

Supplementary Materials

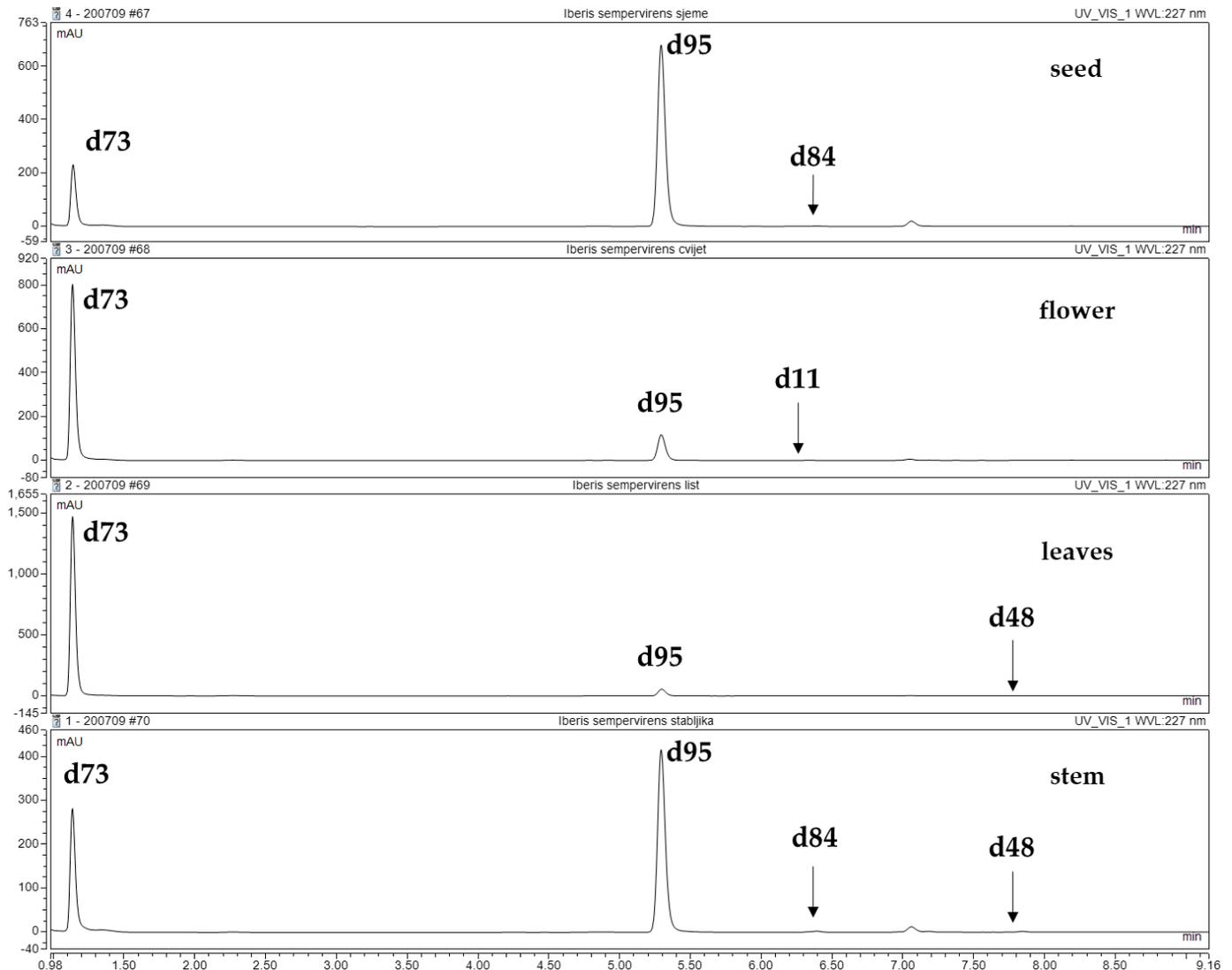
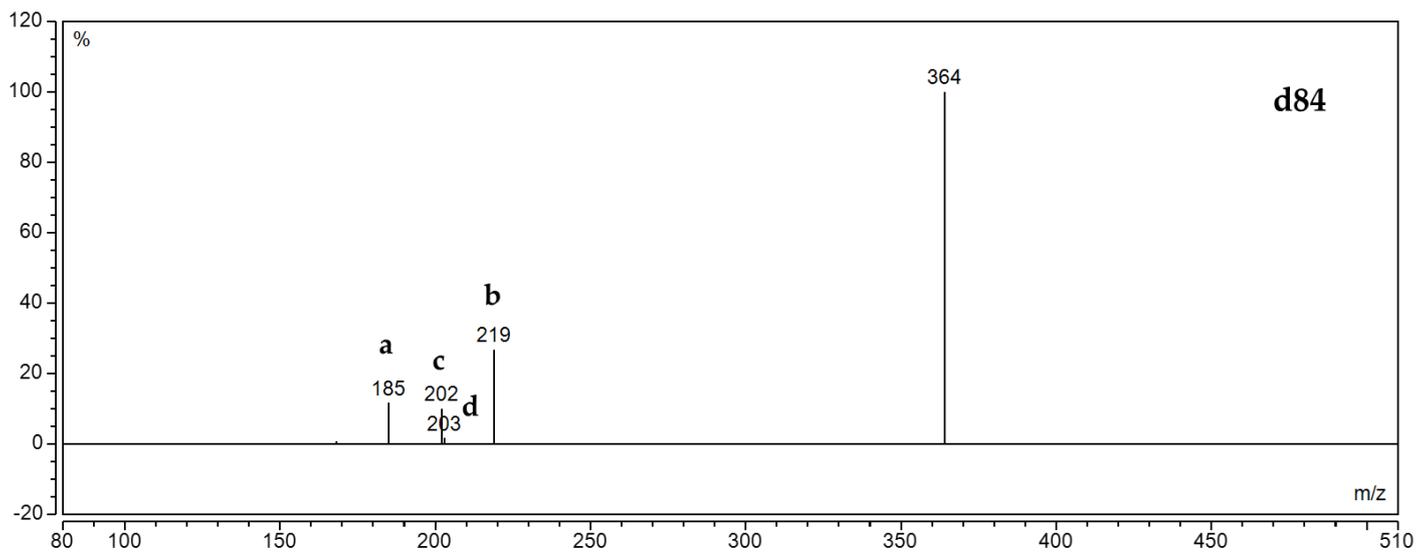
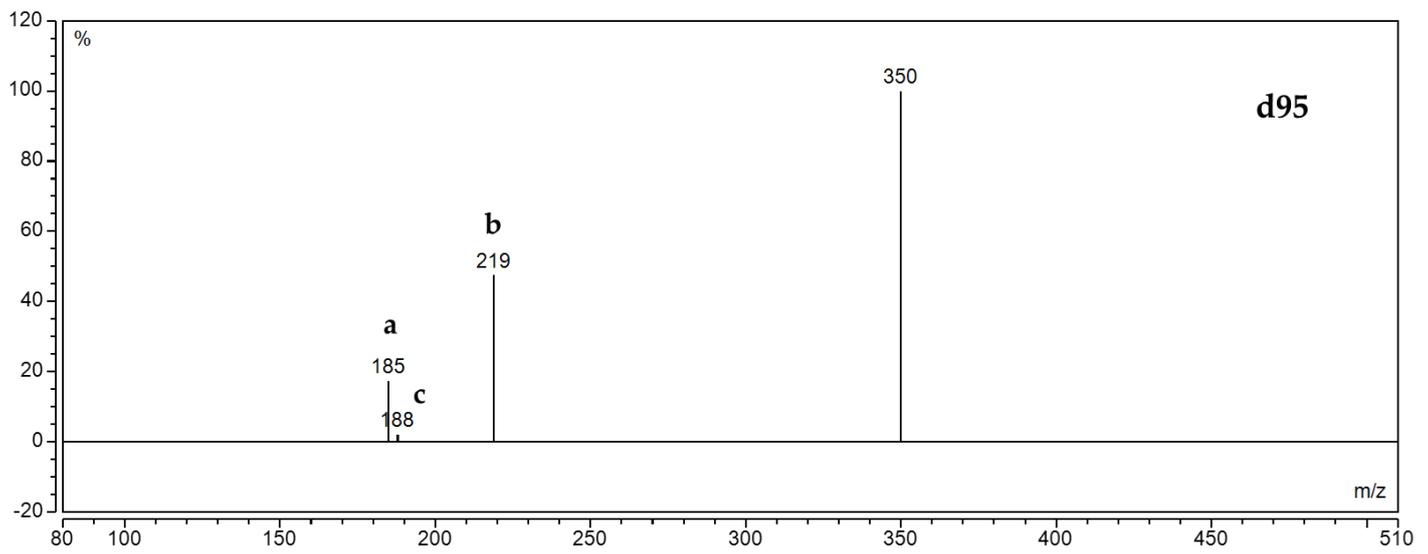
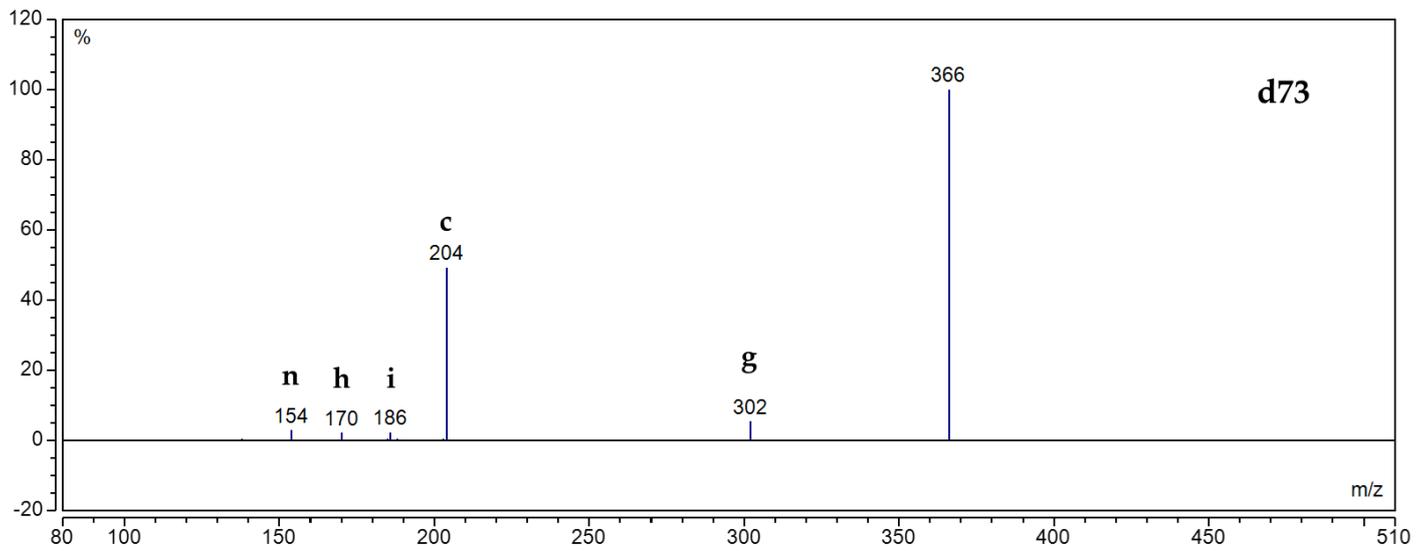


Figure S1. Chromatograms of desulfoglucosinolates (dGSLs) obtained from the different plant parts of *I. sempervirens*. **d73** – 3-(methylsulfinyl)propyl dGSL (desulfoglucoiberin); **d95** – 3-(methylsulfonyl)propyl dGSL (desulfoglucoibervirin); **d84** – 4-(methylsulfonyl)butyl dGSL (desulfoglucoerucin); **d11** – benzyl dGSL (desulfoglucoctropeolin); **d48** – 4-methoxyindol-3-ylmethyl dGSL (desulfo-4-methoxyglucobrassicin).



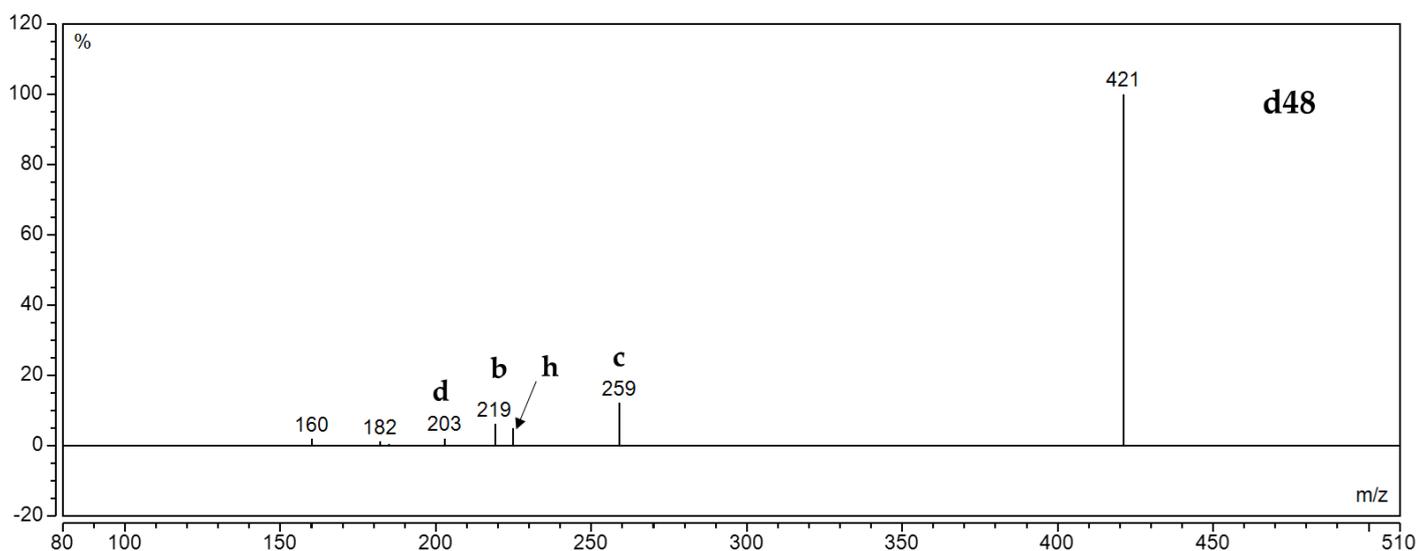
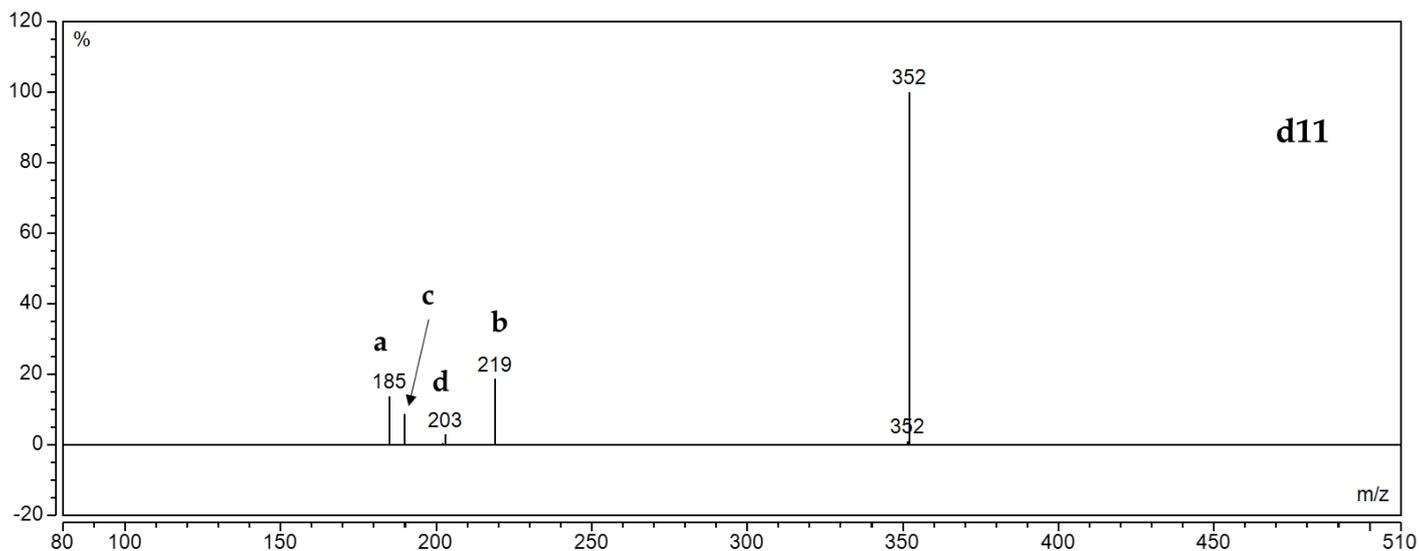


Figure S2. MS² spectra of desulfoglucosinolates from *I. sempervirens*. **d73** – 3-(methylsulfinyl)propyl dGSL (desulfoglucouiberin); **d95** – 3-(methylsulfonyl)propyl dGSL (desulfoglucouibervirin); **d84** – 4-(methylsulfonyl)butyl dGSL (desulfoglucouerucin); **d11** – benzyl dGSL (desulfoglucotropaeolin); **d48** – 4-methoxyindol-3-ylmethyl dGSL (desulfo-4-methoxyglucobrassicin). Fragment types observed, alone or in combination, in MS² spectra desulfoglucosinolates (dGSLs) in positive mode: **a** - Na⁺ adduct of anhydroglucose, C₆H₁₀O₅ (at m/z 185) or an acyl derivative; **b** - Na⁺ adduct of thioglucose, C₆H₁₁O₅SH (at m/z 219) or an acyl derivative; **c** - loss of anhydroglucose (m/z 162) or an acyl derivative; **d** - Na⁺ adduct of glucose, C₆H₁₂O₆ (at m/z 203); **g** - loss of H(SO)CH₃ (m/z 64); **h** - loss of thioglucose (m/z 196); **i** - loss of glucose (m/z 180); **n** - loss of oxo-thioGlc (m/z 212) [1].

Reference

1. Agerbirk, N.; Hansen, C.C.; Olsen, C.E.; Kiefer, C.; Hauser, T. P.; Christensen, S. et al. Glucosinolate profiles and phylogeny in *Barbarea* compared to other tribe Cardamineae (Brassicaceae) and *Reseda* (Resedaceae), based on a library of ion trap HPLC-MS/MS data of reference desulfoglucosinolates. *Phytochemistry*, **2021**, *185*, 112658 <https://doi.org/10.1016/j.phytochem.2021.112658>