
Supplementary Materials

Glucosinolates of *Sisymbrium officinale* and *S. orientale*

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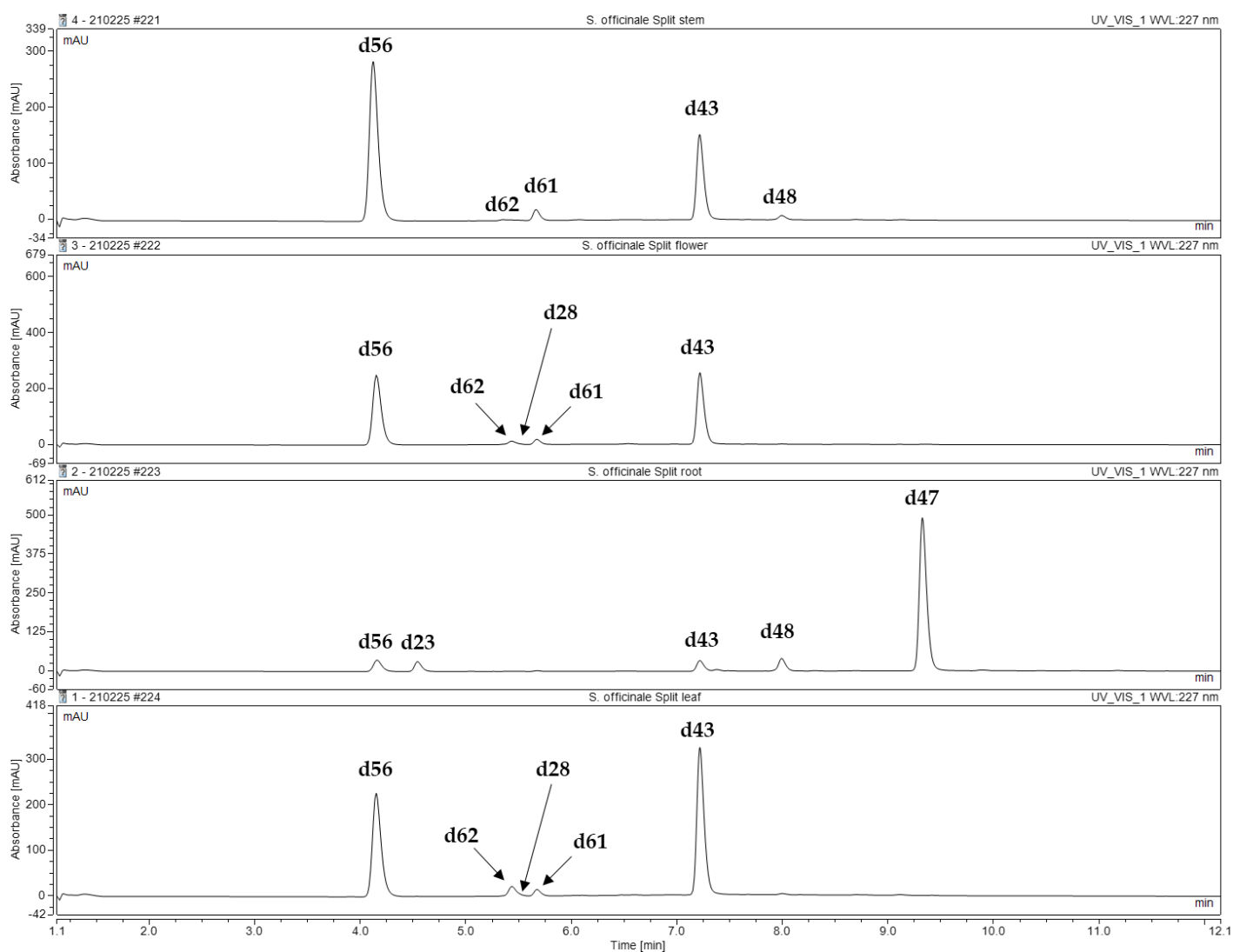


Figure S1. Chromatogram of desulfoglucosinolates obtained from the different plant parts of *S. officinale* from Split:

d56 - desulfoisopropyl GSL (desulfoglucoputranjivin), **d61** - desulfo-*sec*-butyl GSL (desulfoglucocochlearin), **d62** - desulfoisobutyl GSL, **d23** - desulfo-4-hydroxybenzyl GSL (desulfoglucosinalbin), **d28** - desulfo-4-hydroxyindol-3-ylmethyl GSL (desulfo-4-hydroxyglucobrassicin), **d43** - desulfoindol-3-ylmethyl GSL (desulfoglucobrassicin), **d47** - desulfo-*N*-methoxyindol-3-ylmethyl GSL (desulfoneoglucobrassicin), **d48** - desulfo-4-methoxyindol-3-ylmethyl GSL (desulfo-4-methoxyglucobrassicin).

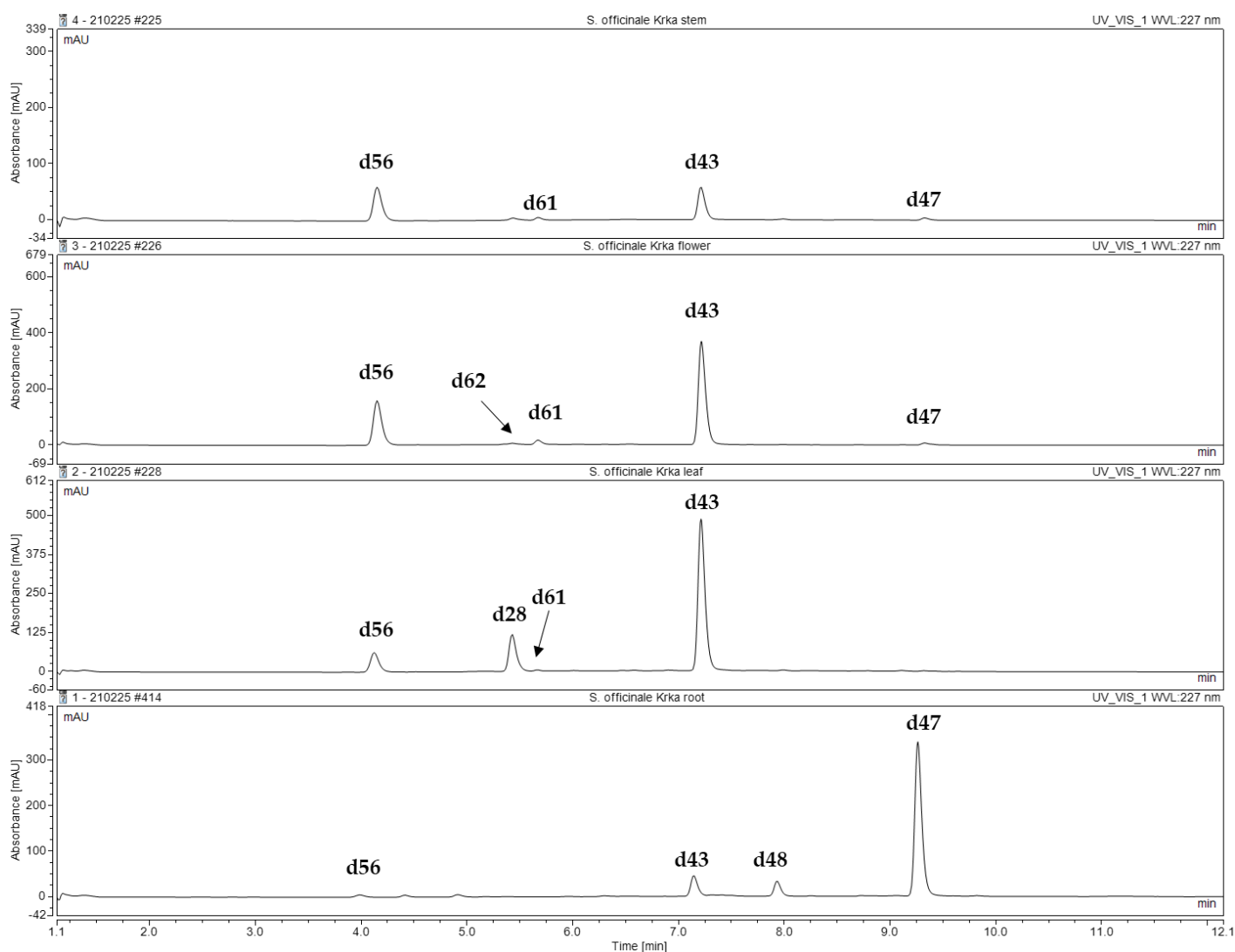


Figure S2. Chromatogram of desulfoglucosinolates obtained from the different plant parts of *S. officinale* from Krka:

d56 - desulfoisopropyl GSL (desulfoglucoputranjivin), **d61** - desulfo-*sec*-butyl GSL (desulfoglucocochlearin), **d62** - desulfoisobutyl GSL, **d28** - desulfo-4-hydroxyindol-3-ylmethyl GSL (desulfo-4-hydroxyglucobrassicin), **d43** - desulfoindol-3-ylmethyl GSL (desulfoglucobrassicin), **d47** - desulfo-*N*-methoxyindol-3-ylmethyl GSL (desulfoneoglucobrassicin), **d48** - desulfo-4-methoxyindol-3-ylmethyl GSL (desulfo-4-methoxyglucobrassicin).

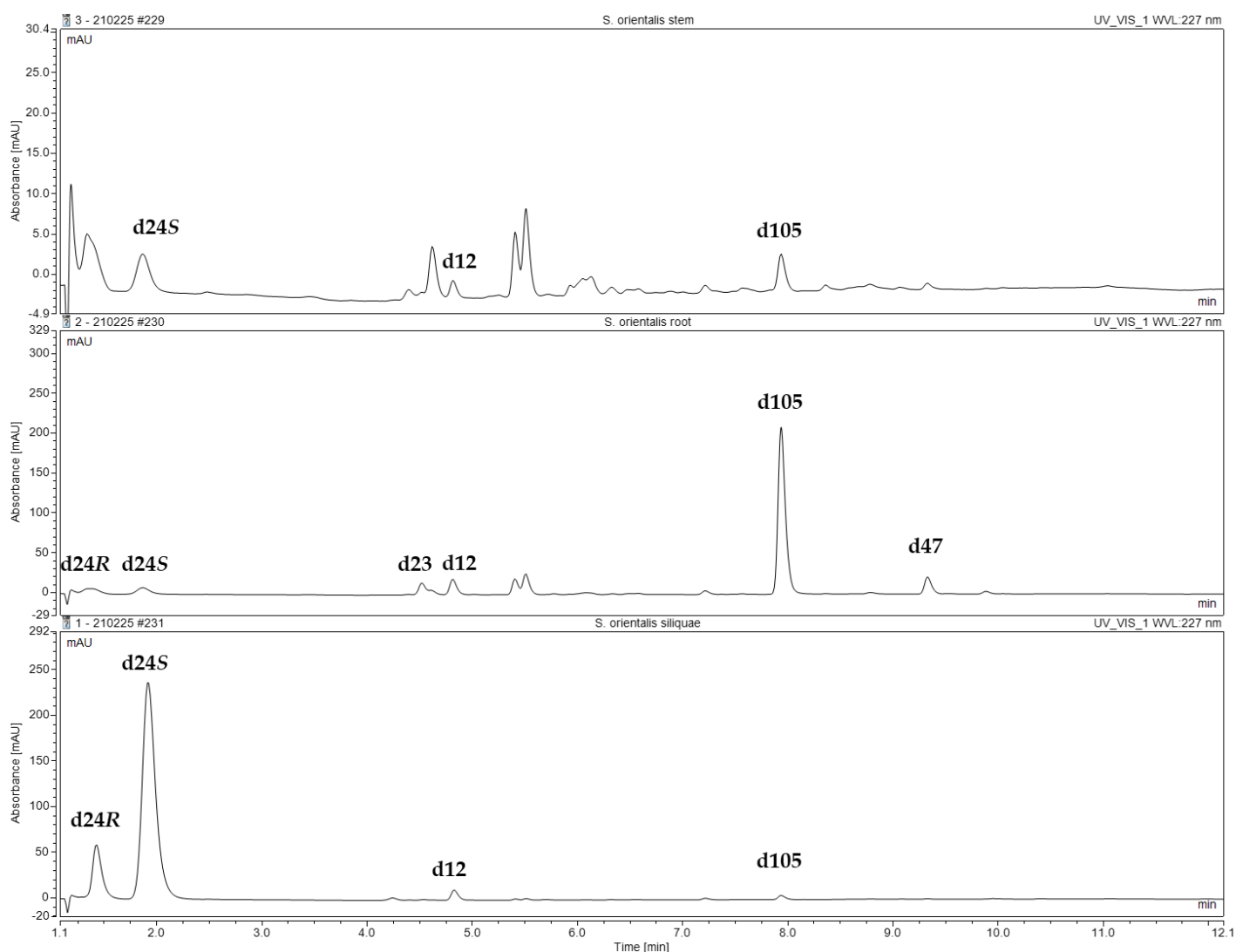


Figure S3. Chromatogram of desulfoglucosinolates obtained from the different plant parts of *S. orientale*:

d12 - desulfobut-3-enyl GSL (desulfogluconapin), **d24R** - desulfo-(2R)-hydroxybut-3-enyl GSL (desulfoprogoitrin), **d24S** - desulfo-(2S)-hydroxybut-3-enyl GSL (desulfoepiprogoitrin), **d23** - desulfo-4-hydroxybenzyl GSL (desulfoglucosinalbin), **d47** - desulfo-N-methoxyindol-3-ylmethyl GSL (desulfoneoglucobrassicin), **d105** - desulfo-2-phenylethyl GSL (desulfogluconasturtiin).

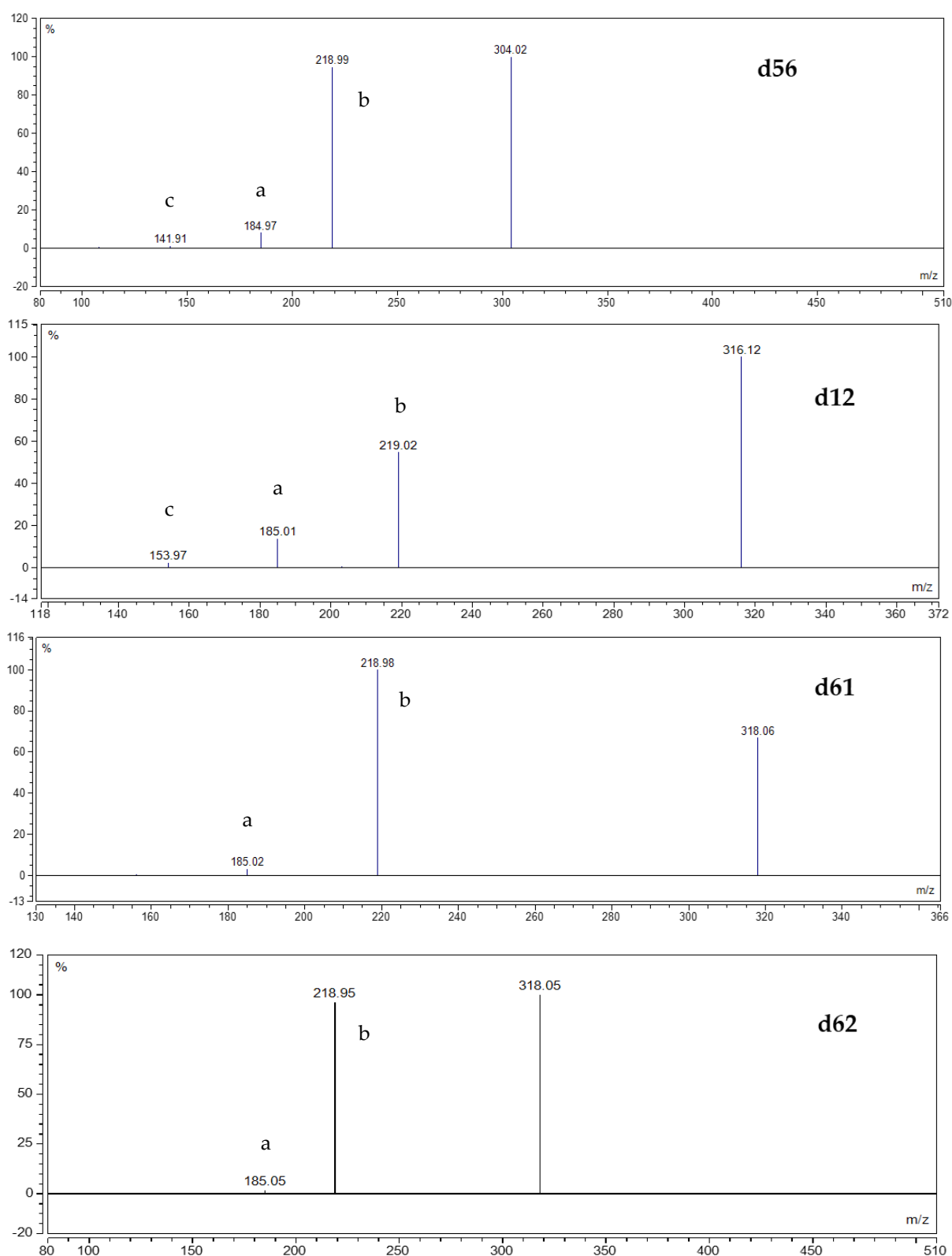


Figure S4. Continuous

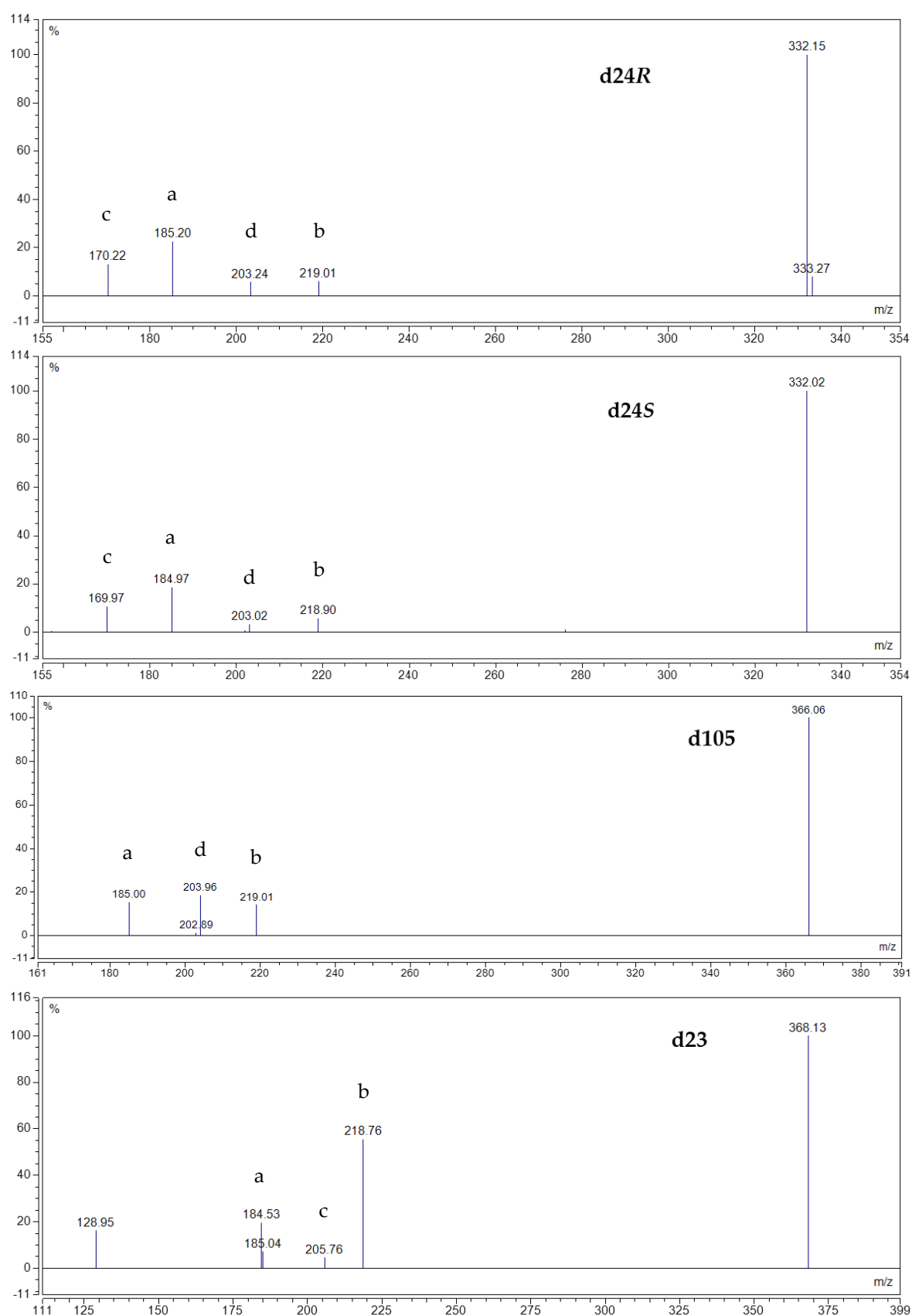


Figure S4. Continuous

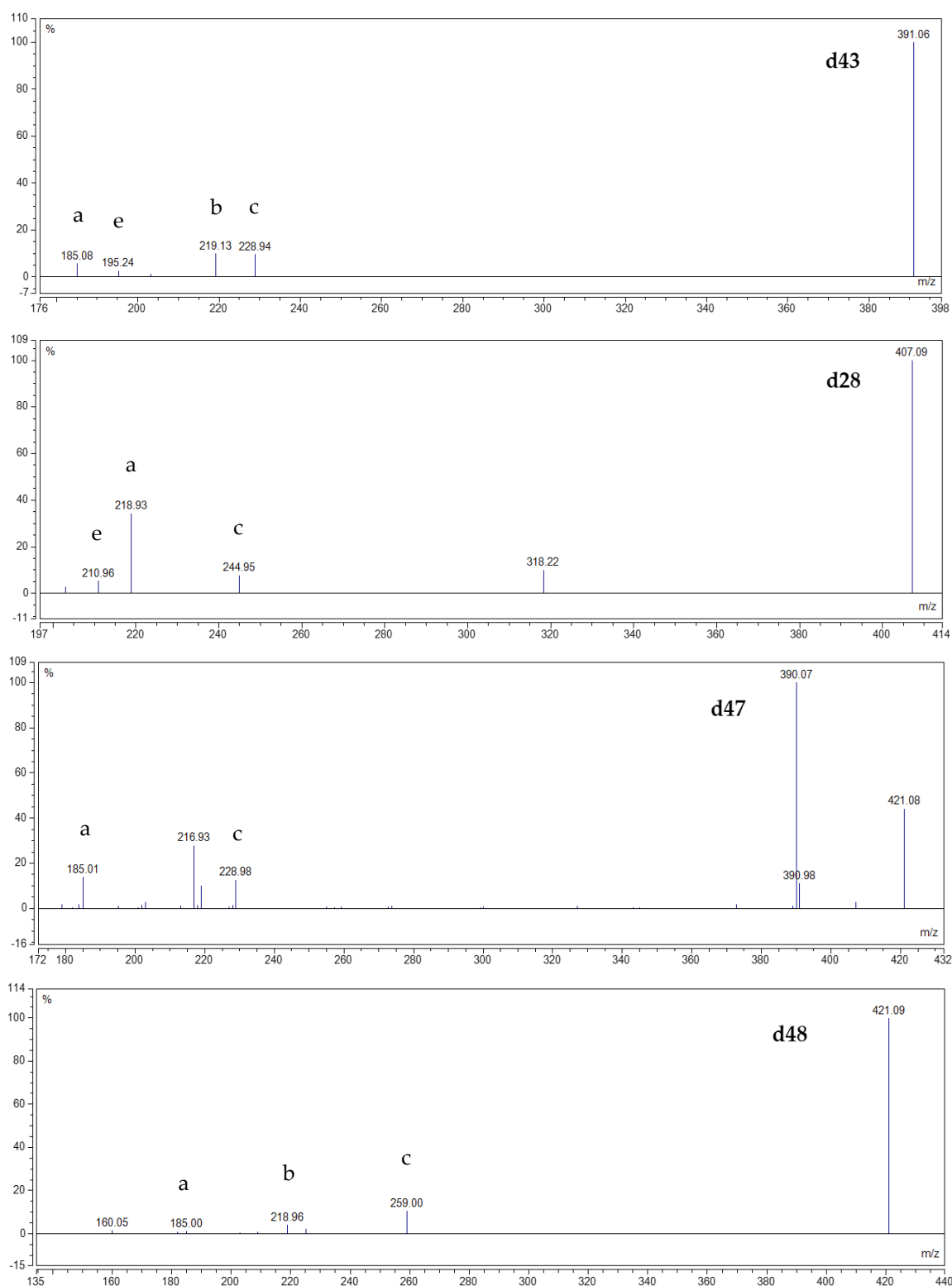


Figure S4. MS² spectra at 15V ionization of detected desulfoglucosinolates. Fragment types observed, alone or in combination, in MS2 spectra desulfoglucosinolates (dGSLs) in positive mode: a - Na⁺ adduct of anhydroGlc, C₆H₁₀O₅ (at m/z 185) or an acyl derivative; b - Na⁺ adduct of thioGlc, C₆H₁₁O₅SH (at m/z 219) or an acyl derivative; c - Loss of anhydroGlc (m/z 162) or an acyl derivative; d - Na⁺ adduct of Glc, C₆H₁₂O₆ (at m/z 203); e - Loss of thioGlc (m/z 196) or an acyl derivative.