Supplemental information

In-depth Sphingomyelin Characterization using Electron Impact Excitation of Ions from Organics (EIEIO) and Mass Spectrometry

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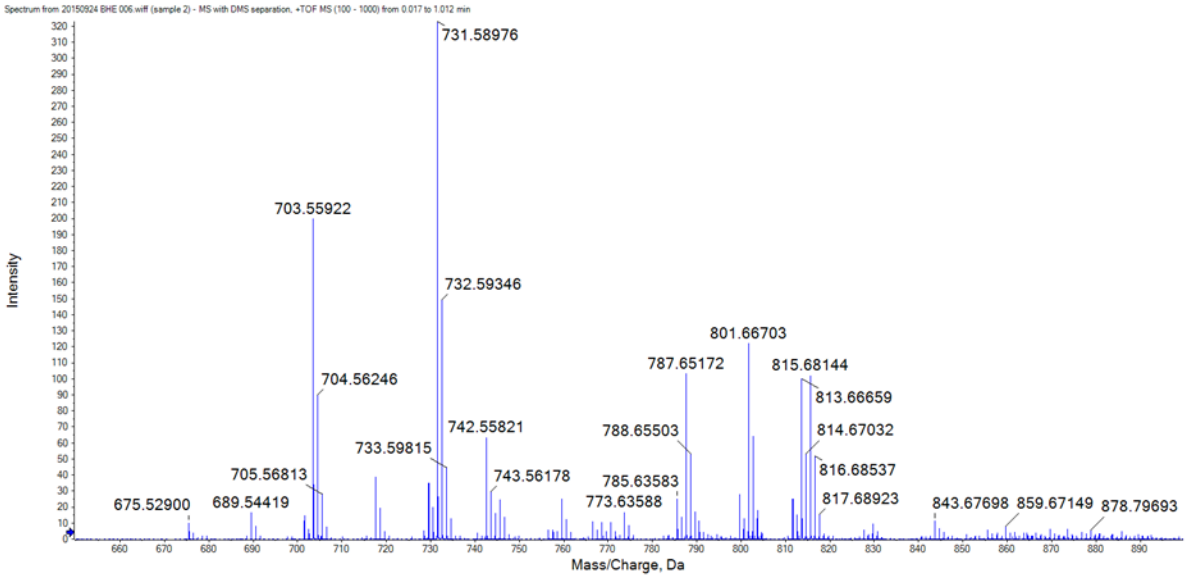
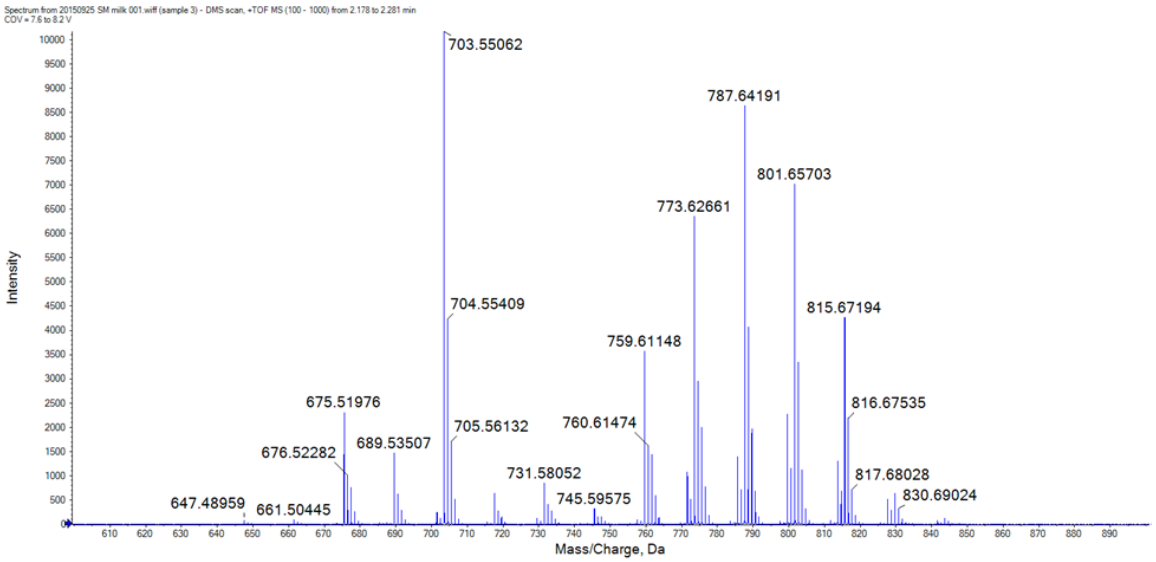
Figure SI-1 MS spectrum and SMs found in BHE



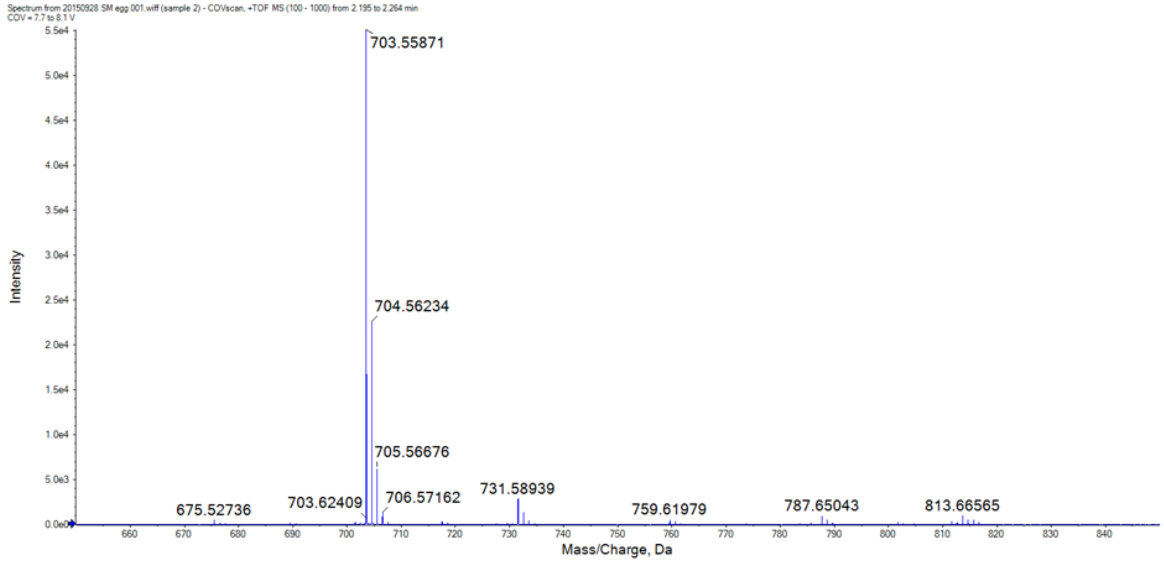
precursor m/z	weight [%] in total	identified sphingomyelins		
675.511	0.008	SM(d16:1,16:0) [70%] (46 sec)		
689.526	0.017	SM(d17:1,16:0) [100%] (14 sec)		
701.526	0.014	SM(d18;2,16:0) [manual]		
703.546	0.186	SM(d18:1,16:0) [95%] (0.086 sec)	SM(d16:1,18:0) [5%] (5 sec)	
717.557	0.038	SM(d17:1,18:0) [100%] (3 sec)		
729.555	0.037	SM(d18:2,18:0) [66%] (11 sec)	SM(d18:1,18:1(n-9)) [34%] (11 sec)	
731.572	0.339	SM(d18:1,18:0) [100%] (0.032 sec)		
745.577	0.036	SM(d19:1,18:0) [77%] (4 sec)	SM(d18:1,19:0) [23%] (6 sec)	
759.588	0.034	SM(d18:1,20:0) [88%] (4 sec)		
773.607	0.021	SM(d17:1,22:0) [48%] (11 sec)	SM(d18:1,21:0) [30%] (11 sec)	SM(d16:1,23:0) [22%] (17 sec)
785.609	0.029	SM(d18:1,22:1) [54%] (14 sec)	SM(d18:2,22:0) [46%] (14 sec)	
787.63	0.129	SM(d18:1,22:0) [92%] (0.346 sec)	SM(d17:1,23:0) [8%] (2 sec)	
799.624	0.035	SM(d18:2,23:0) [44%] (19 sec)	SM(d18:1,23:1) [30%] (19 sec)	SM(d17:1,24:1) [26%] (19 sec)
801.643	0.151	SM(d18:1,23:0) [87%] (0.220 sec)	SM(d19:1,22:0) [7%] (8 sec)	SM(d17:1,24:0) [6%] (2 sec)
811.623	0.032	SM(d18:1,24:2(n-6,-9)) [78%] (14 sec)	SM(d18:2,24:1(n-9)) [22%] (28 sec)	
813.644	0.122	SM(d18:1,24:1(n-9)) [80%] (0.549 sec)	SM(d18:2,24:0) [20%] (2 sec)	
815.655	0.139	SM(d18:1,24:0) [91%] (0.278 sec)	SM(d19:1,23:0) [9%] (5 sec)	
827.628	0.007	PC head group, but may not be a SM.		
829.649	0.016	SM(d19:1,24:0) [51%] (19 sec)	SM(d18:1,25:0) [49%] (19 sec)	
843.636	0.014	PC(17:0,16:3) + 101.11		
855.605	0.010	PC(17:0,16:3) + 113.05		

Figure SI-2 MS spectrum and SMs found in milk SM



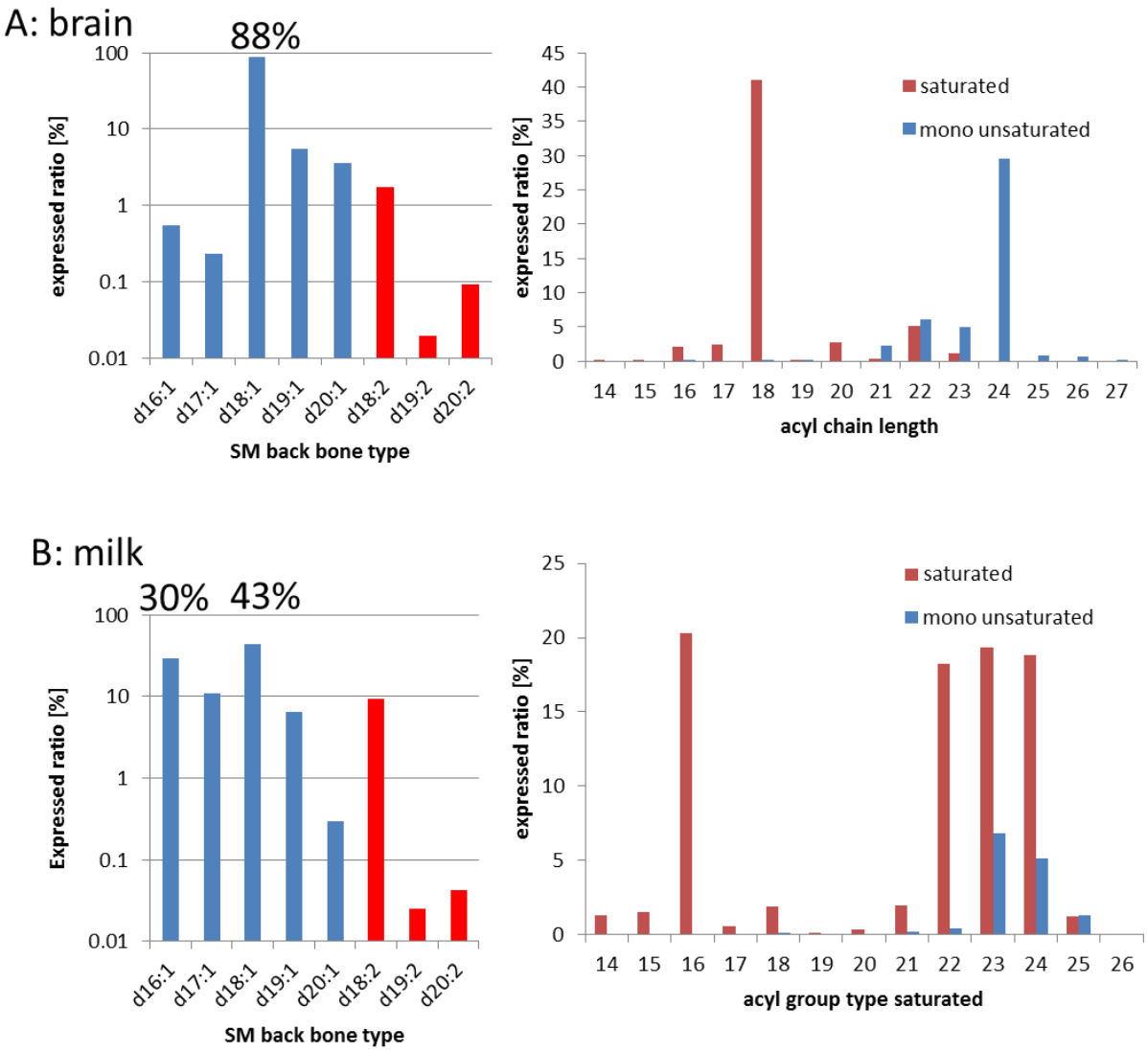
precursor m/z	precursor intensity [%]	identified sphingomyelins				
647.486	0.16	SM(d16:1,14:0) [100%]				
661.502	0.16	SM(d17:1,14:0) [78%]	SM(d16:1,15:0) [22%]			
673.501	0.04	SM(d18:2,14:0) [52%]	SM(d16:1,16:1) [48%]			
675.508	3.98	SM(d16:1,16:0) [72%]	SM(d18:1,14:0) [24%]	SM(d17:1,15:0) [5%]		
685.511	0.05	PC head group, but may not be a SM.				
687.517	0.07	SM(d17:1,16:1) [100%]				
689.524	2.84	SM(d17:1,16:0) [83%]	SM(d18:1,15:0) [13%]			
699.515	0.02	SM(d11:1,18:2) [100%]				
703.53	15.89	SM(d18:1,16:0) [91%]	SM(d19:1,15:0) [9%]			
715.544	0.08	SM(d17:1,18:1) [57%]	SM(d19:2,16:0) [29%]			
717.556	1.07	SM(d19:1,16:0) [43%]	SM(d18:1,17:0) [29%]	SM(d17:1,18:0) [22%]	SM(d20:1,15:0) [4%]	SM(d16:1,19:0) [3%]
727.542	0.02	SM(d18:1,18:2) [100%]				
731.569	1.58	SM(d18:1,18:0) [79%]	SM(d16:1,20:0) [16%]			
741.581	0.03	PC head group				
743.576	0.04	SM(d19:1,18:1) [84%]				
745.586	0.59	SM(d16:1,21:0) [55%]	SM(d19:1,18:0) [23%]	SM(d17:1,20:0) [14%]	SM(d18:1,19:0) [8%]	
755.591	0.06	PC_HG, but may not be a SM .				
757.59	0.22	SM(d16:1,22:1) [81%]	SM(d18:1,20:1) [9%]	SM(d18:2,20:0) [5%]		(n-7)[84%], (n-9)[16%]
759.588	6.84	SM(d16:1,22:0) [88%]	SM(d17:1,21:0) [7%]	SM(d18:1,20:0) [4%]		
769.573	0.09	SM(d16:1,23:2) [100%]				
771.596	2.13	SM(d16:1,23:1) [93%]	SM(d17:1,22:1) [7%]			(n-6)[21%], (n-9)[79%]
773.596	12.23	SM(d16:1,23:0) [79%]	SM(d17:1,22:0) [17%]	SM(d18:1,21:0) [4%]		
783.608	0.16	SM(d16:1,24:2(n-9,*)) [79%]	SM(d18:1,22:2(n-9,*)) [13%]			
785.609	2.73	SM(d16:1,24:1(n-9)) [61%]	SM(d17:1,23:1(n-9)) [22%]	SM(d18:1,22:1(n-9)) [9%]	SM(d18:2,22:0) [8%]	
787.61	15.75	SM(d18:1,22:0) [44%]	SM(d16:1,24:0) [39%]	SM(d17:1,23:0) [17%]		
789.621	4.09	SM(d18:0,22:0) [manual]				
797.623	0.16	SM(d18:2,23:1(n-9)) [56%]	SM(d17:1,24:2) [19%]	SM(d18:1,23:2) [14%]	SM(d16:1,25:2) [11%]	
799.62	3.93	SM(d18:1,23:1) [58%]	SM(d16:1,25:1) [20%]	SM(d17:1,24:1) [10%]	SM(d18:2,23:0) [7%]	(n-6)[6%], (n-9)[94%]
801.621	12.64	SM(d18:1,23:0) [77%]	SM(d17:1,24:0) [12%]	SM(d19:1,22:0) [12%]		
811.633	0.15	SM(d18:1,24:2) [63%]	SM(d18:2,24:1(n-9)) [32%]			
813.637	2.47	SM(d18:1,24:1(n-9)) [71%]	SM(d19:1,23:1(n-9)) [14%]	SM(d18:2,24:0) [8%]	SM(d17:1,25:1(n-9)) [7%]	
815.641	7.59	SM(d18:1,24:0) [80%]	SM(d19:1,23:0) [20%]			
825.642	0.07	SM(d18:2,25:1) [39%]	SM(d19:1,24:2) [21%]	SM(d20:2,23:1) [19%]		
829.667	1.34	SM(d19:1,24:0) [52%]	SM(d18:1,25:0) [33%]	SM(d20:1,23:0) [12%]		
841.674	0.13	SM(d19:1,25:1(n-9)) [53%]	SM(d20:2,24:0) [18%]	SM(d20:1,24:1(n-9)) [16%]		
843.686	0.25	SM(d18:1,26:0) [49%]	SM(d20:1,24:0) [30%]	SM(d19:1,25:0) [21%]		
847.657	0.05	SM possible.				
849.622	0.02	SM possible.				
874.726	0.02	SM(d16:1,23:0)+101.11				
886.698	0.03	SM(d16:1,24:1)+101.11				

Figure SI-3 MS spectrum and SMs found in egg SM

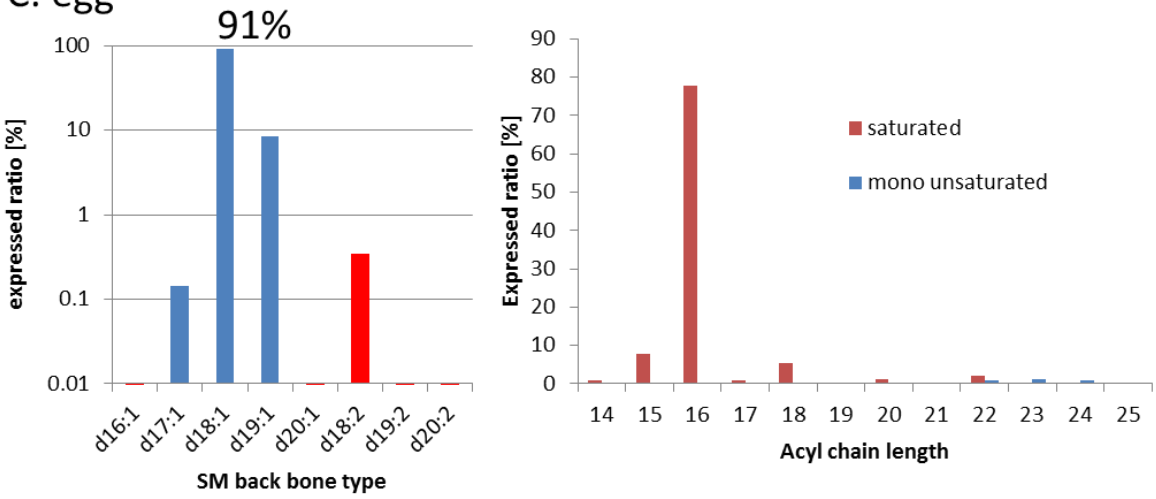


precursor m/z	precursor intensity [%]		identified SM	
675.518	0.90	SM(d18:1,14:0) [100%]		
685.53	0.03	PC head group, but may not be a SM.		
689.535	0.34	SM(d18:1,15:0) [55%]	SM(d17:1,16:0) [41%]	SM(d19:1,14:0) [5%]
699.522	0.02	SM(d18:1,16:2) [manual]		
701.534	0.54	SM(d18:2,16:0) [61%]	SM(d18:1,16:1(n-9)) [39%]	
703.518	83.47	SM(d18:1,16:0) [90%]	SM(d19:1,15:0) [10%]	
715.547	0.03	SM, but chains are not identified.		
717.562	0.62	SM(d18:1,17:0) [85%]	SM(d19:1,16:0) [15%]	
725.531	0.01	SM(d18:1,18:3) [manual]		
727.55	0.20	SM(d18:1,18:2(n-6,-9)) [100%]		
729.564	0.41	SM(d18:1,18:1(n-9)) [94%]	SM(d18:2,18:0) [6%]	
731.57	5.36	SM(d18:1,18:0) [94%]	SM(d19:1,17:0) [6%]	
745.593	0.12	SM(d18:1,19:0) [86%]	SM(d19:1,18:0) [14%]	
755.579	0.02	SM(d18:1,20:2) [100%]		
757.593	0.11	SM(d18:1,20:1(n-9)) [91%]		
759.606	1.06	SM(d18:1,20:0) [94%]	SM(d19:1,19:0) [6%]	
773.623	0.14	SM(d18:1,21:0) [100%]		
781.592	0.02	SM(d18:1,22:3) [100%]		
783.607	0.13	SM(d18:1,22:2(n-6,-9)) [100%]		
785.62	0.29	SM(d18:1,22:1(n-9)) [93%]		
787.631	1.83	SM(d18:1,22:0) [94%]		
799.635	0.07	SM(d18:1,23:1(n-9)) [95%]		
801.648	0.44	SM(d18:1,23:0) [92%]	SM(d19:1,22:0) [8%]	
804.662	0.10	SM(d18:1,16:0)+101.1		
807.613	0.06	SM(d18:1,24:4(n-6,-9,-12,-15)) [100%]		
809.621	0.12	SM(d18:1,24:3(n-6,-9,-12)) [100%]		
811.633	0.66	SM(d18:1,24:2(n-6,-9)) [91%]		
813.643	1.85	SM(d18:1,24:1(n-9)) [94%]		
829.657	0.07	SM(d18:1,25:0) [95%]		

Figure SI-4 sphingolipid backbone and acyl constituents. A: brain SM, B: milk SM, C: egg SM and D: BHE.



C: egg


91%
100
10
1
0.1
0.01
expressed ratio [%]
d16:1
d17:1
d18:1
d19:1
d20:1
d18:2
d19:2
d20:2
SM back bone type
90
80
70
60
50
40
30
20
10
0
Expressed ratio [%]
saturated
mono unsaturated
14
15
16
17
18
19
20
21
22
23
24
25
Acyl chain length

D: BHE

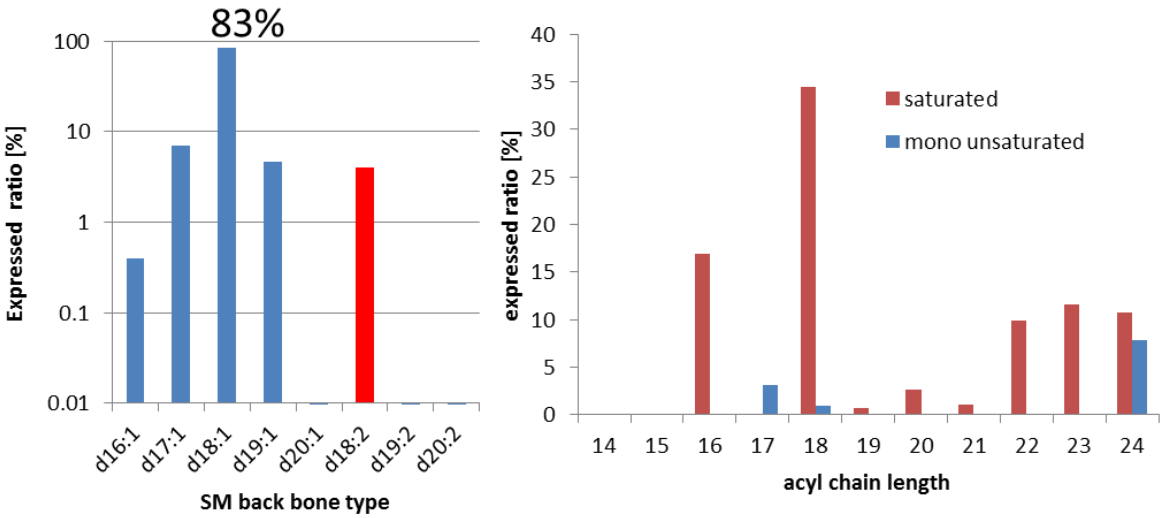

83%
100
10
1
0.1
0.01
Expressed ratio [%]
d16:1
d17:1
d18:1
d19:1
d20:1
d18:2
d19:2
d20:2
SM back bone type
40
35
30
25
20
15
10
5
0
expressed ratio [%]
saturated
mono unsaturated
14
15
16
17
18
19
20
21
22
23
24
acyl chain length

Figure SI-5 milk SM treated iodine vapor

Evapolated Milk SM was exposed to iodine vapor for 10 min. The color changed from white to deep brown. DMS separated the type of modification. (top) non modified SM profile. Hydrogen-iodine replacement reaction was observed in all types of SMs(middle). Double bond opening reaction appeared only in SM with an unsaturated allyl (bottom).