

Supplementary Data 1 Data acquisition parameters from Analyst 1.6.2 Software report

File Information for Sample 221 (MSc-13-L1(1)) of 2018-04-19.wiff

File Name: 2018-04-19.wiff
File Path: D:\Analyst Data\Projects\Multiple
sclerosis\Sclerosis\Data\ Original Name: 2018-04-19.wiff
Software Version: Analyst 1.6.2

Log Information from Devices at Start of acquisition:

Software Application	Shimadzu Instrument driver	0
Time from start =0.0000 min	Mass Spectrometer	3200 Q
TRAP Config Table Version	02	
Firmware Version	MIA3000-----MIL3002 MIB3000	
Component Name	Linear Ion Trap Quadrupole LC/MS/MS Mass	
Spectrometer Component ID	3200 Q TRAP	
Manufacturer	AB Sciex Instruments	
Model	1031491U	
Serial Number	AF26401304	
Time from start =0.0000 min	Mass Spectrometer	3200 Q
TRAP Start of Run - Detailed Status		
Vacuum Status	At Pressure	
Vacuum Gauge (10e-5 Torr)	2.9	
Backing Pump	Ok	
Dual Turbo Pump	Normal	
Sample Introduction Status	Ready	
Source/Ion Path Electronics	On	
Source Type	Turbo Spray	
Source Temperature (at setpoint)	300.0 C	
Source Exhaust Pump	Ok	
Interface Heater	Ready	
Time from start =0.0000 min	Shimadzu Instrument	
driver Injection Volume	14 uL	
System Controller (CBM-20A		
Lite) Power On	On	
Event 1	On	
Event 2	Off	
Pumps	(LC-20AD/LC-20AD)	
Pumping Mode	Binary	
Flow Total Flow	0.01	
mL/min		
B Concentration	80 %	
B Curve	0	
P.Min 1	0 MPa	
P.Max 1	20 MPa	
Pump A		

Pump B

Autosampler (SIL-20AC)

Used	Yes
Rinsing Volume	450 uL
Needle Stroke	52 mm
Rinsing Speed	35 uL/sec
Sampling Speed	15 uL/sec
Purge Time	25 min
Dip Time	0 sec
Rinse Mode	Before and after aspiration
Cooler Temperature	10 C
Control Vial Stroke	52 mm

Time Program

Time (min)	Module	Event	Parameter
0.01	Pumps	Pump B Conc.	80
0.01	Pumps	Total Flow	0.1
0.01	System Controller	Event	0
0.6	Pumps	Total Flow	0.1
0.8	Pumps	Total Flow	0.07
1.5	Pumps	Total Flow	0.07
1.51	Pumps	Total Flow	0.4
1.7	Pumps	Total Flow	0.4
1.71	Pumps	Total Flow	0.1
1.75	System Contr		
oller	Stop		

Mass Spectrometer	3200 Q TRAP	0
End of Run - Detailed Status		
Vacuum Status		At Pressure
Vacuum Gauge (10e-5 Torr)		2.9
Backing Pump		Ok
Dual Turbo Pump		Normal
Sample Introduction Status		Ready
Source/Ion Path Electronics		On
Source Type		Turbo Spray
Source Temperature (at setpoint)		300.0 C
Source Exhaust Pump		Ok
Interface Heater		Ready

Time from start =2.1500 min

Acquisition Info

Acquisition Method:	\Newborn_amino_acyl_allMRM.dam
Acquisition Path:	D:\Analyst Data\Projects\Multiple sclerosis\Sclerosis\Acquisition Methods\

0.01	Pumps	6	Total Flow
0.01	System Controller	0	Event
0.6	Pumps	6	Total Flow
0.8	Pumps	6	Total Flow
1.5	Pumps	6	Total Flow
1.51	Pumps	6	Total Flow
1.7	Pumps	6	Total Flow
1.71	Pumps	6	Total Flow
1.75	System Controller	3	Stop

Pumps
 Pumping Mode: Binary Flow
 P.Min 1: 0 MPa
 P.Max 1: 20 MPa
 Total Flow: 0.01 mL/min
 B Concentration: 80 %
 B Curve: 0

Pump A

Pump B

Autosampler
 Used: Yes
 Rinsing Volume: 450 uL
 Needle Stroke: 52 mm
 Rinsing Speed: 35 uL/sec
 Sampling Speed: 15 uL/sec
 Purge Time: 25 min
 Dip Time: 0 sec
 Rinse Mode: Before and after aspiration
 Enable Cooler: Yes
 Cooler Temperature: 10 C
 Control Vial Stroke: 52 mm

Quantitation Information:

Sample Type: Unknown
 Dilution Factor: 1.000000

Custom Data:

Quantitation Table:

Period 1:

Scans in Period: 37
Relative Start Time: 0.00 msec
Experiments in Period: 1

Period 1 Experiment 1:

Scan Type: MRM (MRM)
Scheduled MRM: No
Polarity: Positive
Scan Mode: N/A
Ion Source: Turbo Spray
Resolution Q1: Unit
Resolution Q3: Unit
Intensity Thres.: 0.00 cps
Settling Time: 0.0000 msec
MR Pause: 5.0070 msec
MCA: No
Step Size: 0.00 Da

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
146.100	Stop	ID		
	44.000	35.00	DP	25.00
	25.00	Alanine	CEP	10.00
	10.00		CE	22.00
	22.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
150.100	Stop	ID		
	48.000	35.00	DP	25.00
	25.00	Alanine std	CEP	12.00
	12.00		CE	22.00
	22.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
231.100	Stop	ID		
	70.100	35.00	DP	48.00
	48.00	Arginine		

			CEP	14.00
	14.00		CE	41.00
	41.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
238.100	77.100	35.00	DP	48.00
	48.00	Arginine std	CEP	14.00
	14.00		CE	41.00
	41.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
246.200	144.100	35.00	DP	28.00
	28.00	Asparagine	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
249.200	147.100	35.00	DP	28.00
	28.00	Asparagine std	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
218.200	85.000	35.00	DP	44.00
	44.00	C:0	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
227.200	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C:0 std	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
428.400	Stop	ID		
	85.000	35.00	DP	56.00
	56.00	C:14	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
431.400	Stop	ID		
	85.000	35.00	DP	56.00
	56.00	C14 std	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
456.400	Stop	ID		
	85.000	35.00	DP	60.00
	60.00	C16	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
	Stop	ID		

459.400	85.000	35.00	DP	60.00
	60.00	C16 std	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
472.400	85.000	35.00	DP	60.00
	60.00	C16_OH	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
260.200	85.000	35.00	DP	36.00
	36.00	C2	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
263.200	85.000	35.00	DP	36.00
	36.00	C2 std	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
274.200	85.000	35.00	DP	56.00
	56.00	C3	CEP	12.00
	12.00			

	38.00		CE	38.00
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
277.200	85.000	35.00	DP	56.00
	56.00	C3 std	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
288.200	85.000	35.00	DP	28.00
	28.00	C4	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
291.200	85.000	35.00	DP	28.00
	28.00	C4 std	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
302.200	85.000	35.00	DP	44.00
	44.00	C5	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
311.200	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C5 std		
			CEP	12.00
	12.00			
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
388.300	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C5_DC		
			CEP	12.00
	12.00			
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
344.300	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C8		
			CEP	12.00
	12.00			
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
347.300	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C8 std		
			CEP	12.00
	12.00			
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
232.100	Stop	ID		
	113.000	35.00	DP	36.00
	36.00	Cit		

			CEP	14.00
	14.00		CE	25.00
	25.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
234.100	115.000	35.00	DP	36.00
	36.00	Cit_istd	CEP	14.00
	14.00		CE	25.00
	25.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
260.200	158.000	35.00	DP	36.00
	36.00	Glu	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
265.200	163.100	35.00	DP	36.00
	36.00	Glu_std	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
132.100	76.100	35.00	DP	26.00
	26.00	Gly	CEP	12.00
	12.00		CE	14.00
	14.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
135.100	79.100	35.00	DP	26.00
	26.00	Gly std	CEP	12.00
	12.00		CE	14.00
	14.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
206.200	104.100	35.00	DP	28.00
	28.00	Met	CEP	12.00
	12.00		CE	26.00
	26.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
209.200	107.100	35.00	DP	28.00
	28.00	Met STD	CEP	12.00
	12.00		CE	26.00
	26.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
189.200	70.100	35.00	DP	31.00
	31.00	Orn	CEP	12.00
	12.00		CE	31.00
	31.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
	Stop	ID		

195.200	76.100	35.00	DP	31.00
	31.00	Orn STD	CEP	12.00
	12.00		CE	31.00
	31.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
222.200	119.900	35.00	DP	28.00
	28.00	Phe	CEP	12.00
	12.00		CE	26.00
	26.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
227.200	125.100	35.00	DP	28.00
	28.00	Phe STD	CEP	12.00
	12.00		CE	26.00
	26.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
238.200	136.100	35.00	DP	28.00
	28.00	Tyr	CEP	12.00
	12.00		CE	26.00
	26.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
242.200	140.100	35.00	DP	28.00
	28.00	Tyr STD	CEP	12.00
	12.00			

	26.00		CE	26.00
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
174.200	72.100	35.00	DP	28.00
	28.00	Val	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
182.200	80.100	35.00	DP	28.00
	28.00	Val STD	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
188.200	86.000	35.00	DP	28.00
	28.00	ile	CEP	12.00
	12.00		CE	26.00
	26.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
191.200	89.000	35.00	DP	28.00
	28.00	ile STD	CEP	12.00
	12.00		CE	26.00
	26.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
394.300	85.000	35.00	DP	44.00
	44.00	C5DC STD	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
316.300	85.000	35.00	DP	44.00
	44.00	C6	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
319.300	85.000	35.00	DP	44.00
	44.00	C6 STD	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
372.400	85.000	35.00	DP	48.00
	48.00	C10	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
375.400	85.000	35.00	DP	48.00
	48.00	C10 STD		

			CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
400.400	85.000	35.00	DP	52.00
	52.00	C12	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
403.400	85.000	35.00	DP	52.00
	52.00	C12 STD	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
484.400	85.000	35.00	DP	60.00
	60.00	C18	CEP	12.00
	12.00		CE	43.00
	43.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
487.400	85.000	35.00	DP	60.00
	60.00	C18 STD	CEP	12.00
	12.00		CE	43.00
	43.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
318.400	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C5OH	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
300.300	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C5:1	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
374.300	Stop	ID		
	85.000	35.00	DP	44.00
	44.00	C4DC	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
482.400	Stop	ID		
	85.000	35.00	DP	60.00
	60.00	C18:1	CEP	51.37
	51.37		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
	Stop	ID		

426.400	85.000	35.00	DP	56.00
	56.00	C14:1		
	12.00		CEP	12.00
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
360.300	85.000	35.00	DP	44.00
	44.00	C3DC		
	12.00		CEP	12.00
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
304.300	85.000	35.00	DP	44.00
	44.00	C4OH		
	12.00		CEP	12.00
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
342.300	85.000	35.00	DP	44.00
	44.00	C8:1		
	12.00		CEP	12.00
	38.00		CE	38.00

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
370.400	85.000	35.00	DP	48.00
	48.00	C10:1		
	12.00		CEP	12.00

			CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
424.400	85.000	35.00	DP	56.00
	56.00	C14:2	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
444.400	85.000	35.00	DP	60.00
	60.00	C14OH	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
454.400	85.000	35.00	DP	60.00
	60.00	C16:1	CEP	12.00
	12.00		CE	38.00
	38.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
470.400	85.000	35.00	DP	60.00
	60.00	C16:1OH	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
498.400	85.000	35.00	DP	60.00
	60.00	C18:1OH	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
496.400	85.000	35.00	DP	60.00
	60.00	C18:2OH	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
500.400	85.000	35.00	DP	60.00
	60.00	C18OH	CEP	12.00
	12.00		CE	38.00
	38.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
172.000	116.000	35.00	DP	24.00
	24.00	Pro	CEP	12.00
	12.00		CE	13.00
	13.00			

Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
179.000	123.000	35.00	DP	24.00
	24.00	Pro STD		

			CEP	12.00
	12.00		CE	13.00
	13.00			
Q1 Mass (Da)	Q3 Mass (Da)	Dwell(msec)	Param	Start
	Stop	ID		
461.600	85.000	35.00	DP	60.00
	60.00	Unknown	CEP	50.32
	50.32		CE	38.00
	38.00			

Parameter Table(Period 1 Experiment 1)

CUR:	20.00
CAD:	Medium
IS:	5000.00
TEM:	300.00
GS1:	30.00
GS2:	30.00
ihe:	ON
EP	10.00
CXP	4.00

Resolution tables

Quad 1 Positive Unit
 Last Modification Date Time: March 23, 2017 13:59:06

IE1	0.800
Mass (Da)	Offset Value
59.050	0.050
175.133	0.122
616.464	0.365
906.673	0.525
1254.925	0.679
1545.134	0.811

Quad 3 Positive Unit
 Last Modification Date Time: April 19, 2018 16:27:42

IE3	2.800
Mass (Da)	Offset Value
59.050	0.033

175.133	0.085
616.464	0.170
906.673	0.293
1254.925	0.345
1545.134	0.305

Calibration tables

Quad 1 Positive Unit Resolution
 Last Modification Date Time: April 19, 2018 16:30:07

Mass (Da)	Dac Value
59.050	1848
175.133	5549
616.464	19629
906.673	28893
1254.925	39996
1545.134	49249

Quad 3 Positive Unit Resolution
 Last Modification Date Time: April 19, 2018 16:30:50

Mass (Da)	Dac Value
59.050	1848
175.133	5561
616.464	19682
906.673	28979
1254.925	40100
1545.134	49380

Instrument Parameters:

Detector Parameters (Positive):
 CEM 2450.0

Keyed Text:

File was created with the software version: Analyst 1.6.2

Supplementary Table S1 Metabolites and stable isotope-labeled internal standards, MRM transitions for derivatives

Precursor ion	Product ion	AA/IS	Product			Compound Name
			Precursor ion	ion	AC/IS	
146,1	44	Alanine	260,2	85	C2	Acetyl-L-carnitine
150,1	48	Alanine-D4	263,2	85	C2-D3	
231,1	70,1	Arginine	274,2	85	C3	Propionyl-L-carnitine
238,1	77,1	Arginine-D7	360,3	85	C3DC	Malonyl-L-carnitine
246,2	144,1	Aspartic acid	277,2	85	C3-D3	
		Aspartic acid-D7				
249,2	147,1		288,2	85	C4	Butyryl-L-carnitine
232,1	113	Cit	374,3	85	C4DC	Succinyl-L-carnitine
234,1	115	Cit-D2	304,3	85	C4OH	Hydroxybutyryl-L-carnitine
260,2	158	Glu	291,2	85	C4-D3	
265,2	163,1	Glu-D5	302,2	85	C5	Valeryl-L-carnitine
132,1	76,1	Gly	318,4	85	C5OH	Hydroxyvaleryl-L-carnitine
135,1	79,1	Gly-13C2-15N1	300,3	85	C5:1	Tiglyl-L-carnitine
206,2	104,1	Met	311,2	85	C5-D9	
209,2	107,1	Met-D3	388,3	85	C5_DC	Glutaryl-L-carnitine
189,2	70,1	Orn	394,3	85	C5DC-D6	
195,2	76,1	Orn-D6	316,3	85	C6	Hexanoyl-L-carnitine
222,2	119,9	Phe	319,3	85	C6-D3	
227,2	125,1	Phe-D5	344,3	85	C8	Octanoyl-L-carnitine
238,2	136,1	Tyr	342,3	85	C8:1	Octenoyl-L-carnitine
242,2	140,1	Tyr-D4	347,3	85	C8-D3	
174,2	72,1	Val	372,4	85	C10	Decanoyl-L-carnitine
182,2	80,1	Val-D8	370,4	85	C10:1	Decenoyl-L-carnitine
188,2	86	xle	375,4	85	C10-D3	
191,2	89	Leu-D3	400,4	85	C12	Dodecanoyl-L-carnitine
172	116	Pro	403,4	85	C12-D3	
179	123	Pro-D7	428,4	85	C14	Tetradecanoyl-L-carnitine
218,2	85	C:0	426,4	85	C14:1	Tetradecenoyl-L-carnitine
227,2	85	C:0-D9	424,4	85	C14:2	Tetradecadienyl-L-carnitine
						Hydroxytetradecanoyl-L-carnitine
			444,4	85	C14OH	
			431,4	85	C14-D3	
			456,4	85	C16	Hexadecanoyl-L-carnitine
						Hydroxyhexadecanoyl-L-carnitine
			472,4	85	C16OH	
			454,4	85	C16:1	Hexadecenoyl-L-carnitine
						Hydroxyhexadecenoyl-L-carnitine
			470,4	85	C16:1OH	
			459,4	85	C16-D3	
			484,4	85	C18	Octadecanoyl-L-carnitine
			482,4	85	C18:1	Octadecenoyl-L-carnitine
						Hydroxyoctadecenoyl-L-carnitine
			498,4	85	C18:1OH	
						Hydroxyoctadecadienyl-L-carnitine
			496,4	85	C18:2OH	
						Hydroxyoctadecanoyl-L-carnitine
			500,4	85	C18OH	
			487,4	85	C18-D3	