

**S5 Table. Characteristic fragments of oxo-2-alkanol esters detected in wheat leaf wax.** The fragments (*m/z*) used to identify different ester homologs and isomers are listed (fraction E).

Compound	Alternative name	Fragments characteristic of homolog ( <i>m/z</i> )	Fragments characteristic of isomer type:	
			regiomer ( <i>m/z</i> )	metamer ( <i>m/z</i> )
2-Hydroxytridecan-8-one stearate	8-oxotridecan-2-ol stearate	-	99 114 424	197 267 285
2-Hydroxytridecan-7-one stearate	7-oxotridecan-2-ol stearate		113 128 410	
2-Hydroxypentadecan-8-one palmitate	8-oxopentadecan-2-ol palmitate		127 142 396	225 239 257
2-Hydroxypentadecan-7-one palmitate	7-oxopentadecan-2-ol palmitate		141 156 382	
2-Hydroxytridecan-8-one arachidate	8-oxotridecan-2-ol arachidate	-	99 114 452	197 295 313
2-Hydroxytridecan-7-one arachidate	7-oxotridecan-2-ol arachidate		113 128 438	
2-Hydroxypentadecan-8-one stearate	8-oxopentadecan-2-ol stearate		127 142 424	225 267 285
2-Hydroxypentadecan-7-one stearate	7-oxopentadecan-2-ol stearate		141 156 410	
2-Hydroxytridecan-8-one behenate	8-oxotridecan-2-ol behenate	-	99 114 480	197 323 341
2-Hydroxytridecan-7-one behenate	7-oxotridecan-2-ol behenate		113 128 466	
2-Hydroxypentadecan-8-one arachidate	8-oxopentadecan-2-ol arachidate		127 142 452	225 295 313
2-Hydroxypentadecan-7-one arachidate	7-oxopentadecan-2-ol arachidate		141 156 438	
2-Hydroxytridecan-8-one lignocerate	8-oxotridecan-2-ol lignocerate	-	99 114 508	197 351 369
2-Hydroxytridecan-7-one lignocerate	7-oxotridecan-2-ol lignocerate		113 128 494	
2-Hydroxypentadecan-8-one behenate	8-oxopentadecan-2-ol behenate		127 142 480	225 323 341
2-Hydroxypentadecan-7-one behenate	7-oxopentadecan-2-ol behenate		141 156 466	
2-Hydroxytridecan-8-one cerotate	8-oxotridecan-2-ol cerotate	-	99 114 536	197 379 397
2-Hydroxytridecan-7-one cerotate	7-oxotridecan-2-ol cerotate		113 128 522	
2-Hydroxypentadecan-8-one lignocerate	8-oxopentadecan-2-ol lignocerate		127 142 508	225 351 369
2-Hydroxypentadecan-7-one lignocerate	7-oxopentadecan-2-ol lignocerate		141 156 494	