# Combined strategy for phytotoxicity enhancement of benzoxazinones

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**SUPPORTING INFORMATION**

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*Physical Data*

*6-Fluoro-4-propyl-(2H)-1,4-benzoxazin-3(4H)-one (6-F-4-Pr-D-DIBOA).* FTIR (cm-1): 1674, 1718. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.8 [d, 2H, J=14 (H-2)], δ 6.65 [dd, 1H, J=2.3, 5.7 (H-5), δ 6.77 [dt, 1H, J=2.3, 4.9, 9 (H-7)], δ 7.00 [dd, 1H, J=4.9, 5.7 (H-8)], δ 2.76 [q, 2H, J=7.4 (H-12)], δ 1.38 [t, 3H, J=7.4 (H-13)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 68.5 [s, (C-2)], 159.6 [s, (C-3)], 100.5 [d, (C-5)], 158.4 [d, (C-6)], 111.1 [d, (C-7)], 118.1 [d, (C-8)], 139.8 [s, (C-9)], 129.0 [s, (C-10)], 170.0 [s, (C-11)], 25.0 [s, (C-12)], 9.16 [s, (C-13)].EI-MS m/z (%):239$[M]^+$; 105$[M\text{-}OH]^+$

*6-Fluoro-4-valeryl-(2H)-1,4-benzoxazin-3(4H)-one (6-F-4-Val-D-DIBOA):* FTIR (cm-1): 1674, 1718. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.8 [d, 2H, J=14 (H-2)], δ 6.65 [dd, 1H, J=2.3, 5.7, 8.4 (H-5), δ 6.78 [dt, 1H, J=2.3, 4.9, 9 (H-7)], δ 7.00 [dd, 1H, J=4.9, 5.7 (H-8)], δ 2.71 [q, 2H, J=8 (H-12)], δ 1.84 [m, 3H, J=8.1 (H-13)], δ 1.53 [m, 3H, J=8.1 (H-14)], δ 1.03 [t, 3H, J=7.3 (H-15)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 68.5 [s, (C-2)], 159.6 [s, (C-3)], 100.5 [d, (C-5)], 158.5 [d, (C-6)], 111.0 [d, (C-7)], 118.1 [d, (C-8)], 139.8 [s, (C-9)], 130.0 [s, (C-10)], 169.3 [s, (C-11)], 31.1 [s, (C-12)], 27.1 [s, (C-13)], 22.5 [s, (C-13)], 13.9 [s, (C-13)]. EI-MS m/z (%): 267$[M]^+$

*2-Ethyl-6-fluoro-(2H)-1,4-benzoxazin-3(4H)-one (6-F-2-Et-D-DIBOA):* FTIR (cm-1): 1677, 3090. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.56 [dd, 1H, J=4.9 (H-2)], δ 6.67 [dd, 1H, J=2.3, 5.7 (H-5), δ 6.85 [dd, 1H, J=2.3, 4.9, 9 (H-7)], δ 7.11 [dd, 1H, J=4.9, 5.7 (H-8)], δ 1.86 [m, 2H, J=4.9, 7.5 (H-11)], δ 0.99 [t, 3H, J=7.5 (H-12)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 79.0 [s, (C-2)], 163.7 [s, (C-3)], 101.9 [d, (C-5)], 158.7 [d, (C-6)], 111.0 [d, (C-7)], 117.5 [d, (C-8)], 139.0 [s, (C-9)], 129.0 [s, (C-10)], 24.0 [s, (C-11)], 9.32 [s, (C-12)]. EI-MS m/z (%): 211$[M]^+$

*6-Fluoro-2-propyl-(2H)-1,4-benzoxazin-3(4H)-one (6-F-2-Pr-D-DIBOA):* FTIR (cm-1): 1677, 3115. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.64 [t, 1H, J=5.4 (H-2)], δ 6.81 [d, 1H, J=2.3, 5.7, 8.4 (H-5), δ 6.93 [dd, 1H, J=2.3, 4.9, 9 (H-7)], δ 7.33 [d, 1H, J=4.9, 5.7 (H-8)], δ 1.77 [m, 2H, J=2.3 (H-11)], δ 1.45 [m, 3H, J=7.4 (H-12)], δ 0.88 [t, 3H, J=7.4 (H-13)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 77.3 [s, (C-2)], 163.5 [s, (C-3)], 102.1 [d, (C-5)], 159.8 [d, (C-6)], 111.0 [d, (C-7)], 117.5 [d, (C-8)], 139.1 [s, (C-9)], 129.3 [s, (C-10)], 32.7 [s, (C-11)], 18.5 [s, (C-12)], 13.9 [s, (C-13)].. EI-MS m/z (%): 211$[M]^+$

*6-Fluoro-2-phenyl-(2H)-1,4-benzoxazin-3(4H)-one (6-F-2-Ph-D-DIBOA):* FTIR (cm-1): 1674, 3110. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 5.71 [s, 1H (H-2)], δ 6.68 [dd, 1H (H-5)], δ 6.89 [dd, 1H (H-7)], δ 7.08 [d, 1H (H-8)], δ 7.31 [dd, 1H (H-12)], δ 7.29 [m, 1H (H-13)], δ 7.27 [m, 1H (H-14)], δ 7.29 [m, 1H (H-15)], δ 31 [dd, 1H (H-16)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 79.2 [s, (C-2)], 161.5 [s, (C-3)], 102.0 [d, (C-5)], 158.8 [d, (C-6)], 111.1 [d, (C-7)], 117.6 [d, (C-8)], 138.7 [s, (C-9)], 134.5 [s, (C-10)], 128.3 [d, (C-11)], 126.9 [s, (C-12)], 128.8 [s, (C-13)], 139.3 [s, (C-14)], 128.8 [s, (C-15)], 126.9 [s, (C-16)]. EI-MS m/z (%):259$[M]^+$

*6-Chloro-4-propyl-(2H)-1,4-benzoxazin-3(4H)-one (6-Cl-4-Pr-D-DIBOA):* FTIR (cm-1): 1670, 1721. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.75 [d, 2H, J=14 (H-2)], δ 6.97 [d, 1H, J=2 (H-5)], δ 6.95 [dd, 1H, J=2, 8.5 (H-7)], δ 6.81 [d, 1H (H-8)], δ 2.69 [q, 2H, J=7.5 (H-12)], δ 1.31 [t, 3H (H-13)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 68.1 [s, (C-2)], 158.9 [s, (C-3)], 117.9 [d, (C-5)], 127.9 [s, (C-6)], 124.5 [s, (C-7)], 112.3 [s, (C-8)], 142.1 [s, (C-9)], 128.8 [s, (C-10)], 24.6 [s, (C-11)], 126.9 [s, (C-12)], 8.7 [s, (C-13)]. EI-MS m/z (%): 255$[M]^+$

*6-Chloro-4-valeryl-(2H)-1,4-benzoxazin-3(4H)-one (6-Cl-4-Val-D-DIBOA):* FTIR (cm-1): 1677, 1718. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.83 [d, 2H, J=14 (H-2)], δ 7.06 [d, 1H, J=2 (H-5)], δ 6.86 [dd, 1H, J=2, 8.5 (H-7)], δ 7.00 [d, 1H, J=8.5 (H-8)], δ 2.75 [m, 2H, J=8 (H-12)], δ 1.86 [m, 2H, J=8.5 (H-13)], δ 1.56 [m, 2H, J=8.5 (H-14)], δ 1.06 [t, 3H, J=7.3 (H-15)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 68.4 [s, (C-2)], 159.2 [s, (C-3)], 118.3 [s, (C-5)], 128.3 [s, (C-6)], 124.8 [s, (C-7)], 112.7 [s, (C-8)], 142.4 [s, (C-9)], 129.1 [s, (C-10)], 169.3 [s, (C-11)], 31.2 [s, (C-12)], 27.0 [s, (C-13)], 22.5 [s, (C-14)], 13.9 [s, (C-15)]. EI-MS m/z (%): 283$[M]^+$

*6-Chloro-2-Ethyl- (2H)-1,4-benzoxazin-3(4H)-one (6-Cl-2-Et-D-DIBOA):* FTIR (cm-1): 1677, 3090. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.70 [t, 2H, J=4.5 (H-2)], δ 7.45 [d, 1H, J=2.7 (H-5)], δ 6.96 [dd, 1H, J=2, 8.5 (H-7)], δ 7.08 [d, 1H, J=8.5 (H-8)], δ 1.97 [q, 2H, J=4.5, 7.5 (H-11)], δ 1.11 [t, 3H, J=7.5 (H-12)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 79.3 [s, (C-2)], 163.3 [s, (C-3)], 117.9 [s, (C-5)], 128.1 [s, (C-6)], 125.0 [s, (C-7)], 114.3 [s, (C-8)], 141.7 [s, (C-9)], 128.8 [s, (C-10)], 24.4 [s, (C-11)], 9.48 [s, (C-12)]. EI-MS m/z (%): 227$[M]^+$

*6-Chloro-2-propyl-(2H)-1,4-benzoxazin-3(4H)-one (6-Cl-2-Pr-D-DIBOA):* FTIR (cm-1): 1677, 3090. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.65 [t, 1H, J=6.4 (H-2)], δ 7.34 [d, 1H, J=2.3, 8.2 (H-5)], δ 6.83 [dd, 1H, J=2.3, 8.5 (H-7)], δ 6.94 [d, 1H, J=8.2 (H-8)], δ 1.78 [m, 2H, J=6.4 (H-11)], δ 1.47 [m, 2H, J=7.2 (H-12)], δ 0.88 [t, 3H, J=7.2 (H-13)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 77.3 [s, (C-2)], 163.5 [s, (C-3)], 102.1 [d, (C-5)], 159.8 [d, (C-6)], 111.0 [d, (C-7)], 117.5 [d, (C-8)], 139.1 [s, (C-9)], 129.3 [s, (C-10)], 32.7 [s, (C-11)], 18.5 [s, (C-12)], 13.9 [s, (C-13)]. EI-MS m/z (%): 241$[M]^+$

*6-Chloro-2-phenyl-(2H)-1,4-benzoxazin-3(4H)-one(6-Cl-2-Ph-D-DIBOA):* FTIR (cm-1): 1674, 3110. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 5.73 [s, 1H (H-2)], δ 6.96 [dd, 1H (H-5)], δ 6.87 [dd, 1H (H-7)], δ 7.29 [d, 1H (H-8)], δ 7.33 [d, 1H (H-12)], δ 7.29 [m, 1H (H-13)], δ 7.29 [m, 1H (H-14)], δ 7.29 [m, 1H (H-15)], δ 7.33 [d, 1H (H-16)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 79.4 [s, (C-2)], 160.9 [s, (C-3)], 118.1 [s, (C-5)], 128.1 [s, (C-6)], 125.0 [s, (C-7)], 114.2 [d, (C-8)], 141.5 [s, (C-9)], 128.3 [s, (C-10)], 134.3 [s, (C-11)], 127.1 [s, (C-12)], 129.1 [s, (C-13)], 129.6 [s, (C-14)], 129.1 [s, (C-15)], 129.1 [s, (C-16)]. EI-MS m/z (%): 275$[M]^+$; 105$[M\text{-}OH]^+$

*8-Chloro-4-propyl-(2H)-1,4-benzoxazin-3(4H)-one (8-Cl-4-Pr-D-DIBOA):* FTIR (cm-1): 1673, 1718. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.84 [d, 2H, J=14 (H-2)], δ 6.73 [dd, 1H, J=1.1, 8.1 (H-5)], δ 6.91 [dd, 1H, J=8.1 (H-6)], δ 7.06 [d, 1H, J=1.1, 8.2 (H-7)], δ 2.67 [q, 2H, J=7.4 (H-12)], δ 1.30 [t, 3H, J=7.4 (H-13)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 68.2 [s, (C-2)], 158.5 [s, (C-3)], 110.5 [d, (C-5)], 122.8 [s, (C-6)], 125.5 [s, (C-7)], 122.2 [s, (C-8)], 139.6 [s, (C-9)], 129.9 [s, (C-10)], 169.7 [s, (C-11)], 24.6 [s, (C-12)], 8.69 [s, (C-13)]. EI-MS m/z (%): 255$[M]^+$

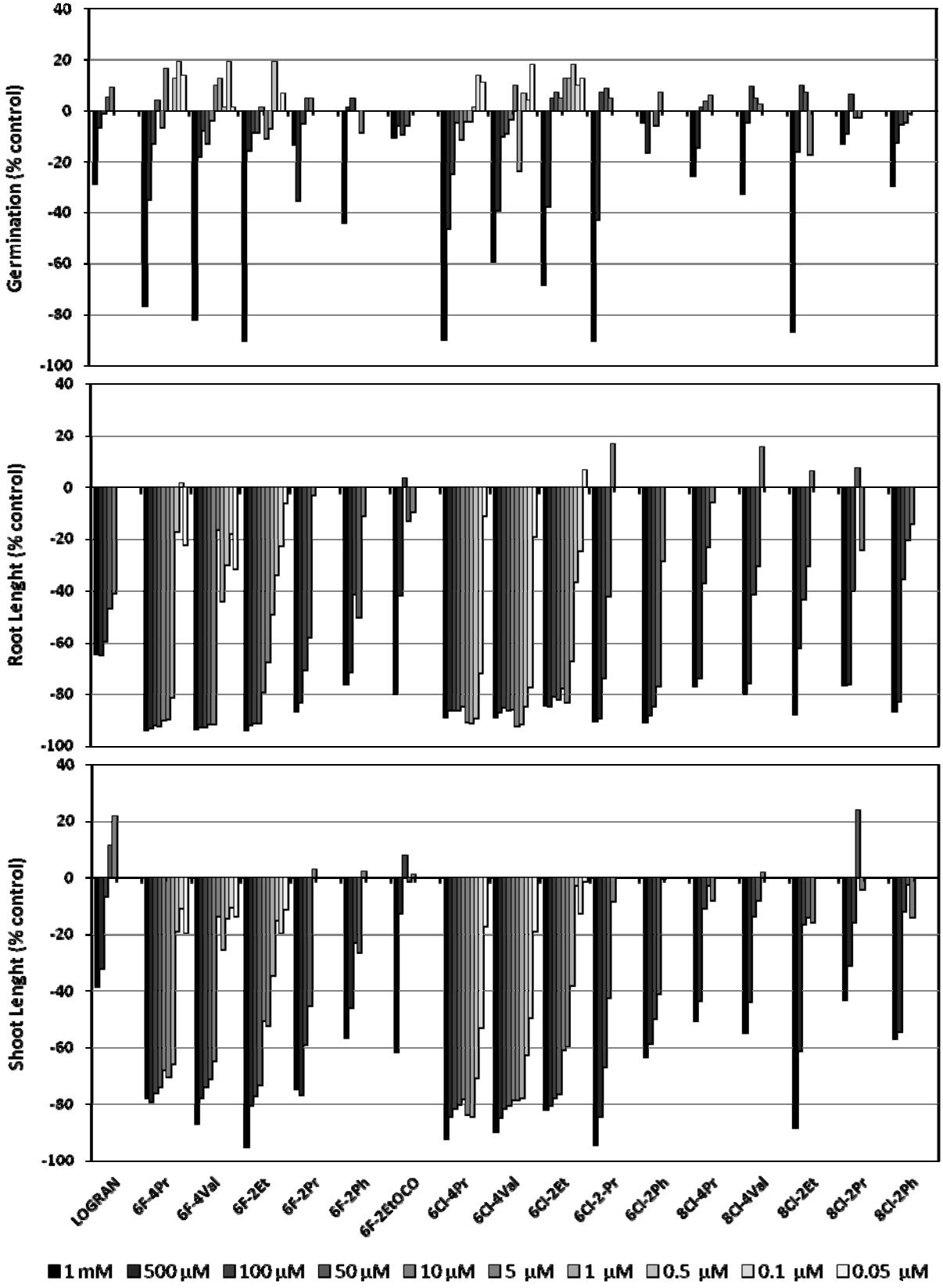
*8-Chloro-4-valeryl-(2H)-1,4-benzoxazin-3(4H)-one (8-Cl-4-Val-D-DIBOA):* FTIR (cm-1): 1673, 1718. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.93 [d, 2H, J=13.9 (H-2)], δ 6.82 [d, 1H, J=8.2 (H-5)], δ 7.17 [d, 1H, J=2, 8.2 (H-6)], δ 7.01 [dd, 1H, J=1.1, 8.2 (H-7)], δ 1.85 [m, 2H, J=8 (H-12)], δ 1.50 [m, 2H, J=8 (H-13)], δ 1.32 [m, 2H, J=7.3 (H-14)], δ 1.02 [t, 3H, J=7.3 (H-15)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 68.6 [s, (C-2)], 158.9 [s, (C-3)], 110.9 [s, (C-5)], 123.2 [s, (C-6)], 125.9 [s, (C-7)], 122.6 [s, (C-8)], 139.8 [s, (C-9)], 129.3 [s, (C-10)], 169.4 [s, (C-11)], 31.2 [s, (C-12)], 27.0 [s, (C-13)], 22.5 [s, (C-14)], 14 [s, (C-15)]. EI-MS m/z (%): 283$[M]^+$

*8-Chloro-2-Ethyl-(2H)-1,4-benzoxazin-3(4H)-one (8-Cl-2-Et-D-DIBOA):* FTIR (cm-1): 1679, 3095. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.80 [m, 2H, J=4.5 (H-2)], δ 7.04 [dd, 1H, J=1.1, 8.1 (H-5)], δ 7.37 [dd, 1H, J=8.1, 8.2 (H-6)], δ 7.15 [d, 1H, J=1.1, 8.2 (H-7)], δ 2.24 [m, 1H (H-11a)], δ 1.95 [m, 1H (H-11b)], δ 1.16 [t, 1H, J=7.3 (H-12)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 79.7 [s, (C-2)], 163.0 [s, (C-3)], 126.1 [s, (C-5)], 123.1 [s, (C-6)], 126.1 [s, (C-7)], 122.3 [s, (C-8)], 139.2 [s, (C-9)], 129.1 [s, (C-10)], 24.5 [s, (C-11)], 9.70 [s, (C-12)]. EI-MS m/z (%): 227$[M]^+$

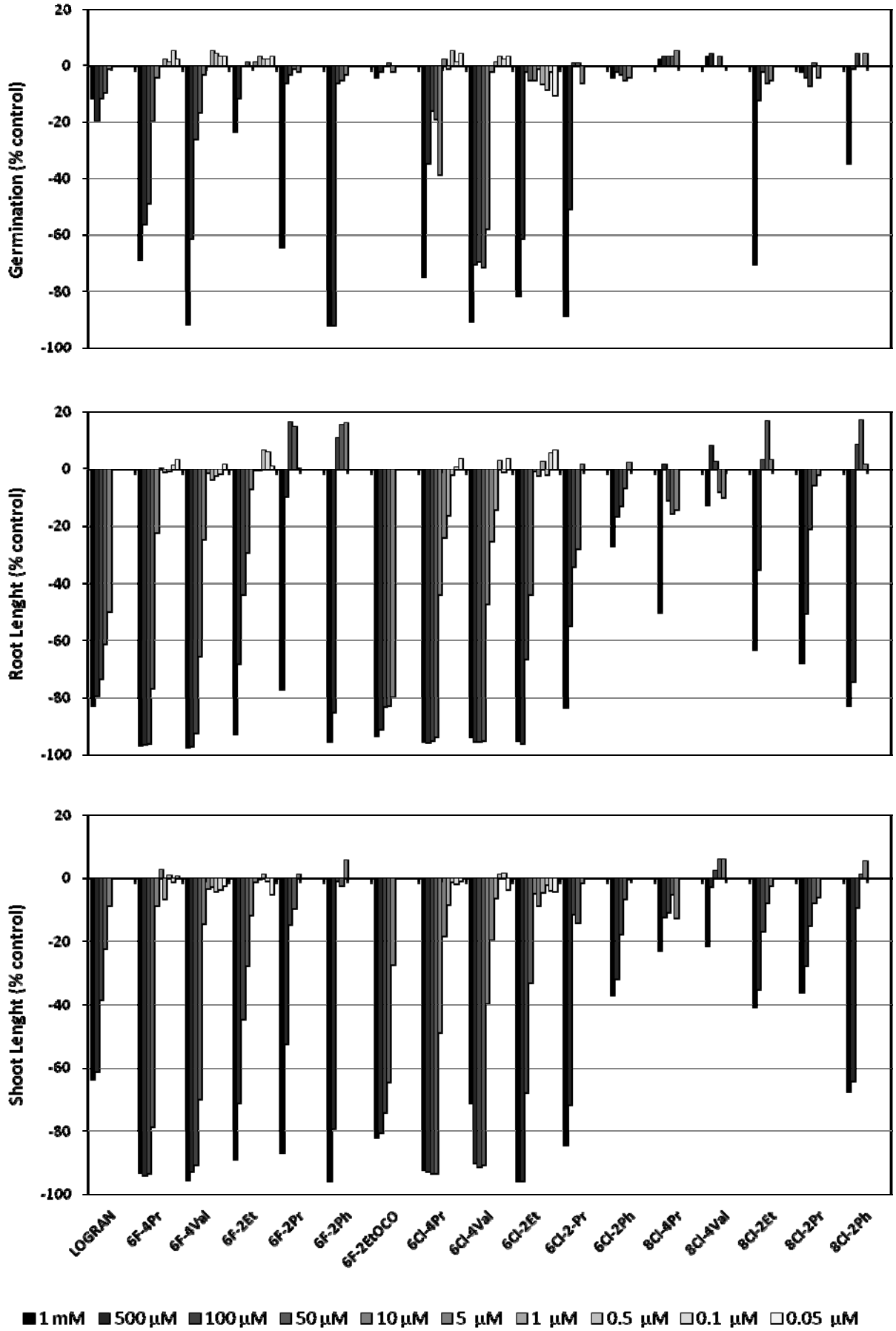
*8-Chloro-2-propyl-(2H)-1,4-benzoxazin-3(4H)-one (8-Cl-2-Pr-D-DIBOA):* FTIR (cm-1): 1677, 3075. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 4.86 [m, 1H, J=4.5 (H-2)], δ 7.00 [dd, 1H, J=1.1, 8.1 (H-5)], δ 7.39 [dd, 1H, J=8.1, 8.2 (H-6)], δ 7.20[d, 1H, J=1.1, 8.2 (H-7)], δ 2.22 [m, 2H, J=7.3 (H-11)], δ 1.86 [m, 2H, J=7.2 (H-12)], δ 1.62 [t, 3H, J=7.2 (H-13)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 78.3 [s, (C-2)], 163.0 [s, (C-3)], 112.5 [d, (C-5)], 123.1 [d, (C-6)], 126.1 [d, (C-7)], 122.3 [d, (C-8)], 139.1 [s, (C-9)], 129.0 [s, (C-10)], 32.9 [s, (C-11)], 18.5 [s, (C-12)], 13.9 [s, (C-13)]. EI-MS m/z (%): 241$[M]^+$

*8-Chloro-2-phenyl-(2H)-1,4-benzoxazin-3(4H)-one (8-Cl-2-Ph-D-DIBOA):* FTIR (cm-1): 1674, 3115. $^{1}$H-NMR ($ClCD_3$, 400 MHz): δ 5.88 [s, 1H (H-2)], δ 6.92 [dd, 1H (H-5)], δ 7.25 [dd, 1H (H-6)], δ 7.07 [dd, 1H (H-7)], δ 7.36 [dd, 1H (H-12)], δ 7.25 [m, 1H (H-13)], δ 7.24 [m, 1H (H-14)], δ 7.25 [m, 1H (H-15)], δ 7.36 [dd, 1H (H-16)]. $^{13}$C-NMR ($ClCD_3$, 100 MHz): 79.0 [s, (C-2)], 160.8 [s, (C-3)], 112.6 [d, (C-5)], 123.0 [d, (C-6)], 125.9 [d, (C-7)], 122.0 [d, (C-8)], 139.0 [s, (C-9)], 128.7 [s, (C-10)], 133.6 [d, (C-11)], 126.3 [s, (C-12)], 128.8 [s, (C-13)], 129.2 [s, (C-14)], 128.8 [s, (C-15)], 126.3 [s, (C-16)]. EI-MS m/z (%): 275$[M]^+$

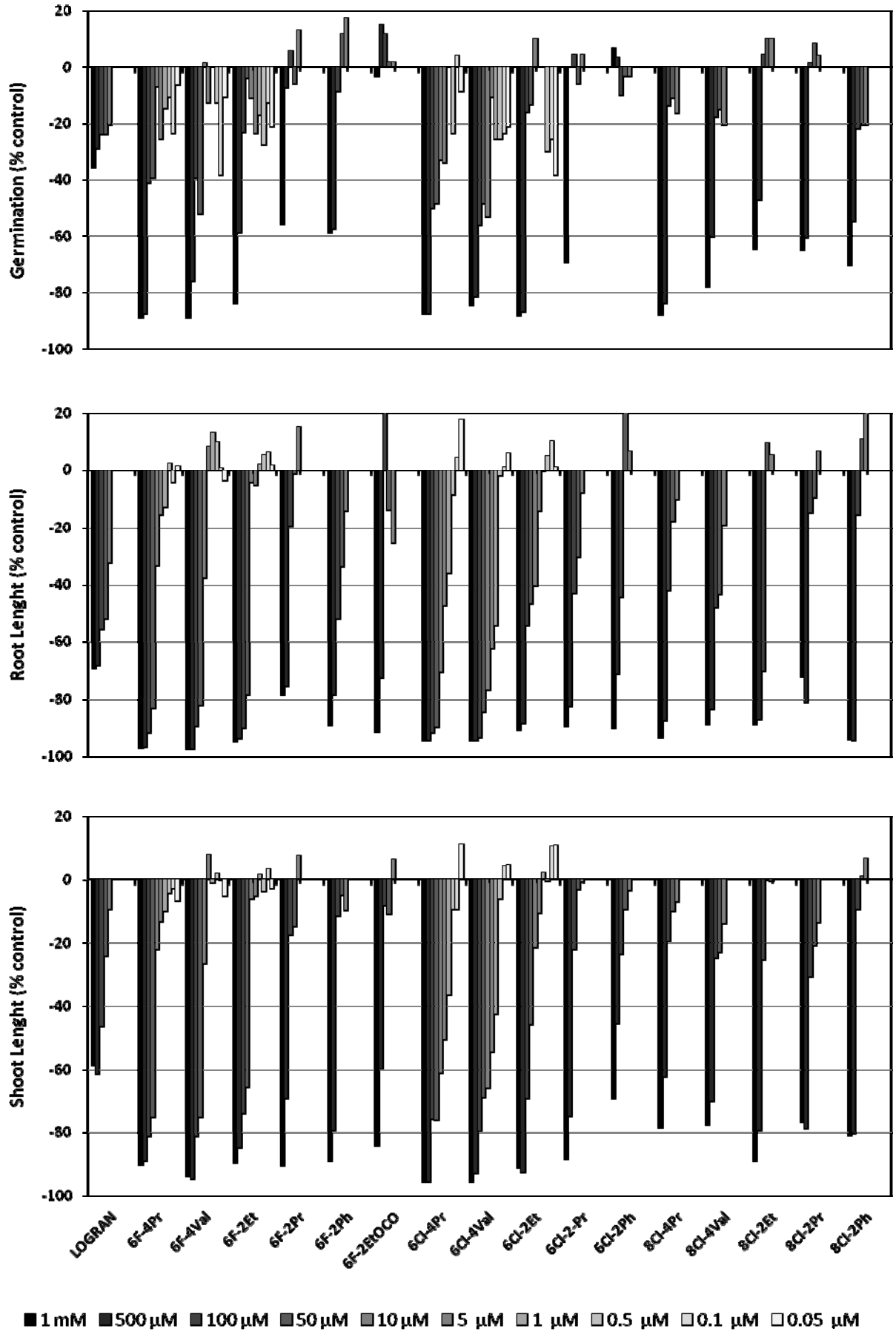
*Lepidium sativum* L.



*Lactuca sativa* L.



*Licopersicon esculentum* L.



*Allium cepa* L.