

Article

A Comparative Study of Milk Fat Extracted from the Milk of Different Goat Breeds in China: Fatty Acids, Triacylglycerols and Thermal and Spectroscopic Characterization

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Table S1. Composition and relative content (%) of TAGs in goat milk fat samples identified according to $[M + NH_4]^+$ by using UPCC-Q-TOF-MS with supercritical carbon dioxide as a mobile phase.

tr (min)	Mass observed (m/z)	Molecular formula	Identified TAGs	[DAG] ⁺ fragment ions ([M-FA + H] ⁺)	Relative content (%)		AC N:D B
					GZG *	XSG **	
4.033	488.3759	C ₂₇ H ₅₄ NO ₆ ⁺	La-Cy-Bu	[Bu-Cy] ⁺ :271.1769; [La-Bu] ⁺ :327.2471; [La-Cy] ⁺ :383.3165	0.04 ± 0.00	ND	24:0
			Ca-Ca-Bu	[Ca-Bu] ⁺ :299.2217; [Ca-Ca] ⁺ :383.3165			
			Cy-Cy-Cy	[Cy-Cy] ⁺ :327.2471			
4.155	516.4219	C ₂₉ H ₅₈ NO ₆ ⁺	P-Co-Bu	[Bu-Co] ⁺ :243.1501; [P-Bu] ⁺ :383.3159; [P-Co] ⁺ :411.3453	0.94 ± 0.02 ^a	0.21 ±	26:0
			La-Ca-Bu	[Bu-Ca] ⁺ :299.2251; [La-Bu] ⁺ :327.2584; [La-Ca] ⁺ : 411.3453		0.02 ^b	
			La-Cy-Co	[Co-Cy] ⁺ :299.2251; [La-Co] ⁺ :355.2927; [La-Cy] ⁺ :383.3159			
			Ca-Cy-Cy	[Cy-Cy] ⁺ :327.2584; [Ca-Cy] ⁺ :355.2927			
			Ca-Ca-Co	[Ca-Co] ⁺ :327.2584; [Ca-Ca] ⁺ :383.3159			
			M-Cy-Bu	[Bu-Cy] ⁺ :271.199; [M-Bu] ⁺ :355.2927; [M-Cy] ⁺ :411.3453			
			S-Bu-Bu	[S-Bu] ⁺ :411.3453; [Bu-Bu] ⁺ :215.1276			
			Ud-Bu-Ud	[Ud-Bu] ⁺ :313.2854; [Ud-Ud] ⁺ :411.3453			
4.345	544.4544	C ₃₁ H ₆₂ NO ₆ ⁺	P-Co-Co	[P-Co] ⁺ :411.3515; [Co-Co] ⁺ :271.1956	0.17 ± 0.00 ^b	0.28 ±	28:0
			La-Cy-Cy	[La-Cy] ⁺ :383.3175; [Cy-Cy] ⁺ :327.2553		0.01 ^a	
			Ca-Ca-Cy	[Ca-Cy] ⁺ :355.2854; [Ca-Ca] ⁺ :383.3175			
			La-Ca-Co	[Co-Ca] ⁺ :327.2553; [La-Co] ⁺ :355.2854; [La-Ca] ⁺ :411.3515			
			Ud-Co-Ud	[Ud-Co] ⁺ :341.2854; [Ud-Ud] ⁺ : 411.3515			
4.555	544.4552	C ₃₁ H ₆₂ NO ₆ ⁺	P-Cy-Bu	[Bu-Cy] ⁺ :271.1963; [P-Bu] ⁺ :383.3179; [P-Cy] ⁺ :439.3792	0.68 ± 0.01 ^b	1.08 ±	28:0
			M-Ca-Bu	[Bu-Ca] ⁺ :299.2235; [M-Bu] ⁺ :355.2839; [M-Ca] ⁺ :439.3792		0.02 ^a	
			La-La-Bu	[La-Bu] ⁺ :327.2560; [La-La] ⁺ :439.3792			
			Ca-Ca-Cy	[Ca-Cy] ⁺ :355.2839; [Ca-Ca] ⁺ :383.3179			
			La-Cy-Cy	[La-Cy] ⁺ :383.3179; [Cy-Cy] ⁺ :327.2560			
4.741	572.4848	C ₃₃ H ₆₆ NO ₆ ⁺	P-Cy-Co	[Co-Cy] ⁺ :299.2246; [P-Co] ⁺ :411.3457; [P-Cy] ⁺ :439.3794	0.59 ± 0.00 ^a	0.43 ±	30:0
			M-Ca-Co	[Co-Ca] ⁺ :327.2537; [M-Co] ⁺ :383.3163; [M-Ca] ⁺ :439.3794		0.02 ^b	
			M-Cy-Cy	[M-Cy] ⁺ :411.3457; [Cy-Cy] ⁺ :327.2537			
			La-Ca-Cy	[Cy-Ca] ⁺ :355.2892; [La-Cy] ⁺ :383.3163; [La-Ca] ⁺ :411.3457			
			Ca-Ca-Ca	[Ca-Ca] ⁺ :383.3163			
			S-Co-Co	[S-Co] ⁺ :439.3794; [Co-Co] ⁺ :271.1898			
4.902	572.4843	C ₃₃ H ₆₆ NO ₆ ⁺	P-Ca-Bu	[Bu-Ca] ⁺ :299.2225; [P-Bu] ⁺ :383.3154; [P-Ca] ⁺ :467.4089	2.92 ± 0.07 ^a	2.81 ±	30:0
						0.12 ^a	
5.056	570.4728	C ₃₃ H ₆₄ NO ₆ ⁺	O-Cy-Bu	[Bu-Cy] ⁺ :271.1865; [O-Bu] ⁺ :409.3291; [O-Cy] ⁺ :465.3960	ND	0.05 ± 0.01	30:1
			Po-Ca-Bu	[Bu-Ca] ⁺ :299.2219; [Po-Bu] ⁺ :381.3013; [Po-Ca] ⁺ :465.3960			
5.139	600.5118	C ₃₅ H ₇₀ NO ₆ ⁺	P-Ca-Co	[Co-Ca] ⁺ :327.25301; [P-Co] ⁺ :411.3429; [P-Ca] ⁺ :467.4076	0.93 ± 0.01 ^b	1.31 ±	32:0
			P-Cy-Cy	[Cy-Cy] ⁺ :327.25301; [P-Cy] ⁺ :439.3754		0.04 ^a	

			M-La-Co	[Co-La] ⁺ :355.2838; [M-Co] ⁺ :383.3129; [M-La] ⁺ :467.4076			
			M-Ca-Cy	[Cy-Ca] ⁺ :355.2838; [M-Cy] ⁺ :411.3429; [M-Ca] ⁺ :439.3754			
			La-La-Cy	[Cy-La] ⁺ :383.3129; [La-La] ⁺ :439.3754			
			La-Ca-Ca	[Ca-Ca] ⁺ :383.3129; [La-Ca] ⁺ :411.3429			
			S-Cy-Co	[Co-Cy] ⁺ :299.2258; [S-Co] ⁺ :439.3754; [S-Cy] ⁺ :467.4076			
5.367	600.5179	C ₃₅ H ₇₀ NO ₆ ⁺	P-La-Bu	[Bu-La] ⁺ :327.2537; [P-Bu] ⁺ :383.3147; [P-La] ⁺ :495.4394	1.27 ± 0.02 ^a	0.12 ±	32:0
			M-M-Bu	[Bu-M] ⁺ :355.2854; [M-M] ⁺ :495.4394		0.01 ^b	
			S-Ca-Bu	[Bu-Ca] ⁺ :299.2253; [S-Bu] ⁺ :411.3483; [S-Ca] ⁺ :495.4394			
			La-Ca-Ca	[Ca-La] ⁺ :411.3483; [Ca-Ca] ⁺ :383.3147			
5.495	598.5066	C ₃₅ H ₆₈ NO ₆ ⁺	O-Ca-Bu	[Bu-Ca] ⁺ :299.2244; [O-Bu] ⁺ :409.3343; [O-Ca] ⁺ :493.4273	0.18 ± 0.00 ^a	0.17 ±	32:1
			Po-La-Bu	[Bu-La] ⁺ :327.2544; [Po-Bu] ⁺ :381.3107; [Po-La] ⁺ :493.4273		0.01 ^a	
			Po-Ca-Co	[Co-Ca] ⁺ :327.2544; [Po-Co] ⁺ :409.3343; [Po-Ca] ⁺ :465.4074			
			Mo-La-Co	[Co-La] ⁺ :355.2873; [Mo-Co] ⁺ :381.3107; [Mo-La] ⁺ :465.4074			
			Lo-Ca-Ca	[Lo-Ca] ⁺ :409.3343; [Ca-Ca] ⁺ :383.3162			
			La-Ca-De	[De-Ca] ⁺ :381.3107; [La-De] ⁺ :409.3343; [La-Ca] ⁺ :411.3531			
5.549	614.5391	C ₃₆ H ₇₂ NO ₆ ⁺	Ma-Ca-Co	[Co-Ca] ⁺ :327.2544; [Ma-Co] ⁺ :425.3617; [Ma-Ca] ⁺ :481.4270	0.12 ± 0.00 ^a	0.12 ±	33:0
			Ma-Cy-Cy	[Ma-Cy] ⁺ :453.3994; [Cy-Cy] ⁺ :327.2544		0.02 ^a	
			Pe-Ca-Cy	[Cy-Ca] ⁺ :355.2870; [Pe-Cy] ⁺ :425.3617; [Pe-Ca] ⁺ :453.3994			
5.604	628.5483	C ₃₇ H ₇₄ NO ₆ ⁺	P-La-Co	[Co-La] ⁺ :355.28939; [P-Co] ⁺ :411.3463; [P-La] ⁺ :495.4414	4.12 ± 0.07 ^a	2.20 ±	34:0
			M-Ca-Ca	[M-Ca] ⁺ :439.3770; [Ca-Ca] ⁺ :383.3161		0.08 ^b	
			M-M-Co	[M-Co] ⁺ :383.3161; [M-M] ⁺ :495.4414			
			M-La-Cy	[Cy-La] ⁺ :383.3161; [M-Cy] ⁺ :411.3463; [M-La] ⁺ :467.4114			
			La-La-Ca	[La-Ca] ⁺ :411.3463; [La-La] ⁺ :439.3770			
			P-Ca-Cy	[Cy-Ca] ⁺ :355.28939; [P-Cy] ⁺ :439.3770; [P-Ca] ⁺ :467.4114			
			S-Ca-Co	[Co-Ca] ⁺ :327.2541; [S-Co] ⁺ :439.3770; [S-Ca] ⁺ :495.4414			
5.850	628.5479	C ₃₇ H ₇₄ NO ₆ ⁺	P-M-Bu	[Bu-M] ⁺ :355.2832; [P-Bu] ⁺ :383.315; [P-M] ⁺ :523.4709	2.03 ± 0.03 ^a	1.81 ±	34:0
						0.09 ^b	
6.004	626.5367	C ₃₇ H ₇₂ NO ₆ ⁺	O-La-Bu	[Bu-La] ⁺ :327.2559; [O-Bu] ⁺ :409.3293; [O-La] ⁺ :521.4564	0.41 ± 0.02 ^a	0.43 ±	34:1
			P-Mo-Bu	[Bu-Mo] ⁺ :353.2786; [P-Bu] ⁺ :383.3224; [P-Mo] ⁺ :521.4564		0.04 ^a	
			P-De-Cy	[Cy-De] ⁺ :353.2786; [P-Cy] ⁺ :439.3788; [P-De] ⁺ :465.3951			
			Po-M-Bu	[Bu-M] ⁺ :355.2857; [Po-Bu] ⁺ :381.3018; [Po-M] ⁺ :521.4564			
			Po-Ca-Cy	[Cy-Ca] ⁺ :355.2857; [Po-Cy] ⁺ :437.3664; [Po-Ca] ⁺ :465.3951			
			Mo-La-Cy	[Cy-La] ⁺ :383.3224; [Mo-Cy] ⁺ :409.3293; [Mo-La] ⁺ :465.3951			
			Mo-Ca-Ca	[Ca-Ca] ⁺ :383.3224; [Mo-Ca] ⁺ :437.3664			
			La-La-De	[De-La] ⁺ :409.3293; [La-La] ⁺ :439.3788			
			Lo-M-Cy	[Cy-M] ⁺ :411.3304; [Lo-Cy] ⁺ :381.3018; [Lo-M] ⁺ :465.3951			
			Lo-La-Ca	[Ca-La] ⁺ :411.3304; [Lo-Ca] ⁺ :409.3293; [Lo-La] ⁺ :437.3664			
6.045	642.5677	C ₃₈ H ₇₆ NO ₆ ⁺	Ma-La-Co	[Co-La] ⁺ :355.2813; [Ma-Co] ⁺ :425.3704; [Ma-La] ⁺ :509.449	0.40 ± 0.01 ^a	0.42 ±	35:0
			Ma-Ca-Cy	[Cy-Ca] ⁺ :355.2813; [Ma-Cy] ⁺ :453.3948; [Ma-Ca] ⁺ :481.4268		0.02 ^a	

			P-Tr-Co	[Co-Tr] ⁺ :369.32967; [P-Co] ⁺ :411.3529; [P-Tr] ⁺ :509.449			
			Pe-M-Co	[Co-M] ⁺ :383.3180; [Pe-Co] ⁺ :397.3285; [Pe-M] ⁺ :509.449			
			Pe-La-Cy	[Cy-La] ⁺ :383.3180; [Pe-Cy] ⁺ :425.3704; [Pe-La] ⁺ :481.4268			
			Pe-Ca-Ca	[Ca-Ca] ⁺ :383.3180; [Pe-Ca] ⁺ :453.3948			
			Tr-La-Ca	[Ca-La] ⁺ :411.3529; [Tr-Ca] ⁺ :425.3704; [Tr-La] ⁺ :453.3948			
			Ma-M-Bu	[Bu-M] ⁺ :355.2813; [Ma-Bu] ⁺ :397.3285; [Ma-M] ⁺ :537.4912			
			P-Pe-Bu	[Bu-Pe] ⁺ :369.32967; [P-Bu] ⁺ :383.3180; [P-Pe] ⁺ :537.4912			
6.087	656.5759	C ₃₉ H ₇₈ NO ₆ ⁺	S-La-Co	[Co-La] ⁺ :355.2856; [S-Co] ⁺ :439.3773; [S-La] ⁺ :523.4716	2.21 ± 0.05 ^a	0.16 ±	36:0
			S-Ca-Cy	[Cy-Ca] ⁺ :355.2856; [S-Cy] ⁺ :467.4088; [S-Ca] ⁺ :495.4409		0.01 ^b	
			P-M-Co	[Co-M] ⁺ :383.3148; [P-Co] ⁺ :411.3462; [P-M] ⁺ :523.4716			
			P-Ca-Ca	[Ca-Ca] ⁺ :383.3148; [P-Ca] ⁺ :467.4088			
			La-La-La	[La-La] ⁺ :439.3773			
			P-La-Cy	[Cy-La] ⁺ :383.3148; [P-Cy] ⁺ :439.3773; [P-La] ⁺ :495.4409			
			M-M-Cy	[Cy-M] ⁺ :411.3462; [M-M] ⁺ :495.4409			
			M-La-Ca	[Ca-La] ⁺ :411.3462; [M-Ca] ⁺ :439.3773; [M-La] ⁺ :467.4088			
6.324	656.5784	C ₃₉ H ₇₈ NO ₆ ⁺	P-P-Bu	[Bu-P] ⁺ :383.3160; [P-P] ⁺ :551.5031	3.66 ± 0.06 ^b	4.12 ±	36:0
			S-M-Bu	[Bu-M] ⁺ :355.2828; [S-Bu] ⁺ :411.3481; [S-M] ⁺ :551.5031		0.21 ^a	
5.561	654.5667	C ₃₉ H ₇₆ NO ₆ ⁺	O-M-Bu	[Bu-M] ⁺ :355.2864; [O-Bu] ⁺ :409.3323; [O-M] ⁺ :549.4913	0.31 ± 0.03 ^b	0.73 ±	36:1
			P-Ca-De	[De-Ca] ⁺ :381.3026; [P-De] ⁺ :465.3986; [P-Ca] ⁺ :467.3167		0.02 ^a	
			Po-Ca-Ca	[Ca-Ca] ⁺ :383.3195; [Po-Ca] ⁺ :465.3986			
			S-Mo-Bu	[Bu-Mo] ⁺ :353.2727; [S-Bu] ⁺ :411.3439; [S-Mo] ⁺ :549.4913			
6.179	670.6010	C ₄₀ H ₈₀ NO ₆ ⁺	Ma-M-Co	[Co-M] ⁺ :383.3148; [Ma-Co] ⁺ :425.3634; [Ma-M] ⁺ :537.4920	0.77 ± 0.02 ^b	1.02 ±	37:0
			Ma-La-Cy	[Cy-La] ⁺ :383.3148; [Ma-Cy] ⁺ :453.3986; [Ma-La] ⁺ :509.4580		0.00 ^a	
			Ma-Ca-Ca	[Ca-Ca] ⁺ :383.3148; [Ma-Ca] ⁺ :481.4275			
			P-Pe-Co	[Co-Pe] ⁺ :397.3317; [P-Co] ⁺ :411.3488; [P-Pe] ⁺ :537.4920			
			Pe-M-Cy	[Cy-M] ⁺ :411.3488; [Pe-Cy] ⁺ :425.3634; [Pe-M] ⁺ :509.4580			
			Pe-La-Ca	[Ca-La] ⁺ :411.3488; [Pe-Ca] ⁺ :453.3986; [Pe-La] ⁺ :481.4275			
6.446	668.5842	C ₄₀ H ₇₈ NO ₆ ⁺	O-Pe-Bu	[Bu-Pe] ⁺ :369.3046; [O-Bu] ⁺ :409.3241; [O-Pe] ⁺ :563.5032	0.24 ± 0.02 ^a	0.20 ±	37:1
			H-P-Bu	[Bu-P] ⁺ :383.3158; [H-Bu] ⁺ :395.3169; [H-P] ⁺ :563.5032		0.00 ^b	
6.798	684.6094	C ₄₁ H ₈₂ NO ₆ ⁺	S-M-Co	[Co-M] ⁺ :383.3141; [S-Co] ⁺ :439.3789; [S-M] ⁺ :551.5022	6.63 ± 0.01 ^b	10.94 ±	38:0
			S-La-Cy	[Cy-La] ⁺ :383.3141; [S-Cy] ⁺ :467.4089; [S-La] ⁺ :523.4722		0.02 ^a	
			S-Ca-Ca	[Ca-Ca] ⁺ :383.3141; [S-Ca] ⁺ :495.4402			
			P-P-Co	[Co-P] ⁺ :411.3452; [P-P] ⁺ :551.5022			
			P-M-Cy	[Cy-M] ⁺ :411.3452; [P-Cy] ⁺ :439.3789; [P-M] ⁺ :523.4722			
			P-La-Ca	[Ca-La] ⁺ :411.3452; [P-Ca] ⁺ :467.4089; [P-La] ⁺ :495.4402			
			M-M-Ca	[Ca-M] ⁺ :439.3789; [M-M] ⁺ :495.4402			
			M-La-La	[La-La] ⁺ :439.3789; [M-La] ⁺ :467.4089			
7.026	682.5958	C ₄₁ H ₈₀ NO ₆ ⁺	O-P-Bu	[Bu-P] ⁺ :383.3148; [O-Bu] ⁺ :409.3311; [O-P] ⁺ :577.5208	1.04 ± 0.01 ^b	2.33 ±	38:1
			Po-Ca-La	[La-Ca] ⁺ :411.3484; [Po-La] ⁺ :493.4255; [Po-Ca] ⁺ :465.3936		0.09 ^a	
			P-De-La	[La-De] ⁺ :409.3311; [P-La] ⁺ :495.4426; [P-De] ⁺ :465.3936			
			Po-S-Bu	[Bu-S] ⁺ :411.3484; [Po-Bu] ⁺ :381.3070; [Po-S] ⁺ :577.5208			
7.381	712.6441	C ₄₃ H ₈₆ NO ₆ ⁺	S-La-Ca	[Ca-La] ⁺ :411.3467; [S-Ca] ⁺ :495.4438; [S-La] ⁺ :523.4278			40:0

			P-M-Ca	[Ca-M] ⁺ :439.3803; [P-Ca] ⁺ :467.4105; [P-M] ⁺ :523.4278	10.49 ±	9.30 ±	
			M-M-La	[La-M] ⁺ :467.4105; [M-M] ⁺ :495.4438	0.15 ^a	0.40 ^b	
			Co-S-P	[P-S] ⁺ :579.5377; [Co-P] ⁺ :411.3467; [Co-S] ⁺ :439.3803			
			Cy-P-P	[P-P] ⁺ :551.5048; [Cy-P] ⁺ :439.3803			
			Bu-S-S	[S-S] ⁺ :607.5707; [Bu-S] ⁺ :411.3467			
			Ar-Ca-Ca	[Ca-Ca] ⁺ :383.3145; [Ar-Ca] ⁺ :523.4278			
			Ar-P-Bu	[Bu-P] ⁺ :383.3145; [Ar-Bu] ⁺ :439.3803; [Ar-P] ⁺ :607.5707			
			Ar-La-Cy	[Cy-La] ⁺ :383.3145; [Ar-Cy] ⁺ :495.4438; [Ar-La] ⁺ :551.5048			
7.508	710.6297	C ₄₃ H ₈₄ NO ₆ ⁺	S-O-Bu	[Bu-O] ⁺ :409.3309; [S-Bu] ⁺ :411.3476; [S-O] ⁺ :605.5447	3.41 ± 0.10 ^a	3.69 ±	40:1
			S-Po-Co	[Co-Po] ⁺ :409.3309; [S-Co] ⁺ :439.3791; [S-Po] ⁺ :577.5255		0.24 ^a	
			S-Mo-Cy	[Cy-Mo] ⁺ :409.3309; [S-Cy] ⁺ :467.4131; [S-Mo] ⁺ :549.4871			
			S-Lo-Ca	[Ca-Lo] ⁺ :409.3309; [S-Ca] ⁺ :495.4399; [S-Lo] ⁺ :521.4576			
			O-P-Co	[Co-P] ⁺ :411.3476; [O-Co] ⁺ :437.3657; [O-P] ⁺ :577.5255			
			O-M-Cy	[Cy-M] ⁺ :411.3476; [O-Cy] ⁺ :465.3920; [O-M] ⁺ :549.4871			
			O-La-Ca	[Ca-La] ⁺ :411.3476; [O-Ca] ⁺ :493.4264; [O-La] ⁺ :521.4576			
			P-Po-Cy	[Cy-Po] ⁺ :437.3657; [P-Cy] ⁺ :439.3791; [P-Po] ⁺ :549.4871			
			P-Mo-Ca	[Ca-Mo] ⁺ :437.3657; [P-Ca] ⁺ :467.4131; [P-Mo] ⁺ :521.4576			
			P-La-Lo	[Lo-La] ⁺ :437.3657; [P-Lo] ⁺ :493.4264; [P-La] ⁺ :495.4399			
			Po-M-Ca	[Ca-M] ⁺ :439.3791; [Po-Ca] ⁺ :465.3920; [Po-M] ⁺ :521.4576			
			Po-La-La	[La-La] ⁺ :439.3791; [Po-La] ⁺ :493.4264			
			M-M-Lo	[Lo-M] ⁺ :465.3920; [M-M] ⁺ :495.4399			
			M-Mo-La	[La-Mo] ⁺ :465.3920; [M-La] ⁺ :467.4131; [M-Mo] ⁺ :493.4264			
			De-M-P	[P-M] ⁺ :523.4660; [De-P] ⁺ :465.3920; [De-M] ⁺ :437.3657			
			De-S-La	[La-S] ⁺ :523.4660; [De-La] ⁺ :409.3309; [De-S] ⁺ :493.4264			
7.855	708.6151	C ₄₃ H ₈₂ NO ₆ ⁺	O-O-Bu	[Bu-O] ⁺ :409.3301; [O-O] ⁺ :603.5345	1.92 ± 0.01 ^b	2.60 ±	40:2
			O-Po-Co	[Co-Po] ⁺ :409.3301; [O-Co] ⁺ :437.3416; [O-Po] ⁺ :575.4874		0.08 ^a	
			O-Mo-Cy	[Cy-Mo] ⁺ :409.3301; [O-Cy] ⁺ :465.3869; [O-Mo] ⁺ :547.4874			
			O-Lo-Ca	[Ca-Lo] ⁺ :409.3301; [O-Ca] ⁺ :493.4282; [O-Lo] ⁺ :519.4453			
			P-Lo-Lo	[Lo-Lo] ⁺ :435.3163; [P-Lo] ⁺ :493.4282			
			Po-Po-Cy	[Cy-Po] ⁺ :437.3416; [Po-Po] ⁺ :547.4874			
			Po-Mo-Ca	[Ca-Mo] ⁺ :437.3416; [Po-Ca] ⁺ :465.3869; [Po-Mo] ⁺ :519.4453			
			Po-La-Lo	[Lo-La] ⁺ :437.3416; [Po-Lo] ⁺ :491.4105; [Po-La] ⁺ :493.4282			
			M-Mo-Lo	[Lo-Mo] ⁺ :463.3733; [M-Lo] ⁺ :465.3869; [M-Mo] ⁺ :493.4282			
			Mo-Mo-La	[La-Mo] ⁺ :465.3869; [Mo-Mo] ⁺ :491.4105			
			Ca-L-La	[La-L] ⁺ :519.4453; [Ca-La] ⁺ :411.3484; [Ca-L] ⁺ :491.4105			
			L-P-Co	[Co-P] ⁺ :411.3484; [L-Co] ⁺ :435.3163; [L-P] ⁺ :575.4874			
			L-M-Cy	[Cy-M] ⁺ :411.3484; [L-Cy] ⁺ :463.3733; [L-M] ⁺ :547.4874			
7.919	706.6003	C ₄₃ H ₈₀ NO ₆ ⁺	O-L-Bu	[Bu-L] ⁺ :407.3161; [O-Bu] ⁺ :409.3340; [O-L] ⁺ :601.5182	0.28 ± 0.01 ^b	0.44 ±	40:3
						0.07 ^a	
7.950	726.6642	C ₄₄ H ₈₈ NO ₆ ⁺	S-Pe-Cy	[Cy-Pe] ⁺ :425.3679; [S-Cy] ⁺ :467.4133; [S-Pe] ⁺ :565.5246	1.12 ± 0.01 ^b	1.18 ±	41:0
			Ma-P-Cy	[Cy-P] ⁺ :439.3772; [Ma-Cy] ⁺ :453.3950; [Ma-P] ⁺ :565.5246		0.01 ^a	
			Ma-M-Ca	[Ca-M] ⁺ :439.3772; [Ma-Ca] ⁺ :481.4189; [Ma-M] ⁺ :537.4926			

7.982	740.6712	C ₄₇ H ₉₄ NO ₆ ⁺	P-Pe-Ca	[Ca-Pe] ⁺ :453.3950; [P-Ca] ⁺ :467.4133; [P-Pe] ⁺ :537.4926			
			S-M-Ca	[Ca-M] ⁺ :439.3820; [S-Ca] ⁺ :495.4424; [S-M] ⁺ :551.5062	14.10 ±	6.15 ±	42:0
			P-P-Ca	[Ca-P] ⁺ :467.4118; [P-P] ⁺ :551.5062	0.27 ^a	0.07 ^b	
			S-P-Cy	[Cy-P] ⁺ :439.3820; [S-Cy] ⁺ :467.4118; [S-P] ⁺ :579.5339			
8.100	738.6609	C ₄₅ H ₈₈ NO ₆ ⁺	P-M-La	[La-M] ⁺ :467.4118; [P-La] ⁺ :495.4424; [P-M] ⁺ :523.4738			
			O-P-Cy	[Cy-P] ⁺ :439.3777; [O-Cy] ⁺ :465.3987; [O-P] ⁺ :577.5211	3.63 ± 0.03 ^a	1.69 ±	42:1
			O-M-Ca	[Ca-M] ⁺ :439.3777; [O-Ca] ⁺ :493.4267; [O-M] ⁺ :549.4893		0.02 ^b	
			O-La-La	[La-La] ⁺ :439.3777; [O-La] ⁺ :521.4584			
			P-Po-Ca	[Ca-Po] ⁺ :465.3987; [P-Ca] ⁺ :467.4155; [P-Po] ⁺ :549.4893			
			P-M-Lo	[Lo-M] ⁺ :465.3987; [P-Lo] ⁺ :493.4267; [P-M] ⁺ :523.4753			
			P-Mo-La	[La-Mo] ⁺ :465.3987; [P-La] ⁺ :495.4426; [P-Mo] ⁺ :521.4584			
			Po-M-La	[La-M] ⁺ :467.4155; [Po-La] ⁺ :493.4267; [Po-M] ⁺ :521.4584			
			P-P-De	[De-P] ⁺ :465.3987; [P-P] ⁺ :551.4984			
			M-S-De	[De-S] ⁺ :493.4267; [M-De] ⁺ :437.3618; [M-S] ⁺ :551.4984			
			Ar-Po-Co	[Co-Po] ⁺ :409.3284; [Ar-Co] ⁺ :467.4155; [Ar-Po] ⁺ :605.5229			
			Ar-Mo-Cy	[Cy-Mo] ⁺ :409.3284; [Ar-Cy] ⁺ :495.4426; [Ar-Mo] ⁺ :577.5211			
			Ar-Lo-Ca	[Ca-Lo] ⁺ :409.3284; [Ar-Ca] ⁺ :523.4753; [Ar-Lo] ⁺ :549.4893			
			S-Pe-Ca	[Ca-Pe] ⁺ :453.3826; [S-Ca] ⁺ :495.4454; [S-Pe] ⁺ :565.52	0.05 ± 0.00 ^b	0.68 ±	43:0
8.456	754.6943	C ₄₆ H ₉₂ NO ₆ ⁺	Ma-P-Ca	[Ca-P] ⁺ :467.4119; [Ma-Ca] ⁺ :481.4261; [Ma-P] ⁺ :565.5233		0.00 ^a	
			Ma-M-La	[La-M] ⁺ :467.4119; [Ma-La] ⁺ :509.4608; [Ma-M] ⁺ :537.4890			
			P-Pe-La	[La-Pe] ⁺ :481.4261; [P-La] ⁺ :495.4454; [P-Pe] ⁺ :537.4890			
			S-Ma-Cy	[Cy-Ma] ⁺ :453.3826; [S-Cy] ⁺ :467.4119; [S-Ma] ⁺ :593.5556			
8.456	752.6806	C ₄₆ H ₉₀ NO ₆ ⁺	O-Pe-Ca	[Ca-Pe] ⁺ :453.3947; [O-Ca] ⁺ :493.4262; [O-Pe] ⁺ :563.5102	ND	0.73 ± 0.02	43:1
			H-P-Ca	[Ca-P] ⁺ :467.4101; [H-Ca] ⁺ :479.4143; [H-P] ⁺ :563.5102			
			Po-Pe-La	[La-Pe] ⁺ :481.4284; [Po-La] ⁺ :493.4262; [Po-Pe] ⁺ :535.4798			
			Pen-P-La	[La-P] ⁺ :495.4410; [Pen-La] ⁺ :479.4143; [Pen-P] ⁺ :535.4798			
			Mo-Pe-M	[M-Pe] ⁺ :509.4605; [Mo-M] ⁺ :493.4262; [Mo-Pe] ⁺ :507.4648			
			Pe-P-Lo	[Lo-P] ⁺ :493.4262; [Pe-Lo] ⁺ :479.4143; [Pe-P] ⁺ :537.4852			
			S-Pe-De	[De-Pe] ⁺ :451.3820; [S-De] ⁺ :493.4262; [S-Pe] ⁺ :565.5132			
			S-De-Pen	[Pen-De] ⁺ :451.3820; [S-Pen] ⁺ :565.5132; [S-De] ⁺ :495.4410			
			O-M-De	[De-M] ⁺ :437.3683; [O-De] ⁺ :491.4168; [O-M] ⁺ :549.4951	0.03 ± 0.00 ^b	0.59 ±	42:2
			O-Mo-Ca	[Ca-Mo] ⁺ :437.3683; [O-Ca] ⁺ :493.4271; [O-Mo] ⁺ :547.4724		0.01 ^a	
8.574	736.6495	C ₄₅ H ₈₆ NO ₆ ⁺	L-M-Ca	[Ca-M] ⁺ :439.3786; [L-Ca] ⁺ :491.4168; [L-M] ⁺ :547.4724			
			P-Po-De	[De-Po] ⁺ :463.3842; [P-De] ⁺ :465.4016; [P-Po] ⁺ :549.4951			
			M-Mo-Mo	[Mo-Mo] ⁺ :491.4168; [M-Mo] ⁺ :493.4271			
			Go-Mo-Cy	[Cy-Mo] ⁺ :409.3611; [Go-Cy] ⁺ :493.4271; [Go-Mo] ⁺ :575.4996			
			S-Mo-De	[De-Mo] ⁺ :435.3509; [S-De] ⁺ :493.4271; [S-Mo] ⁺ :549.4951			
			O-Po-Cy	[Cy-Po] ⁺ :437.3683; [O-Cy] ⁺ :465.4016; [O-Po] ⁺ :575.4996			
			L-P-Cy	[Cy-P] ⁺ :439.3786; [L-Cy] ⁺ :463.3842; [L-P] ⁺ :575.4996			
			Go-P-Co	[Co-P] ⁺ :409.3611; [Go-Co] ⁺ :463.3842; [Go-P] ⁺ :603.5459			

8.646	768.7093	C ₄₇ H ₉₄ NO ₆ ⁺	S-P-Ca	[Ca-P] ⁺ :467.4120; [S-Ca] ⁺ :495.4405; [S-P] ⁺ :579.5398	3.56 ± 0.03 ^a	0.11 ±	44:0
			S-S-Cy	[Cy-S] ⁺ :467.4120; [S-S] ⁺ :607.5645		0.01 ^b	
			Ar-P-Cy	[Cy-P] ⁺ :439.3648; [Ar-Cy] ⁺ :495.4405; [Ar-P] ⁺ :607.5645			
8.720	768.7053	C ₄₇ H ₉₄ NO ₆ ⁺	S-M-La	[La-M] ⁺ :467.4118; [S-La] ⁺ :523.4743; [S-M] ⁺ :551.5044	1.06 ± 0.01 ^a	0.97 ±	44:0
			P-M-M	[M-M] ⁺ :495.4416; [P-M] ⁺ :523.4743		0.02 ^b	
8.811	766.6907	C ₄₇ H ₉₂ NO ₆ ⁺	O-P-Ca	[Ca-P] ⁺ :467.4088; [O-Ca] ⁺ :493.4244; [O-P] ⁺ :577.5208	0.38 ± 0.03 ^b	5.18 ±	44:1
			O-M-La	[La-M] ⁺ :467.4088; [O-La] ⁺ :521.4575; [O-M] ⁺ :549.4867		0.14 ^a	
			P-Po-La	[La-Po] ⁺ :493.4244; [P-La] ⁺ :495.4409; [P-Po] ⁺ :549.4867			
			P-M-Mo	[Mo-M] ⁺ :493.4244; [P-Mo] ⁺ :521.4575; [P-M] ⁺ :523.4719			
			Po-M-M	[M-M] ⁺ :495.4409; [Po-M] ⁺ :521.4575			
			S-P-De	[De-P] ⁺ :465.3907; [S-De] ⁺ :493.4244; [S-P] ⁺ :579.5267			
			S-Mo-La	[La-Mo] ⁺ :465.3907; [S-La] ⁺ :523.4719; [S-Mo] ⁺ :549.4867			
			O-S-Cy	[Cy-S] ⁺ :467.4088; [O-Cy] ⁺ :465.3907; [O-S] ⁺ :605.5510			
			S-Po-Ca	[Ca-Po] ⁺ :465.3907; [S-Ca] ⁺ :495.4409; [S-Po] ⁺ :577.5208			
9.285	764.6772	C ₄₇ H ₉₀ NO ₆ ⁺	O-Po-Ca	[Ca-Po] ⁺ :465.3941; [O-Ca] ⁺ :493.4220; [O-Po] ⁺ :575.5020	0.77 ± 0.00 ^b	0.88 ±	44:2
			L-P-Ca	[Ca-P] ⁺ :467.4126; [L-Ca] ⁺ :491.4115; [L-P] ⁺ :575.5020		0.01 ^a	
			L-S-Cy	[Cy-S] ⁺ :467.4126; [L-Cy] ⁺ :463.3744 ; [L-S] ⁺ :603.5362			
			L-P-De	[De-P] ⁺ :467.4126; [L-De] ⁺ :491.4115; [L-P] ⁺ :577.5207			
			S-Po-De	[De-Po] ⁺ :463.3744; [S-De] ⁺ :493.4220; [S-Po] ⁺ :577.5207			
9.378	762.6606	C ₄₇ H ₈₈ NO ₆ ⁺	O-L-Cy	[Cy-L] ⁺ :463.3793; [O-Cy] ⁺ :465.397; [O-L] ⁺ :601.5299	0.24 ± 0.01 ^a	0.21 ±	44:3
			O-Po-De	[De-Po] ⁺ :463.3793; [O-De] ⁺ :491.4095; [O-Po] ⁺ :575.4979		0.00 ^b	
			L-P-De	[De-P] ⁺ :465.397; [L-De] ⁺ :489.3885; [L-P] ⁺ :575.4979			
			L-Po-Ca	[Ca-Po] ⁺ :465.397; [L-Ca] ⁺ :491.4095; [L-Po] ⁺ :573.4914			
			Ln-P-Ca	[Ca-P] ⁺ :467.4094; [Ln-Ca] ⁺ :489.3885; [Ln-P] ⁺ :573.4914			
9.425	782.7233	C ₄₈ H ₉₆ NO ₆ ⁺	S-Ma-Ca	[Ca-Ma] ⁺ :481.4243; [S-Ca] ⁺ :495.4471; [S-Ma] ⁺ :593.5403	0.37 ± 0.01 ^b	0.43 ±	45:0
			S-Pe-La	[La-Pe] ⁺ :481.4243; [S-La] ⁺ :523.4765; [S-Pe] ⁺ :565.5621		0.02 ^a	
			Ma-P-La	[La-P] ⁺ :495.4471; [Ma-La] ⁺ :509.4581; [Ma-P] ⁺ :565.5621			
			P-Pe-M	[M-Pe] ⁺ :509.4581; [P-M] ⁺ :523.4765; [P-Pe] ⁺ :537.4824			
9.448	780.7103	C ₄₈ H ₉₄ NO ₆ ⁺	O-Ma-Ca	[Ca-Ma] ⁺ :481.4223; [O-Ca] ⁺ :493.4251; [O-Ma] ⁺ :591.5336	0.24 ± 0.00 ^b	0.89 ±	45:1
			O-Pe-La	[La-Pe] ⁺ :481.4223; [O-La] ⁺ :521.4601; [O-Pe] ⁺ :563.4905		0.01 ^a	
			Ma-Po-La	[La-Po] ⁺ :493.4251; [Ma-La] ⁺ :509.4567; [Ma-Po] ⁺ :563.4905			
			Ma-M-Mo	[Mo-M] ⁺ :493.4251; [Ma-Mo] ⁺ :535.4616; [Ma-M] ⁺ :537.4751			
			H-P-La	[La-P] ⁺ :495.4432; [H-La] ⁺ :507.4404; [H-P] ⁺ :563.4905			
			H-M-M	[M-M] ⁺ :495.4432; [H-M] ⁺ :535.4616			
9.471	796.7405	C ₄₉ H ₉₆ NO ₆ ⁺	S-P-La	[La-P] ⁺ :495.4413; [S-La] ⁺ :523.4727; [S-P] ⁺ :579.5362	8.93 ± 0.30 ^a	0.88 ±	46:0
			P-P-M	[M-P] ⁺ :523.4727; [P-P] ⁺ :551.5046		0.01 ^b	
			Ar-P-Ca	[Ca-P] ⁺ :467.4126; [Ar-Ca] ⁺ :523.4727; [Ar-P] ⁺ :607.5650			
			Beh-M-Ca	[Ca-M] ⁺ :439.3787; [Beh-Ca] ⁺ :551.5046; [Beh-M] ⁺ :607.5650			
9.663	794.7227	C ₄₉ H ₉₆ NO ₆ ⁺	S-O-Ca	[Ca-O] ⁺ :493.4302; [S-Ca] ⁺ :495.4447; [S-O] ⁺ :605.5582	1.18 ± 0.04 ^a	1.28 ±	46:1
						0.05 ^a	
9.754	794.7258	C ₄₉ H ₉₆ NO ₆ ⁺	O-P-La	[La-P] ⁺ :495.44409; [O-La] ⁺ :521.4586; [O-P] ⁺ :577.5190	0.32 ± 0.01 ^b		46:1

9.909	792.7107	C ₄₉ H ₉₄ NO ₆ ⁺	O-M-M	[M-M] ⁺ :495.44409; [O-M] ⁺ :549.4893	1.18 ±		
			P-Po-M	[M-Po] ⁺ :521.4586; [P-M] ⁺ :523.4734; [P-Po] ⁺ :549.4893	0.03 ^a		
			P-P-Mo	[Mo-P] ⁺ :521.4586; [P-P] ⁺ :551.5009			
			Go-M-La	[La-M] ⁺ :467.4145; [Go-La] ⁺ :549.4893; [Go-M] ⁺ :577.5190			
			O-O-Ca	[Ca-O] ⁺ :493.4272; [O-O] ⁺ :603.5304	1.47 ± 0.04 ^b	4.37 ±	46:2
			O-Po-La	[La-Po] ⁺ :493.4272; [O-La] ⁺ :521.4590; [O-Po] ⁺ :575.5083	0.19 ^a		
			P-Po-Mo	[Mo-Po] ⁺ :519.4435; [P-Mo] ⁺ :521.4590; [P-Po] ⁺ :549.4917			
			O-Mo-M	[M-Mo] ⁺ :493.4272; [O-M] ⁺ :549.4917; [O-Mo] ⁺ :547.4738			
			S-Po-Lo	[Lo-Po] ⁺ :491.3987; [S-Lo] ⁺ :521.4590; [S-Po] ⁺ :577.5272			
			S-O-De	[De-O] ⁺ :491.3987; [S-De] ⁺ :493.4272; [S-O] ⁺ :605.5482			
			Po-Po-M	[M-Po] ⁺ :521.4590; [Po-Po] ⁺ :547.4738			
			S-Mo-Mo	[Mo-Mo] ⁺ :491.3987; [S-Mo] ⁺ :549.4917			
			L-P-La	[La-P] ⁺ :495.4438; [L-La] ⁺ :519.4435; [L-P] ⁺ :575.5083			
			L-M-M	[M-M] ⁺ :495.4438; [L-M] ⁺ :547.4738			
10.33 2	790.6936	C ₄₉ H ₉₂ NO ₆ ⁺	O-O-De	[De-O] ⁺ :491.4067; [O-O] ⁺ :603.5139	0.11 ± 0.00 ^b	0.44 ±	46:3
			O-L-Ca	[Ca-L] ⁺ :491.4067; [O-Ca] ⁺ :493.4273; [O-L] ⁺ :601.5186	0.02 ^a		
			O-Po-Lo	[Lo-Po] ⁺ :491.4067; [O-Lo] ⁺ :519.4462; [O-Po] ⁺ :575.4924			
			Ln-S-Ca	[Ca-S] ⁺ :495.4396; [Ln-Ca] ⁺ :489.3986; [Ln-S] ⁺ :601.5186			
			L-S-De	[De-S] ⁺ :493.4273; [L-De] ⁺ :489.3986; [L-S] ⁺ :603.5139			
			Po-Po-Mo	[Mo-Po] ⁺ :519.4462; [Po-Po] ⁺ :547.4758			
10.44 7	810.7181	C ₅₀ H ₁₀₀ NO ₆ +	S-Pe-M	[M-Pe] ⁺ :509.5443; [S-M] ⁺ :551.5043; [S-Pe] ⁺ :565.5245	0.37 ± 0.03 ^a	0.19 ±	47:0
			Ma-P-M	[M-P] ⁺ :523.4802; [Ma-M] ⁺ :537.4909; [Ma-P] ⁺ :565.5245	0.01 ^b		
10.50 4	808.7416	C ₅₀ H ₉₈ NO ₆ ⁺	No-M-M	[M-M] ⁺ :495.4455; [No-M] ⁺ :563.4995	0.35 ± 0.03 ^b	0.43 ±	47:1
			O-Pe-M	[M-Pe] ⁺ :509.4578; [O-M] ⁺ :549.4913; [O-Pe] ⁺ :563.4995	0.00 ^a		
			Ma-Po-M	[M-Po] ⁺ :521.4575; [Ma-M] ⁺ :537.4875; [Ma-Po] ⁺ :563.4995			
			Ma-Pe-Pen	[Pen-Pe] ⁺ :521.4575; [Ma-Pen] ⁺ :549.4913; [Ma-Pe] ⁺ :551.5023			
			H-Pe-Pe	[Pe-Pe] ⁺ :523.4760; [H-Pe] ⁺ :549.4913			
10.56 2	824.7719	C ₅₁ H ₁₀₂ NO ₆ +	P-Po-Pe	[Pe-Po] ⁺ :535.4694; [P-Pe] ⁺ :537.4875; [P-Po] ⁺ :549.4913			
			S-P-M	[M-P] ⁺ :523.4703; [S-M] ⁺ :551.5020; [S-P] ⁺ :579.5310	0.03 ± 0.00 ^b	0.09 ±	48:0
			P-P-P	[P-P] ⁺ :551.5020	0.00 ^a		
			Ar-P-La	[La-P] ⁺ :495.4424; [Ar-La] ⁺ :551.5020; [Ar-P] ⁺ :607.5682			
			Ar-M-M	[M-M] ⁺ :495.4424; [Ar-M] ⁺ :579.5310			
10.67 2	822.7561	C ₅₁ H ₁₀₀ NO ₆ +	O-P-M	[M-P] ⁺ :523.4706; [O-M] ⁺ :549.4868; [O-P] ⁺ :577.5182	2.24 ± 0.05 ^b	2.44 ±	48:1
			S-Po-M	[M-Po] ⁺ :521.4626; [S-M] ⁺ :551.5020; [S-Po] ⁺ :577.5182	0.08 ^a		
			S-Mo-P	[P-Mo] ⁺ :521.4626; [S-P] ⁺ :579.5309; [S-Mo] ⁺ :549.4868			
			P-P-Po	[Po-P] ⁺ :549.4868; [P-P] ⁺ :551.5020			
			S-S-Lo	[Lo-S] ⁺ :521.4626; [S-S] ⁺ :607.5341			
10.91 7	820.7415	C ₅₁ H ₉₈ NO ₆ ⁺	O-O-La	[La-O] ⁺ :521.4549; [O-O] ⁺ :603.5394	0.59 ± 0.03 ^b	0.76 ±	48:2
			O-P-Mo	[Mo-P] ⁺ :521.4549; [O-Mo] ⁺ :547.4785; [O-P] ⁺ :577.5272	0.00 ^a		
			O-Po-M	[M-Po] ⁺ :521.4549; [O-M] ⁺ :549.4933; [O-Po] ⁺ :575.5081			
			P-Po-Po	[Po-Po] ⁺ :547.4785; [P-Po] ⁺ :549.4933			

			S-Po-Mo	[Mo-Po] ⁺ :519.4585; [S-Mo] ⁺ :549.4933; [S-Po] ⁺ :577.5272			
			S-O-Lo	[Lo-O] ⁺ :519.4585; [S-Lo] ⁺ :521.4549; [S-O] ⁺ :605.5237			
			L-S-La	[La-S] ⁺ :523.4719; [L-La] ⁺ :519.4585; [L-S] ⁺ :603.5394			
			L-P-M	[M-P] ⁺ :523.4719; [L-M] ⁺ :547.4785; [L-P] ⁺ :575.5081			
11.02 4	818.7282	C ₅₁ H ₉₆ NO ₆ ⁺	O-L-La	[La-L] ⁺ :519.4471; [O-La] ⁺ :521.4567; [O-L] ⁺ :601.5184	0.23 ± 0.01 ^a	0.17 ±	48:3
			O-Po-Mo	[Mo-Po] ⁺ :519.4471; [O-Mo] ⁺ :547.4750; [O-Po] ⁺ :575.5078		0.00 ^b	
			L-P-Mo	[Mo-P] ⁺ :521.4567; [L-Mo] ⁺ :545.4654; [L-P] ⁺ :575.5078			
			L-Po-M	[M-Po] ⁺ :521.4567; [L-M] ⁺ :547.4750; [L-Po] ⁺ :573.4930			
			Ln-P-M	[M-P] ⁺ :523.4727; [Ln-M] ⁺ :545.4654; [Ln-P] ⁺ :573.4930			
11.07 7	838.7857	C ₅₂ H ₁₀₄ NO ₆	S-Ma-M	[M-Ma] ⁺ :537.4852; [S-M] ⁺ :551.5049; [S-Ma] ⁺ :593.5395	0.09 ± 0.01 ^b	0.12 ±	49:0
		+	S-P-Pe	[Pe-P] ⁺ :537.4852; [S-P] ⁺ :579.5416; [S-Pe] ⁺ :565.5264		0.00 ^a	
			Ma-Ma-Pe	[Pe-Ma] ⁺ :551.5049; [Ma-Ma] ⁺ :579.5416			
11.13 0	836.7768	C ₅₂ H ₁₀₂ NO ₆	S-H-M	[M-H] ⁺ :535.7930; [S-M] ⁺ :551.5072; [S-H] ⁺ :591.5445	0.14 ± 0.00 ^b	0.20 ±	49:1
		+	O-P-Pe	[Pe-P] ⁺ :537.4899; [O-Pe] ⁺ :563.5214; [O-P] ⁺ :577.5214		0.00 ^a	
			Ma-H-Pe	[Pe-H] ⁺ :549.4925 ; [Ma-Pe] ⁺ :551.5072; [Ma-H] ⁺ :577.5214			
			H-P-P	[P-P] ⁺ :551.5072; [H-P] ⁺ :563.5214			
			S-Ma-Mo	[Mo-Ma] ⁺ :535.7930; [S-Mo] ⁺ :549.4925; [S-Ma] ⁺ :593.5431			
			O-S-Tr	[Tr-S] ⁺ :537.4899; [O-Tr] ⁺ :535.7930; [O-S] ⁺ :605.5498			
11.36 5	834.7649	C ₅₂ H ₁₀₀ NO ₆	O-H-M	[M-H] ⁺ :535.4683; [O-M] ⁺ :549.4814; [O-H] ⁺ :589.5240	ND	0.08 ± 0.00	49:2
		+	O-Po-Pe	[Pe-Po] ⁺ :535.4683; [O-Pe] ⁺ :563.5098; [O-Po] ⁺ :575.4991			
			L-Ma-M	[M-Ma] ⁺ :537.4938; [L-M] ⁺ :547.4705; [L-Ma] ⁺ :589.5240			
			L-P-Pe	[Pe-P] ⁺ :537.4938; [L-Pe] ⁺ :561.4965; [L-P] ⁺ :575.4991			
			H-H-Pe	[Pe-H] ⁺ :549.4814; [H-H] ⁺ :575.4991			
			H-P-Po	[Po-P] ⁺ :549.4814; [H-Po] ⁺ :561.4965; [H-P] ⁺ :563.5098			
			O-Ma-Mo	[Mo-Ma] ⁺ :535.4683; [O-Mo] ⁺ :547.4705; [O-Ma] ⁺ :591.5600			
11.51 9	852.8041	C ₅₃ H ₁₀₆ NO ₆	S-P-P	[P-P] ⁺ :551.5048; [S-P] ⁺ :579.5347	0.45 ± 0.03 ^b	0.66 ±	50:0
		+	Ar-P-M	[M-P] ⁺ :523.4764; [Ar-M] ⁺ :579.5347; [Ar-P] ⁺ :607.5732		0.01 ^a	
			Beh-M-M	[M-M] ⁺ :495.4517; [Beh-M] ⁺ :607.5732			
11.59 3	850.7817	C ₅₃ H ₁₀₄ NO ₆	S-O-M	[M-O] ⁺ :549.4885; [S-M] ⁺ :551.5026; [S-O] ⁺ :605.5463	4.82 ± 0.07 ^a	3.46 ±	50:1
		+	O-P-P	[P-P] ⁺ :551.5026; [O-P] ⁺ :577.5152		0.01 ^b	
			Go-P-M	[M-P] ⁺ :523.4730; [Go-M] ⁺ :577.5152; [Go-P] ⁺ :605.5463			
			S-S-Mo	[Mo-S] ⁺ :549.4885; [S-S] ⁺ :607.5656			
			S-P-Po	[Po-P] ⁺ :549.4885; [S-Po] ⁺ :577.5152; [S-P] ⁺ :579.5328			
11.83 0	848.7693	C ₅₃ H ₁₀₂ NO ₆	O-P-Po	[Po-P] ⁺ :549.4889; [O-Po] ⁺ :575.5103; [O-P] ⁺ :577.5217	0.42 ± 0.06 ^b	1.17 ±	50:2
		+	O-O-M	[M-O] ⁺ :549.4889; [O-O] ⁺ :603.5364		0.03 ^a	
			S-O-Mo	[Mo-O] ⁺ :547.4779; [S-Mo] ⁺ :549.4889; [S-O] ⁺ :605.5458			
11.94 9	846.7548	C ₅₃ H ₁₀₀ NO ₆	O-O-Mo	[Mo-O] ⁺ :547.4079; [O-O] ⁺ :603.5284	0.08 ± 0.01 ^b	0.28 ±	50:3
		+	O-L-M	[M-L] ⁺ :547.4079; [O-M] ⁺ :549.4863; [O-L] ⁺ :601.5201		0.01 ^a	
			L-P-Po	[Po-P] ⁺ :549.4863; [L-Po] ⁺ :573.4880; [L-P] ⁺ :575.5060			
			Ln-P-P	[P-P] ⁺ :551.5009; [Ln-P] ⁺ :573.4880			
12.06 8	864.8017	C ₅₄ H ₁₀₆ NO ₆	No-Ma-Pe	[Pe-Ma] ⁺ :551.5150; [No-Pe] ⁺ :577.5186; [No-Ma] ⁺ :605.5285	ND	0.26 ± 0.01	51:1

			No-P-P	[P-P] ⁺ :551.5150; [No-P] ⁺ :591.5280			
			S-O-Pe	[Pe-O] ⁺ :563.5051; [S-Pe] ⁺ :565.5168; [S-O] ⁺ :605.5285			
			O-Ma-P	[P-Ma] ⁺ :565.5168; [O-P] ⁺ :577.5186; [O-Ma] ⁺ :591.5280			
12.25	862.7877	C ₅₄ H ₁₀₄ NO ₆	O-O-Pe	[Pe-O] ⁺ :563.5052; [O-O] ⁺ :603.5369	0.05 ± 0.01 ^b	0.10 ±	51:2
1		+	O-Ma-Po	[Po-Ma] ⁺ :563.5052; [O-Po] ⁺ :575.4844; [O-Ma] ⁺ :591.5364		0.00 ^a	
			O-H-P	[P-H] ⁺ :563.5052; [O-P] ⁺ :577.5157; [O-H] ⁺ :589.5279			
			L-Ma-P	[P-Ma] ⁺ :565.5178; [L-P] ⁺ :575.4844; [L-Ma] ⁺ :589.5279			
			No-H-Pe	[Pe-H] ⁺ :549.4899; [No-Pe] ⁺ :577.5157; [No-H] ⁺ :603.5369			
			No-Ma-Pen	[Pen-Ma] ⁺ :549.4899; [No-Pen] ⁺ :575.4844; [No-Ma] ⁺ :605.5588			
			No-S-Mo	[Mo-S] ⁺ :549.4899; [No-Mo] ⁺ :561.4742; [No-S] ⁺ :619.7220			
			No-O-M	[M-O] ⁺ :549.4899; [No-M] ⁺ :563.5052; [No-O] ⁺ :617.5646			
			L-S-Pe	[Pe-S] ⁺ :565.5178; [L-Pe] ⁺ :561.4742; [L-S] ⁺ :603.5369			
			Po-S-H	[H-S] ⁺ :591.5364; [Po-H] ⁺ :561.4742; [Po-S] ⁺ :577.5157			
12.36	860.7770	C ₅₄ H ₁₀₂ NO ₆	O-L-Pe	[Pe-L] ⁺ :561.4814; [O-L] ⁺ :601.5345; [O-Pe] ⁺ :563.5072	0.10 ± 0.00 ^a	0.10 ±	51:3
3		+	O-H-Po	[Po-H] ⁺ :561.4814; [O-Po] ⁺ :575.5125; [O-H] ⁺ :589.5167		0.02 ^a	
12.47	880.8372	C ₅₅ H ₁₁₀ NO ₆	Ar-P-P	[P-P] ⁺ :551.5081; [Ar-P] ⁺ :607.5637	0.32 ± 0.02 ^a	0.03 ±	52:0
3		+	S-S-P	[P-S] ⁺ :579.5384; [S-S] ⁺ :607.5637		0.00 ^b	
12.63	878.8212	C ₅₅ H ₁₀₈ NO ₆	S-O-P	[P-O] ⁺ :577.5182; [S-P] ⁺ :579.5346; [S-O] ⁺ :605.5522	0.28 ± 0.02 ^b	0.90 ±	52:1
8		+	Ar-P-Po	[Po-P] ⁺ :549.4811; [Ar-Po] ⁺ :605.5522; [Ar-P] ⁺ :607.5670		0.01 ^a	
			Go-P-P	[P-P] ⁺ :551.5057; [Go-P] ⁺ :605.5522			
12.71	876.8040	C ₅₅ H ₁₀₆ NO ₆	O-P-O	[O-P] ⁺ :577.5212; [O-O] ⁺ :603.5396	4.09 ± 0.31 ^b	6.44 ±	52:2
0		+	L-P-S	[S-P] ⁺ :579.5291; [L-S] ⁺ :603.5396; [L-P] ⁺ :575.5015		0.20 ^a	
13.14	874.7872	C ₅₅ H ₁₀₄ NO ₆	O-L-P	[P-L] ⁺ :575.5043; [O-P] ⁺ :577.5184; [O-L] ⁺ :601.5167	0.55 ± 0.05 ^b	1.03 ±	52:3
9		+	Di-P-P	[P-P] ⁺ :551.4954; [Di-P] ⁺ :601.5167		0.04 ^a	
			Ln-S-P	[P-S] ⁺ :579.5158; [Ln-P] ⁺ :573.4679; [Ln-S] ⁺ :601.5167			
			S-L-Po	[Po-L] ⁺ :573.4679; [S-Po] ⁺ :577.5184; [S-L] ⁺ :603.5374			
			O-O-Po	[Po-O] ⁺ :575.5043; [O-O] ⁺ :603.5374			
13.38	872.7766	C ₅₅ H ₁₀₂ NO ₆	ARA-P-P	[P-P] ⁺ :551.5228; [ARA-P] ⁺ :599.5119	0.03 ± 0.00 ^b	0.20 ±	52:4
7		+	O-L-Po	[Po-L] ⁺ :573.4722; [O-Po] ⁺ :575.4924; [O-L] ⁺ :601.5225		0.01 ^a	
			O-Ln-P	[P-Ln] ⁺ :573.4722; [O-P] ⁺ :577.5264; [O-Ln] ⁺ :599.5119			
			L-L-P	[P-L] ⁺ :575.4924; [L-L] ⁺ :599.5119			
13.47	890.8211	C ₅₆ H ₁₀₈ NO ₆	No-Ma-H	[H-Ma] ⁺ :577.5147; [No-H] ⁺ :603.5295; [No-Ma] ⁺ :605.5561	0.21 ± 0.01 ^b	0.32 ±	53:2
6		+	O-O-Ma	[Ma-O] ⁺ :591.5372; [O-O] ⁺ :603.5295		0.00 ^a	
13.56	888.8082	C ₅₆ H ₁₀₆ NO ₆	O-O-H	[H-O] ⁺ :589.5126; [O-O] ⁺ :603.5280	0.11 ± 0.01 ^a	0.11 ±	53:3
4		+	O-L-Ma	[Ma-L] ⁺ :589.5126; [O-Ma] ⁺ :591.5402; [O-L] ⁺ :601.5248		0.01 ^a	
13.62	906.8683	C ₅₇ H ₁₁₂ NO ₆	Beh-P-Po	[Po-P] ⁺ :549.4929; [Beh-Po] ⁺ :633.5734; [Beh-P] ⁺ :635.5895	0.19 ± 0.01 ^b	0.28 ±	54:1
4		+	Er-P-P	[P-P] ⁺ :551.4932; [Er-P] ⁺ :633.5734		0.01 ^a	
			Ar-S-Po	[Po-S] ⁺ :577.5233; [Ar-Po] ⁺ :605.5491; [Ar-S] ⁺ :635.5895			
			Ar-O-P	[P-O] ⁺ :577.5233; [Ar-P] ⁺ :607.5693; [Ar-O] ⁺ :633.5734			
			Go-S-P	[P-S] ⁺ :579.5262; [Go-P] ⁺ :605.5491; [Go-S] ⁺ :633.5734			
	904.8342		S-O-O	[O-O] ⁺ :603.5375; [S-O] ⁺ :605.5510	0.13 ± 0.01 ^b		54:2

13.74		C ₅₇ H ₁₁₀ NO ₆	L-S-S	[S-S]*:607.5631; [L-S]*:603.5375		0.39 ±	
3		+				0.02 ^a	
13.87	902.8211	C ₅₇ H ₁₀₈ NO ₆	O-O-O	[O-O]*:603.5378	0.39 ± 0.04 ^b	2.61 ±	54:3
0		+				0.11 ^a	
14.30	902.8203	C ₅₇ H ₁₀₈ NO ₆	S-O-L	[L-O]*:601.5290; [S-L]*:603.5383; [S-O]*:605.5518	0.23 ± 0.01 ^b	0.33 ±	54:3
9		+	Ln-S-S	[S-S]*:607.5652; [Ln-S]*:601.5290		0.00 ^a	
14.36	900.8062	C ₅₇ H ₁₀₆ NO ₆	O-O-L	[L-O]*:601.5163; [O-O]*:603.5383	0.18 ± 0.01 ^b	2.02 ±	54:4
6		+	Ln-O-S	[S-O]*:605.5476; [Ln-S]*:601.5163; [Ln-O]*:599.5190		0.09 ^a	
			L-L-S	[S-L]*:603.5383; [L-L]*:599.5190			
14.85	898.7900	C ₅₇ H ₁₀₄ NO ₆	Gln-O-O	[O-O]*:603.5295; [Gln-O]*:599.5087	ND	0.04 ± 0.00	54:5
6		+	ARA-O-P	[P-O]*:577.5115; [ARA-P]*:599.5087; [ARA-O]*:625.5305			

tr, retention time (min); * GZG, Guanzhong goat milk; ** XSG, Xinong Saanen goat milk; ACN, acyl carbon number; DB, double bonds number; abbreviations of FAs used in structure of TAGs: Bu, butyric acid (C4:0); Co, caproic acid (C6:0); Cy, caprylic acid (C8:0); Ca, capric acid (C10:0); De, decanoic acid (C10:1); Ud, undecanoic acid (C11:0); La, lauric acid (C12:0); Lo, lauroleic acid (C12:1); Tr, tridecanoic acid (C13:0); M, myristic acid (C14:0); Mo, myristoleic acid (C14:1 n-5c); Pe, pentadecylic acid (C15:0); Pen, pentadecenoic acid (C15:1 n-5c); P, palmitic acid (C16:0); Po, palmitoleic acid (C16:1 n-7c); Ma, margaric acid (C17:0); H, heptadecenoic acid (C17:1 n-7t); S, stearic acid (C18:0); O, oleic acid (C18:1 n-9c); L, linoleic acid (C18:2 n-6c); Ln, alpha-linolenic acid (C18:3 n-3c); Gln, gamma-linolenic acid (C18:3 n-6c); N, nonadecanoic acid (C19:0); No, nonadecenoic acid (C19:1); Ar, arachidic acid (C20:0); Go, gadoleic acid (C20:1); ARA, arachidonic acid (C20:4 n-6c); Beh, behenic acid (C22:0); Er, erucic acid (C22:1). X–Y–Z: structure of TAGs, i.e., O–P–Cy stands for oleoyl–palmitoyl–capryloyl–glycerol structure; regiospecificity of the FAs in the TAGs was not determined. Results represent mean ± standard deviation, n = 3. Presented values with the different superscript letters (within a row) are significantly different by independent samples *t*-test (*p* ≤ 0.05). ND, not detected.