 4.79	96.88 ± 8.75	70.82 ± 6.04	87.59 ± 7.80	92.57 ± 8.16	35.22 ± 2.77