Table 1: Mass Spectrometer settings for in Negative Ion Mode for Multiple Reaction Monitoring and Enhance product Ion with the AB Sciex 5500 Q TRAP

AB Sciex 5500 Q TRAP		
Parameter	**MRM**	**EPI**
Curtain Gas	35	35
Collision Gas	Medium	Medium
Ion Spray Voltage	-3500	-3500
Temperature	550 °C	550 °C
Ion Source Gas 1	30	30
Ion Source Gas 2	75	75

Table 2: Mass Spectrometer settings used in Negative Ion Mode for Multiple Reaction Monitoring and Enhance product Ion with the AB Sciex 6500+ Q TRAP

AB Sciex 6500+ Q TRAP		
Parameter	**MRM**	**EPI**
Curtain Gas	30	30
Collision Gas	Medium	Medium
Ion Spray Voltage	-4500	-4500
Temperature	440 °C	440 °C
Ion Source Gas 1	45	45
Ion Source Gas 2	70	70

Table 3: Mass Spectrometer settings for Multiple Reaction Monitoring for AB Sciex 5500 Q TRAP

			Individual parameter			
Compound	Q1	Q3	DP	EP	CE	CXP
DHA Metabolome						
RvD1	375	233	-70	-10	-20.5	-19
RvD2	375	141	-64	-10	-22.5	-14
RvD3	375	147	-90	-10	-26	-13
RvD4	375	101	-70	-10	-23	-11
RvD5	359	199	-76	-10	-22.5	-17
RvD6	359	101	-80	-10	-23	-14
17R -RvD1	375	233	-70	-10	-20.5	-19
17R -RvD3	375	147	-90	-10	-26	-13
PD1	359	153	-80	-10	-21.5	-13
PDX	359	153	-80	-10	-21.5	-13
17R-PD1	359	153	-80	-10	-21.5	-13
22-OH-PD1	375	153	-70	-10	-24.5	-12
PCTR1	650	231	80	9	28	15
PCTR2	521	231	80	5	23.5	13
PCTR3	464	231	80	5	23.5	13
MaR1	359	221	-75	-10	-20	-18
MaR2	359	191	-80	-10	-20	-16
7S,14S-diHDHA	359	221	-75	-10	-20	-18
4S,14S-diHDHA	359	101	-80	-10	-23	-11
22-OH-MaR1	375	221	-70	-10	-24	-12
14-oxo-MaR1	357	248	-80	-10	-20	-11
MCTR1	650	191	80	9	28	15
MCTR2	521	191	80	5	23.5	13
MCTR3	464	191	80	5	23.5	13
4-HDHA	343	101	-80	-10	-17	-15
7-HDHA	343	141	-80	-10	-18	-15
14-HDHA	343	205	-80	-10	-17	-14
17-HDHA	343	245	-80	-10	-17	-14
n-3 DPA Metabolome						
RvT1	377	193	-70	-10	-26.8	-19
RvT2	377	197	-64	-10	-22.5	-14
RvT3	377	197	-64	-10	-22.5	-14
RvT4	361	211	-70	-10	-23	-12
$RvD1_{n\text{-}3\ DPA}$	377	143	-70	-10	-20.5	-13
$RvD2_{n\text{-}3\ DPA}$	377	261	-80	-10	-24	-13
$RvD5_{n\text{-}3\ DPA}$	361	199	-80	-10	-22.5	-13
$PD1_{n\text{-}3\ DPA}$	361	183	-75	-10	-24	-11
10S, 17S-diHDPA	361	183	-75	-10	-24	-11
$MaR1_{n\text{-}3\ DPA}$	361	249	-75	-10	-22	-15
7-HDPA	345	143	-80	-10	-17	-15
14-HDPA	345	207	-80	-10	-17	-15
17-HDPA	345	247	-80	-10	-17	-15
EPA Metabolome						
RvE1	349	161	-75	-10	-23.5	-13.5
RvE2	333	199	-80	-10	-25.5	-18
RvE3	333	201	-75	-10	-22	-16
5-HEPE	317	115	-80	-10	-18	-12
12-HEPE	317	179	-80	-10	-19	-12
15-HEPE	317	219	-80	-10	-18	-12
18-HEPE	317	259	-80	-10	-16	-23
AA Metabolome						
LXA_4	351	115	-80	-10	-19.5	-11
LXB_4	351	221	-75	-10	-22.5	-15
5S,15S-diHETE	335	115	-80	-10	-22	-13

15-epi-LXA_4	351	115	-80	-10	-19.5	-11
15-epi-LXB_4	351	221	-75	-10	-22.5	-15
LTB_4	335	195	-90	-10	-23	-16
5S,12S-diHETE	335	195	-90	-10	-23	-16
6-trans-LTB_4	335	195	-90	-10	-23	-16
12-epi-6-trans-LTB_4	335	195	-90	-10	-23	-16
20-OH-LTB_4	335	195	-100	-10	-25	-16
20-COOH-LTB_4	351	195	-80	-10	-19	-15
LTC_4	626	189	80	9	28	15
LTD_4	497	189	80	5	23.5	13
LTE_4	440	189	80	5	23.5	13
PGD_2	351	189	-70	-10	-27.5	-13
PGE_2	351	189	-70	-10	-26	-16
$PGF_{2\alpha}$	353	193	-90	-10	-34.5	-16
TXB_2	369	169	-70	-10	-25	-15
5-HETE	319	115	-80	-10	-19	-12
12-HETE	319	179	-80	-10	-19	-12
15-HETE	319	219	-80	-10	-19	-12
d_4-PGE_2	355	193	-70	-10	-27	-16
d_5-LXA_4	356	115	-90	-5	-20	-12
d_5-RvD2	380	141	-70	-10	-20.7	-12
d_4-LTB_4	339	197	-85	-10	-23.4	-15
d_8-5S-HETE	327	116	-49	-12	-19.8	-14.2
d_5-LTC_4	631	194	70	10	30	15
d_5-LTD_4	502	194	94	8	26.8	15
d_5-LTE_4	445	194	60	10	21.6	20

Table 4: Mass Spectrometer settings for Multiple Reaction Monitoring for AB Sciex 6500+ Q TRAP

			Individual parameter			
Compound	Q1	Q3	DP	EP	CE	CXP
DHA Metabolome						
RvD1	375	233	-33	-4.8	-20.5	-10
RvD2	375	141	-33	-4.8	-21.5	-10
RvD3	375	147	-33	-4.8	-26	-10
RvD4	375	101	-33	-4.8	-23	-10
RvD5	359	199	-33	-4.8	-22.5	-10
RvD6	359	101	-33	-4.8	-23	-10
17R -RvD1	375	233	-33	-4.8	-20.5	-10
17R -RvD3	375	147	-33	-4.8	-26	-10
PD1	359	153	-33	-4.8	-21.5	-10
PDX	359	153	-33	-4.8	-21.5	-10
17R-PD1	359	153	-33	-4.8	.21.5	-10
22-OH-PD1	375	153	-33	-4.8	-24.5	-10
PCTR1	650	231	40	9	28	15
PCTR2	521	231	40	5	23.5	13
PCTR3	464	231	40	5	23.5	13
MaR1	359	221	-33	-4.8	-19	-10
MaR2	359	191	-33	-4.8	-19	-10
7S,14S-diHDHA	359	221	-33	-4.8	-19	-10
4S,14S-diHDHA	359	101	-33	-4.8	-23	-10
22-OH-MaR1	375	221	-33	-4.8	-24.5	-10
14-oxo-MaR1	357	248	-33	-4.8	-20	-10
MCTR1	650	191	40	9	28	15
MCTR2	521	191	40	5	23.5	13
MCTR3	464	191	40	5	23.5	13
4-HDHA	343	101	-33	-4.8	-17	-10
7-HDHA	343	141	-33	-4.8	-18	-10
14-HDHA	343	205	-33	-4.8	-17	-10
17-HDHA	343	245	-33	-4.8	-17	-10
n-3 DPA Metabolome						
RvT1	377	193	-33	-4.8	-26.8	-10
RvT2	377	197	-33	-4.8	-22.5	-10
RvT3	377	197	-33	-4.8	-30	-10
RvT4	361	211	-33	-4.8	-23	-10
$RvD1_{n\text{-}3\ DPA}$	377	215	-33	-4.8	-26.8	-10
$RvD2_{n\text{-}3\ DPA}$	371	261	-33	-4.8	-24	-10
$RvD5_{n\text{-}3\ DPA}$	361	199	-33	-4.8	-22.5	-10
$PD1_{n\text{-}3\ DPA}$	361	183	-33	-4.8	-24	-10
10S, 17S-diHDPA	361	183	-33	-4.8	-24	-10
$MaR1_{n\text{-}3\ DPA}$	361	249	-33	-4.8	-24.2	-10
7-HDPA	345	143	-33	-4.8	-17	-10
14-HDPA	345	207	-33	-4.8	-17	-10
17-HDPA	345	247	-33	-4.8	-17	-10
EPA Metabolome						
RvE1	349	195	-33	-4.8	-23.5	-10
RvE2	333	159	-33	-4.8	-25	-10
RvE2	333	201	-33	-4.8	-22	-10
5-HEPE	317	115	-33	-4.8	-17	-10
12-HEPE	317	179	-33	-4.8	-17	-10
15-HEPE	317	219	-33	-4.8	-17	-10
18-HEPE	317	259	-33	-4.8	-17	-10
AA Metabolome						
LXA_4	351	115	-33	-4.8	-19.5	-10
LXB_4	351	221	-33	-4.8	-21.5	-10

5S,15S-diHETE	335	235	-33	-4.8	-22	-10
15-epi-LXA_4	351	115	-33	-4.8	-19.5	-10
15-epi-LXB_4	351	221	-33	-4.8	-21.5	-10
LTB_4	335	195	-33	-4.8	-23	-10
5S,12S-diHETE	335	195	-33	-4.8	-23	-10
6-trans-LTB_4	335	195	-33	-4.8	-23	-10
12-epi-6-trans-LTB_4	335	195	-33	-4.8	-23	-10
20-OH-LTB_4	351	195	-33	-4.8	-25	-10
20-COOH-LTB_4	369	195	-33	-4.8	-19	-10
LTC_4	626	189	40	9	28	15
LTD_4	497	189	40	5	23.5	13
LTE_4	440	189	40	5	23.5	13
PGD_2	351	189	-33	-4.8	-27.5	-10
PGE_2	351	189	-33	-4.8	-26	-10
$PGF_{2\alpha}$	353	193	-33	-4.8	-34.5	-10
TXB_2	369	169	-33	-4.8	-25	-10
5-HETE	319	115	-33	-4.8	-17	-10
12-HETE	319	179	-33	-4.8	-17	-10
15-HETE	319	219	-33	-4.8	-17	-10
d_4-PGE_2	355	193	-33	-4.8	-24.3	-10
d_5-LXA_4	356	115	-33	-4.8	-18	-10
d_5-RvD2	380	141	-33	-4.8	-21.5	-10
d_4-LTB_4	339	197	-33	-4.8	-21.5	-10
d_8-5S-HETE	327	116	-33	-4.8	-18.1	-10
d_5-LTC_4	631	194	34	6	28.5	13
d_5-LTD_4	502	194	32	7	22.6	13
d_5-LTE_4	445	194	26	8.7	21.9	13

Table 5: Mass Spectrometer settings used in Positive Ion Mode for Multiple Reaction Monitoring and Enhance product Ion with the AB Sciex 5500 Q TRAP

AB Sciex 5500 Q TRAP		
Parameter	**MRM**	**EPI**
Curtain Gas	25	25
Collision Gas	Medium	Medium
Ion Spray Voltage	2200	2200
Temperature	470 °C	470 °C
Ion Source Gas 1	30	30
Ion Source Gas 2	65	65

Table 6: Mass Spectrometer settings used in Positive Ion Mode for Multiple Reaction Monitoring and Enhance product Ion with the AB Sciex 6500+ Q TRAP

AB Sciex 6500+ Q TRAP		
Parameter	**MRM**	**EPI**
Curtain Gas	30	30
Collision Gas	Medium	Medium
Ion Spray Voltage	5500	5500
Temperature	390 °C	390 °C
Ion Source Gas 1	60	60
Ion Source Gas 2	80	80