

**S3 Table. Characteristic fragments of esterified diols with one primary and one secondary hydroxyl function detected in wheat leaf wax.** The fragments ( $m/z$ ) of trimethylsilyl ether derivatives used to identify different diol ester homologs and isomers are listed (fraction C).

Compound	Fragments characteristic of homolog ( $m/z$ )	Fragments characteristic of isomer ( $m/z$ )
Octacosane-1,20-diol palmitate	239 257 313 329	215 623
Octacosane-1,19-diol palmitate		229 609
Octacosane-1,18-diol palmitate		243 595
Octacosane-1,17-diol palmitate		257 581
Octacosane-1,16-diol palmitate		271 567
Octacosane-1,15-diol palmitate		285 553
Octacosane-1,14-diol palmitate		299 539
Octacosane-1,20-diol stearate	267 285 341 357	215 651
Octacosane-1,19-diol stearate		229 637
Octacosane-1,18-diol stearate		243 623
Octacosane-1,17-diol stearate		257 609
Octacosane-1,16-diol stearate		271 595
Octacosane-1,15-diol stearate		285 581
Octacosane-1,14-diol stearate		299 567
Octacosane-1,20-diol arachidate	295 313 369 385	215 679
Octacosane-1,19-diol arachidate		229 665
Octacosane-1,18-diol arachidate		243 651
Octacosane-1,17-diol arachidate		257 637
Octacosane-1,16-diol arachidate		271 623
Octacosane-1,15-diol arachidate		285 609
Octacosane-1,14-diol arachidate		299 595
Octacosane-1,20-diol behenate	323 341 397 413	215 707
Octacosane-1,19-diol behenate		229 693
Octacosane-1,18-diol behenate		243 679
Octacosane-1,17-diol behenate		257 665
Octacosane-1,16-diol behenate		271 651
Octacosane-1,15-diol behenate		285 637
Octacosane-1,14-diol behenate		299 623
Octacosane-1,20-diol lignocerate	351 369 425 441	215 735
Octacosane-1,19-diol lignocerate		229 721
Octacosane-1,18-diol lignocerate		243 707
Octacosane-1,17-diol lignocerate		257 693
Octacosane-1,16-diol lignocerate		271 679
Octacosane-1,15-diol lignocerate		285 665
Octacosane-1,14-diol lignocerate		299 651