Appendix A. Supplementary data

Unveiling the phytoalexin biosynthetic puzzle in salt cress: Unprecedented incorporation of glucobrassicin into wasalexins A and B

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MS-ESI of [2,2,4',5',6',7'-2H₆]glucobrassicin (12a) feedings and control feedings
MS-ESI of [2,2,4',5',6',7'-\text{H}_6]glucobrassicin (12a) feedings and control feedings
MS-ESI of \([^{2}H_3C-S\ 4',5',6',7'-^2H_4]-1\)-methoxybrassinin (6a) feedings and control feedings
'H NMR spectrum of [2,2,4',5',6',7'-2H6]Glucobrassicin in D2O
The image contains a chemical structure and a 13C NMR spectrum of [2,2',4',5',6',7'-2H6]Glucobrassicin in D2O. The spectrum shows the presence of various carbon atoms labeled with their corresponding chemical shifts. The structure includes a glucosinolate moiety with multiple hydroxyl groups, a nitrogen atom, and a sulfur atom. The spectrum highlights the chemical shifts of C-1 to C-7' and C-1'' to C-6''.
Demethoxydihydrowasalexin - $^1$H NMR (CD$_2$Cl$_2$)
Demethoxydihydrowasalexin - $^1$H NMR (CD$_2$Cl$_2$)
Demethoxydihydrowasalexin - $^1$H NMR (CD$_2$Cl$_2$)
Demethoxydihydrowasalexin – $^{13}$C NMR (CD$_2$Cl$_2$)

$^{13}$C NMR (CD$_2$Cl$_2$) spectrum showing peaks at various ppm values, with an annotation indicating $X = \text{impurity}$. The spectrum highlights a peak at 53.6 ppm.
Demethoxywasalexins A and B - $^1$H NMR (CD$_2$Cl$_2$)
Demethoxywasalexins A and B - $^1$H NMR (CD$_2$Cl$_2$)
Demethoxywasalexins A and B – $^{13}$C NMR