

Supplemental data:

Figure S1, related to Figure 1. The high resolution ESI-MS spectrum of the $[M - H]^-$ ions of sulfolipids of *M. tuberculosis* H37Rv grown in modified Wong-Weinzirl broth. The spectrum was obtained with an Orbitrap Velos ion-trap instrument. The high resolution ($R=100,000$) partially separated the SL-I (monoisotopic ions marked with “*”) class from SL-II (monoisotopic ions marked with “▼”), which is again the principal sulfolipid class. However, the base peak shifts 56 Da (from m/z 2459 to m/z 2515), as compared to Figure 2), indicating that length of the hydroxyphthioceranoyl substituents of the sulfolipids changes dependent on the growth condition.

Figure S1

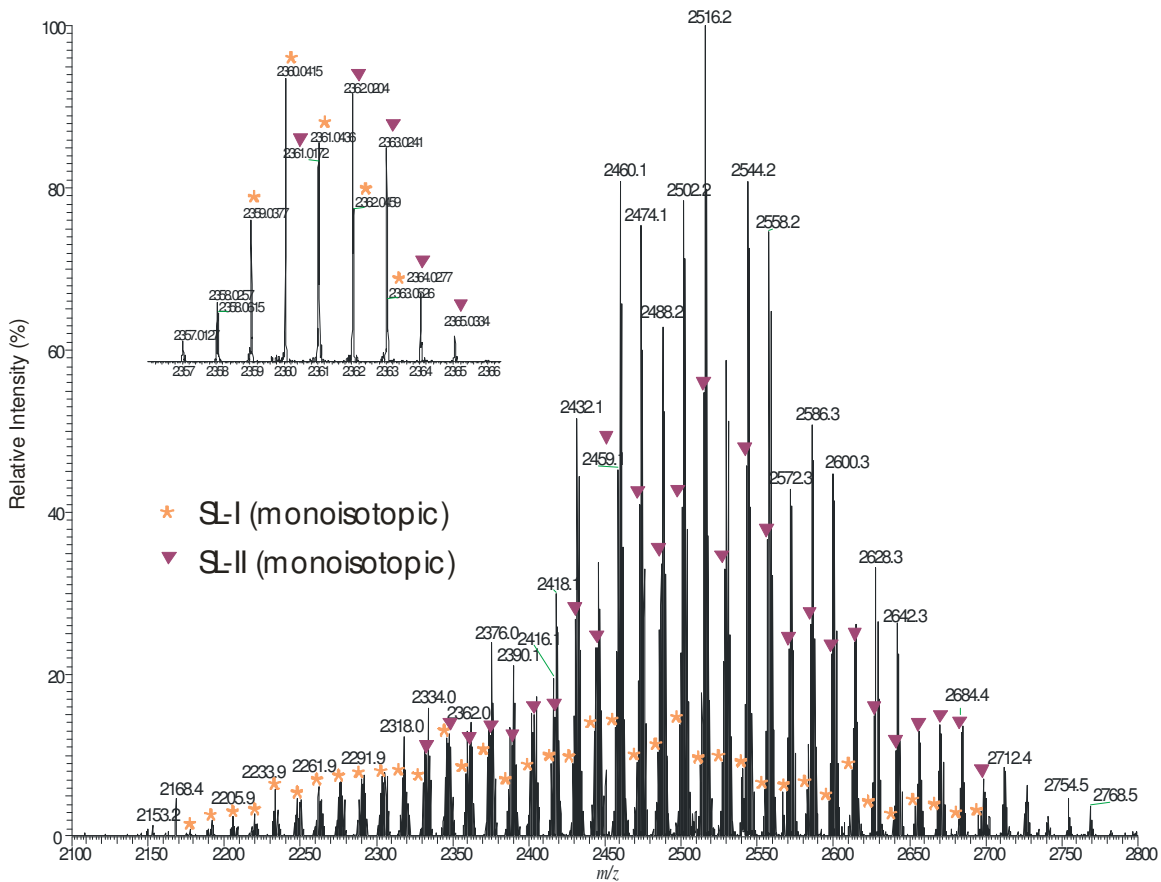


Figure S2, related to Figure 2. The MS² spectrum of the ion at m/z 2122.8 (a), its MS³ spectra of the ion of m/z 1356 (2122 → 1356) (b), and of the ion at m/z 1384 (2123 → 1384) (c). The m/z 2122 represents the lightest SL-II that was characterized

Figure S2

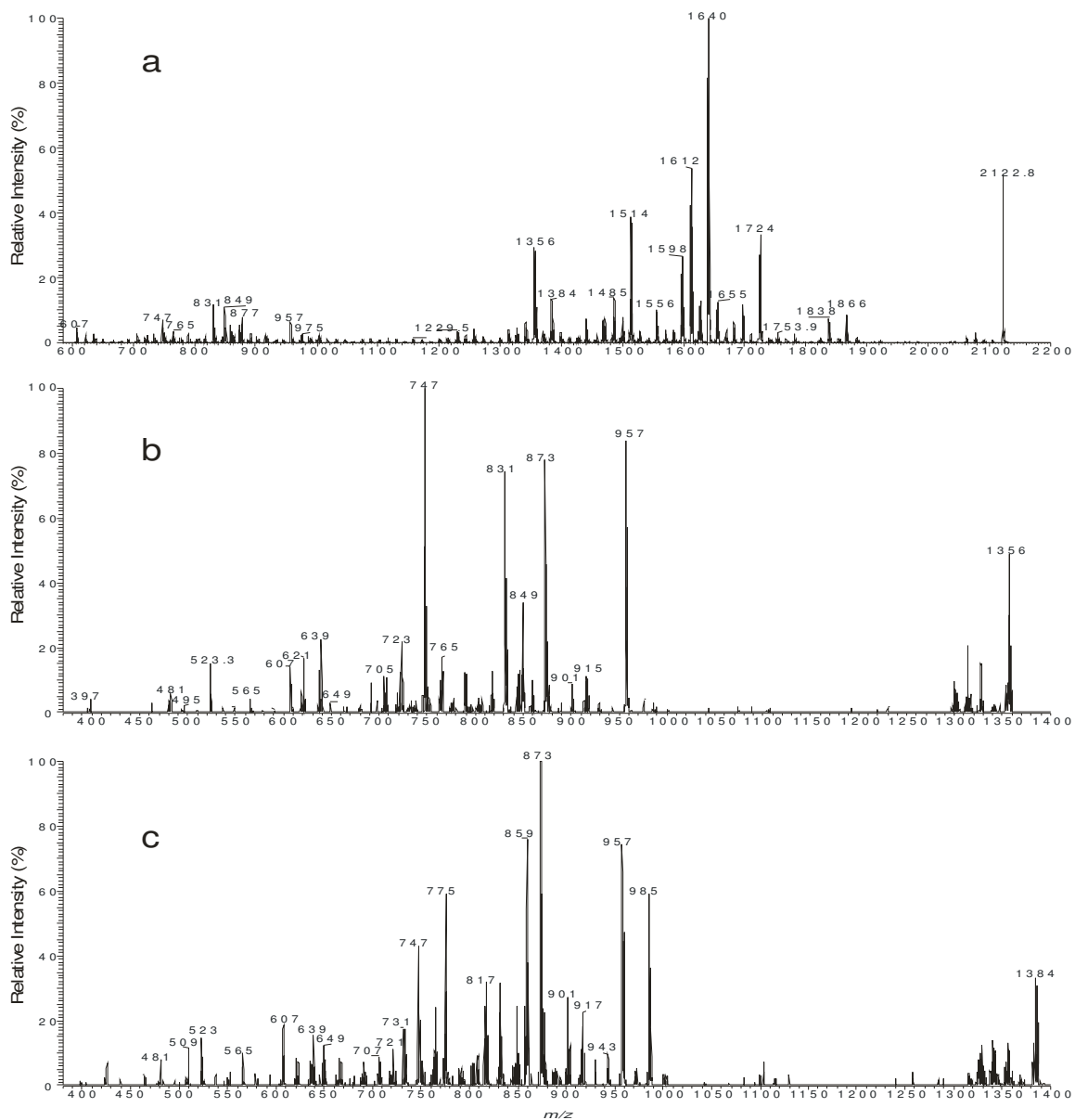


Figure S3, related to Figure 3. The MS² spectrum of the ion at m/z 2795.5 (a), its MS³ spectra of the ion of m/z 1776 (2795 → 1776) (b), and of the ion at 1818 (2795 → 1818) (c). The ion of m/z 2795 represents the heaviest SL-II that was characterized in this study.

Figure S3

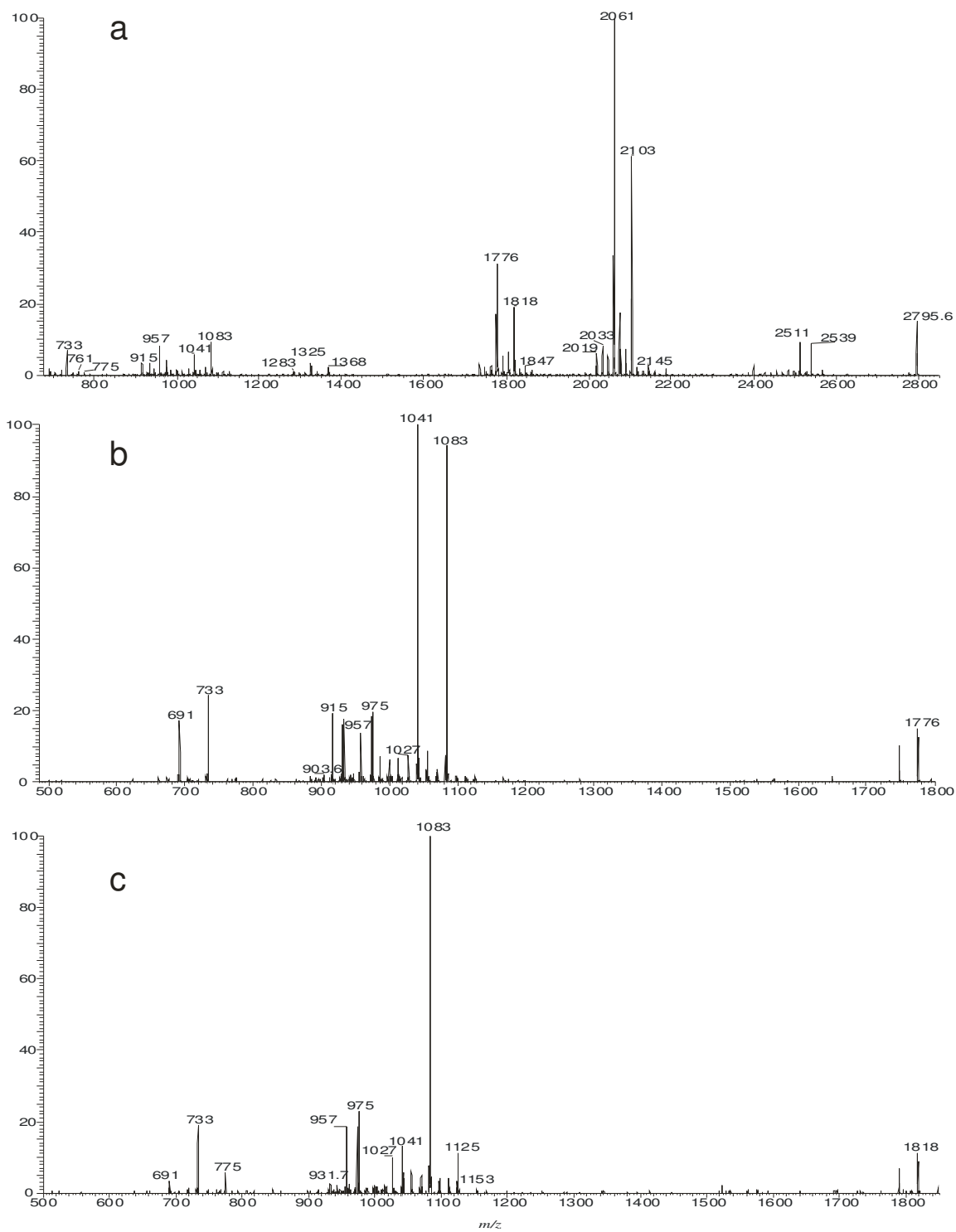


Table S1, related to Figure 2.

Table S1. The elemental compositions (deduced from accurate mass measurements) of the [M -H]⁻ ions of the SLs and the assigned major structures

measured m/z (Da)	calculated m/z (Da)	Composition	deviation (mmu)	Relative Intensity (%)	species	*major structures
2188.8723	2188.8714	C133 H255 O19 S	0.92	0.75	SL-I'	
2190.8502	2190.8467	C132 H253 O20 S	0.45	0.92	SL-I	18:0, hC ₃₃ , hC ₄₀ , C ₃₁
2204.8644	2204.8663	C133 H255 O20 S	-1.90	1.05	SL-I	
2218.8828	2218.8819	C134 H257 O20 S	0.86	0.75	SL-I	
2220.8600	2220.8812	C133 H255 O21 S	-1.21	0.82	SL-II	16:0, hC ₄₀ , hC ₄₀ , hC ₂₅ ;16:0, hC ₄₀ , hC ₃₁ , hC ₃₄
2232.8956	2232.8976	C135 H259 O20 S	-2.00	3.27	SL-I	16:0, hC ₄₀ , hC ₃₄ , C ₃₃ ;18:0, hC ₄₀ , hC ₃₄ , C ₃₁
2234.8776	2234.8769	C134 H257 O21 S	0.74	1.63	SL-II	
2246.9155	2246.9132	C136 H261 O20 S	2.25	2.65	SL-I	
2248.8915	2248.8925	C135 H259 O21 S	-1.01	1.92	SL-II	18:0, hC ₃₁ , hC ₄₀ , hC ₃₄ ;16:0, hC ₃₃ , hC ₄₀ , hC ₃₄
2258.9494	2258.9496	C138 H265 O19 S	-0.23	0.70	SL-I'	
2260.9286	2260.9289	C137 H263 O20 S	-0.30	2.14	SL-I	18:0, hC ₄₀ , hC ₃₄ , C ₃₃
2262.9109	2262.9082	C136 H261 O21 S	2.74	2.88	SL-II	
2272.9639	2272.9653	C139 H267 O19 S	-1.38	1.32	SL-I'	18:0, hC ₄₀ , hC ₃₃ , hC ₃₁
2274.9451	2274.9445	C138 H265 O20 S	0.55	4.84	SL-I	
2276.9229	2276.9238	C137 H263 O21 S	-0.91	4.14	SL-II	18:0, hC ₄₀ , hC ₃₄ , hC ₃₁
2288.9630	2288.9602	C139 H267 O20 S	2.80	4.52	SL-I	
2290.9396	2290.9395	C138 H265 O21 S	0.14	2.40	SL-II	16:0, hC ₄₀ , hC ₄₀ , hC ₃₀ ;18:0, hC ₄₀ , hC ₃₄ , hC ₃₄
2302.9750	2302.9758	C140 H269 O20 S	-0.85	5.32	SL-I	
2304.9553	2304.9551	C139 H267 O21 S	0.19	5.47	SL-II	16:0, hC ₄₀ , hC ₄₀ , hC ₃₁
2316.9897	2316.9915	C141 H271 O20 S	-1.80	7.37	SL-I	18:0, hC ₄₀ , hC ₄₀ , C ₃₁ ; 16:0, hC ₄₀ , hC ₄₀ , C ₃₃
2318.9724	2318.9708	C140 H269 O21 S	1.64	2.81	SL-II	
2329.0263	2329.0279	C143 H275 O19 S	-1.58	0.88	SL-I'	
2331.0072	2331.0071	C142 H273 O20 S	0.05	6.58	SL-I	18:0, hC ₄₀ , hC ₄₀ , hC ₃₀
2332.9870	2332.9864	C141 H271 O21 S	0.59	8.21	SL-II	
2343.0437	2343.0435	C144 H277 O19 S	0.17	0.99	SL-I'	18:0, hC ₄₀ , hC ₄₀ , hC ₃₁
2345.0234	2345.0228	C143 H275 O20 S	0.60	7.26	SL-I	18:0, hC ₄₀ , hC ₄₀ , C ₃₃
2347.0013	2347.0021	C142 H273 O21 S	-0.76	7.15	SL-II	16:0, hC ₄₀ , hC ₄₀ , hC ₃₄
2359.0380	2359.0384	C144 H277 O20 S	-0.45	7.81	SL-I	18:0, hC ₄₀ , hC ₄₀ , C ₃₄
2361.0171	2361.0177	C143 H275 O21 S	-0.61	9.77	SL-II	18:0, hC ₄₀ , hC ₄₀ , hC ₃₃
2373.0542	2373.0541	C145 H279 O20 S	0.10	9.67	SL-I	
2375.0337	2375.0334	C144 H277 O21 S	0.34	12.71	SL-II	18:0, hC ₄₀ , hC ₄₀ , hC ₃₄
2387.0696	2387.0697	C146 H281 O20 S	-0.15	5.86	SL-I	
2389.0494	2389.0490	C145 H279 O21 S	0.39	11.13	SL-II	16:0, hC ₄₀ , hC ₄₃ , hC ₃₄
2401.0860	2401.0854	C147 H283 O20 S	0.60	7.94	SL-I	
2403.0656	2403.0647	C146 H281 O21 S	0.94	10.32	SL-II	18:0, hC ₄₀ , hC ₄₂ , hC ₃₄
2415.0995	2415.1010	C148 H285 O20 S	-1.55	9.04	SL-I	
2417.0794	2417.0080	C147 H283 O21 S	-0.91	13.31	SL-II	18:0, hC ₄₀ , hC ₄₀ , hC ₃₇
2429.1174	2429.1167	C149 H287 O20 S	0.70	8.99	SL-I	
2431.0957	2431.0960	C148 H285 O21 S	-0.26	26.95	SL-II	16:0, hC ₄₀ , hC ₄₀ , hC ₄₀
2443.1313	2443.1323	C150 H289 O20 S	-1.05	13.30	SL-I	
2445.1123	2445.1116	C149 H287 O21 S	0.69	16.60	SL-II	16:0, hC ₄₀ , hC ₄₀ , hC ₄₁
2457.1473	2457.1480	C151 H291 O20 S	-0.70	13.45	SL-I	
2459.1273	2459.1273	C150 H289 O21 S	0.04	45.05	SL-II	18:0, hC ₄₀ , hC ₄₀ , hC ₄₀ ;16:0, hC ₄₀ , hC ₄₂ , hC ₄₀
2471.1631	2471.1636	C152 H293 O20 S	-0.55	9.22	SL-I	
2473.1428	2473.1429	C151 H291 O21 S	-0.11	41.14	SL-II	16:0, hC ₄₀ , hC ₄₃ , hC ₄₀
2485.1790	2485.1793	C153 H295 O20 S	-0.30	10.49	SL-I	
2487.1585	2487.1586	C152 H293 O21 S	0.06	33.62	SL-II	18:0, hC ₄₀ , hC ₄₂ , hC ₄₀
2499.1939	2499.1949	C154 H297 O20 S	-1.05	14.09	SL-I	
2501.1747	2501.1742	C153 H295 O21 S	0.49	40.90	SL-II	18:0, hC ₄₀ , hC ₄₃ , hC ₄₀
2513.2097	2513.2106	C155 H299 O20 S	-0.90	8.86	SL-I	
2515.1897	2525.1899	C154 H297 O21 S	-0.16	49.31	SL-II	16:0, hC ₄₀ , hC ₄₃ , hC ₄₃ ;16:0, hC ₄₀ , hC ₄₆ , hC ₄₀
2527.2261	2527.2262	C156 H301 O20 S	-0.15	9.09	SL-I	
2529.2056	2599.2055	C155 H299 O21 S	0.09	33.00	SL-II	18:0, hC ₄₀ , hC ₄₃ , hC ₄₂
2541.2426	2541.2419	C157 H303 O20 S	0.70	8.50	SL-I	
2543.2208	2543.2212	C156 H301 O21 S	-0.36	42.38	SL-II	18:0, hC ₄₀ , hC ₄₃ , hC ₄₃ ;18:0, hC ₄₀ , hC ₄₆ , hC ₄₀
2555.2565	2555.2575	C158 H305 O20 S	-1.05	5.70	SL-I	
2557.2366	2557.2368	C157 H303 O21 S	-0.21	34.97	SL-II	16:0, hC ₄₀ , hC ₄₃ , hC ₄₆
2569.2693	2569.2372	C159 H307 O20 S	-3.90	5.44	SL-I	
2571.2522	2571.2525	C158 H305 O21 S	-0.26	23.54	SL-II	18:0, hC ₄₀ , hC ₄₂ , hC ₄₆
2583.2872	2583.2888	C160 H309 O20 S	-1.65	4.90	SL-I	
2585.2700	2585.2681	C159 H307 O21 S	1.89	22.92	SL-II	18:0, hC ₄₀ , hC ₄₃ , hC ₄₆
2597.3047	2597.3045	C161 H311 O20 S	0.20	3.53	SL-I	
2599.2833	2599.2838	C160 H309 O21 S	-0.46	22.49	SL-II	16:0, hC ₄₀ , hC ₄₆ , hC ₄₆ ;16:0, hC ₄₃ , hC ₄₃ , hC ₄₆
2611.3177	2611.3201	C162 H313 O20 S	-2.45	2.30	SL-I	
2613.3009	2613.2994	C161 H311 O21 S	1.49	13.43	SL-II	18:0, hC ₄₀ , hC ₄₆ , hC ₄₅ ;18:0, hC ₄₆ , hC ₄₃ , hC ₄₂
2625.3322	2625.3358	C163 H315 O20 S	-3.60	2.58	SL-I	
2627.3177	2627.3151	C162 H313 O21 S	2.64	14.88	SL-II	18:0, hC ₄₀ , hC ₄₆ , hC ₄₆
2639.3490	2639.3151	C164 H317 O20 S	-2.45	0.82	SL-I	
2641.3339	2641.3307	C163 H315 O21 S	3.19	10.55	SL-II	16:0, hC ₄₃ , hC ₄₆ , hC ₄₆ ;18:0, hC ₄₆ , hC ₄₃ , hC ₄₄
2653.3653	2653.3671	C165 H319 O20 S	-1.80	1.21	SL-I	
2655.3466	2655.3464	C164 H317 O21 S	0.24	6.47	SL-II	18:0, hC ₄₃ , hC ₄₆ , hC ₄₆
2669.3632	2669.3620	C165 H319 O21 S	1.19	8.02	SL-II	18:0, hC ₄₆ , hC ₄₃ , hC ₄₆ ;18:0, hC ₄₆ , hC ₄₆ , hC ₄₉
2683.3777	2683.3777	C166 H321 O21 S	0.04	6.09	SL-II	16:0, hC ₄₆ , hC ₄₆ , hC ₄₆ ;16:0, hC ₄₃ , hC ₄₆ , hC ₄₉
2697.3926	2697.3933	C167 H323 O21 S	-0.71	3.00	SL-II	18:0, hC ₄₆ , hC ₄₆ , hC ₄₅
2711.4094	2711.4090	C168 H325 O21 S	0.44	3.92	SL-II	18:0, hC ₄₆ , hC ₄₆ , hC ₄₆
2725.4262	2725.4246	C169 H327 O21 S	1.59	2.87	SL-II	16:0, hC ₄₆ , hC ₄₆ , hC ₄₉ ;16:0, hC ₄₃ , hC ₄₉ , hC ₄₉
2739.4379	2739.4402	C170 H329 O21 S	-2.36	0.80	SL-II	18:0, hC ₄₆ , hC ₄₆ , hC ₄₈
2753.4550	2753.4559	C171 H331 O21 S	-0.91	2.00	SL-II	18:0, hC ₄₆ , hC ₄₆ , hC ₄₉
2767.4740	2767.4716	C172 H333O21 S	2.44	0.50	SL-II	16:0, hC ₄₆ , hC ₄₉ , hC ₄₉

*Only major structures are listed; structures of SL-I and SL-I' not complete