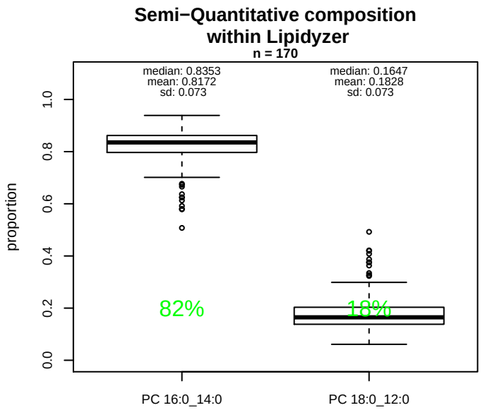
PC aa C28:1 = R

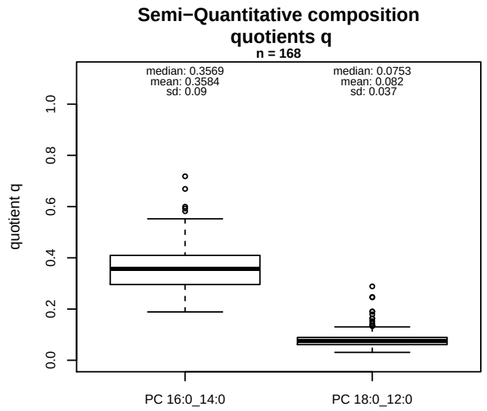
No independent Variable measured.

Qualitative composition

PC aa C28:1 consists of:
PC 10:0_18:1, PC 12:0_16:1, PC 13:0_15:1, PC 14:0_14:1, [13C1]SM 32:1
and further compounds

PC aa C30:0 = PC 16:0_14:0 + PC 18:0_12:0 + R





Semi−Quantitative composition: Lipidyzer

PC aa C30:0 consists of:
PC 16:0_14:0 81.7%
PC 18:0_12:0 18.3%
and of (not quantified):
PC 10:0_20:0, PC 11:0_19:0, PC 13:0_17:0, PC 15:0_15:0,
PC 9:0_21:0, PC O−16:0_15:0, PC O−18:0_13:0, [13C1]SM
and further compounds

Composition: mean of proportions q

conc(PC aa C30:0) * 0.3584 = conc(PC 16:0_14:0) [var(q)=0.3584]
Percentiles: 5%−>0.2248, 25%−>0.2958, 75%−>0.4096, 95%−>0.5098
conc(PC aa C30:0) * 0.082 = conc(PC 18:0_12:0) [var(q)=0.082]
Percentiles: 5%−>0.0462, 25%−>0.0612, 75%−>0.089, 95%−>0.1495

Linear model

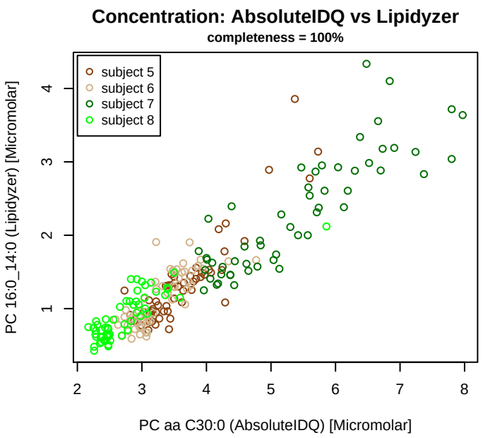
```
PC aa C30:0 ~ b * ( PC 16:0_14:0
   + PC 18:0_12:0 )
```

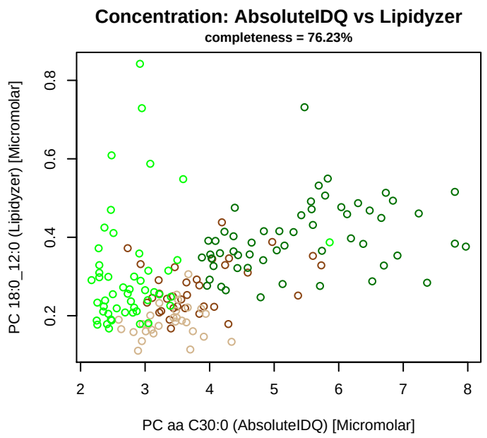
b = 1.30545

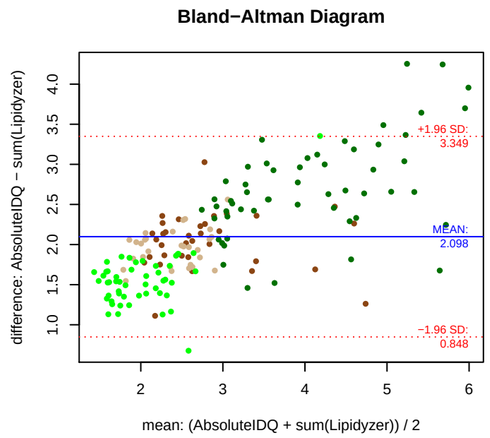
R^2 = 0.83347

Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	2.17	0.6	1.57
Max	7.97	4.8	3.17
Mean	3.77	1.85	1.91
Median	3.42	1.65	1.77
SD	1.25	0.89	0.36





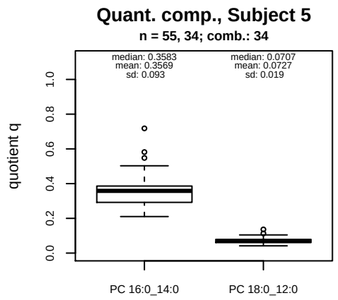


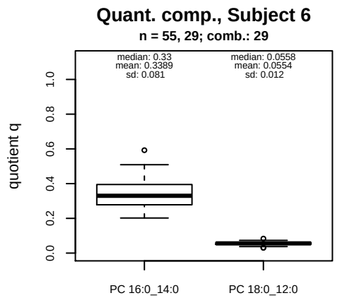
Stability of composition

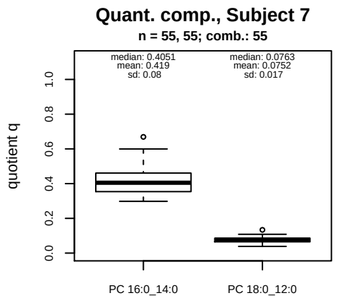
(PC 16:0_14:0 + PC 18:0_12:0) / PC aa C30:0
Shapiro−Wilk Test of log quotients, pv: 0.42442; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.70763; EQUAL
Wilcoxon: Challenge; fasting: 0.5; sport: 0.125; OLTT: 0.5

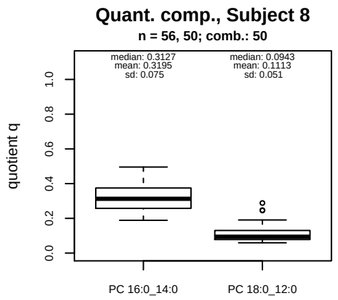
PC 18:0_12:0 / PC aa C30:0
Shapiro−Wilk Test of log quotients, pv: 3e−05; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.5; sport: 0.125; OLTT: 0.5

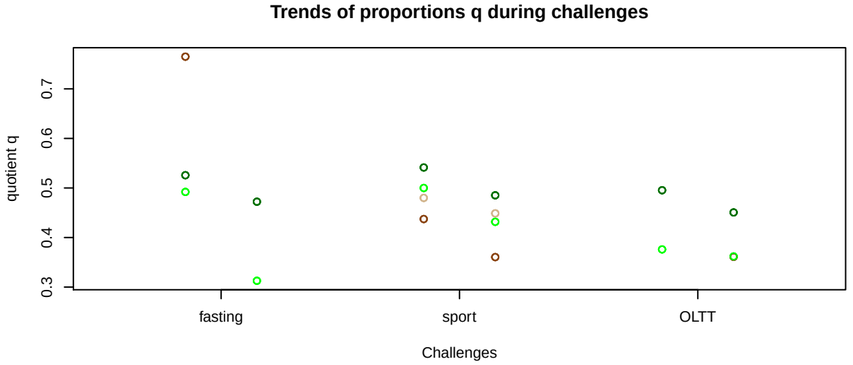
PC 16:0_14:0 / PC aa C30:0
Shapiro−Wilk Test of log quotients, pv: 0.69141; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.47349; EQUAL
Wilcoxon: Challenge; fasting: 0.125; sport: 0.125; OLTT: 0.625

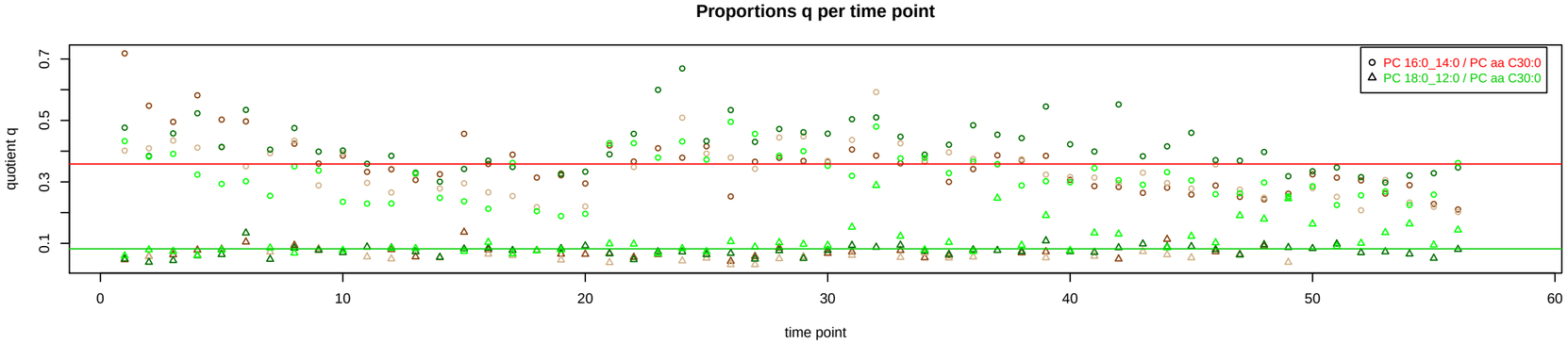




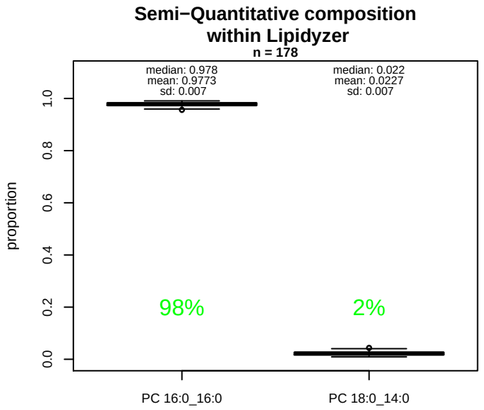


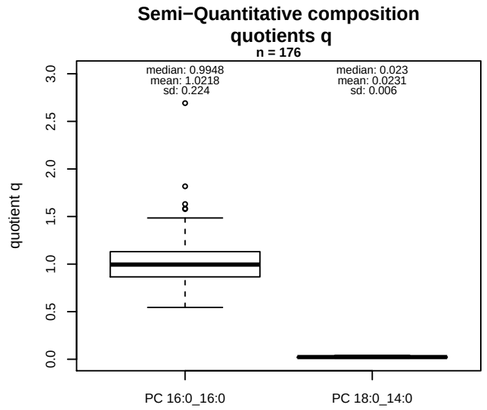






PC aa C32:0 = PC 16:0_16:0 + PC 18:0_14:0 + R





Semi−Quantitative composition: Lipidyzer

PC aa C32:0 consists of:
PC 16:0_16:0 97.7%
PC 18:0_14:0 2.3%
and of (not quantified):
PC 10:0_22:0, PC 11:0_21:0, PC 12:0_20:0, PC 13:0_19:0,
PC 15:0_17:0, PC 9:0_23:0, PC O−16:0_17:0, PC O−18:0_1
[13C1]SM 36:0
and further compounds

Composition: mean of proportions q

conc(PC aa C32:0) * 1.0218 = conc(PC 16:0_16:0) [var(q)=1.0218]
Percentiles: 5%−>0.7561, 25%−>0.8661, 75%−>1.1308, 95%−>1.3897
conc(PC aa C32:0) * 0.0231 = conc(PC 18:0_14:0) [var(q)=0.0231]
Percentiles: 5%−>0.0138, 25%−>0.0173, 75%−>0.0274, 95%−>0.0347

Linear model

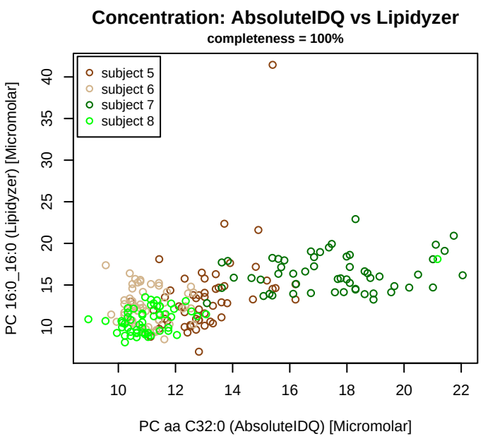
```
PC aa C32:0 ~ b * ( PC 16:0_16:0
   + PC 18:0_14:0 )
```

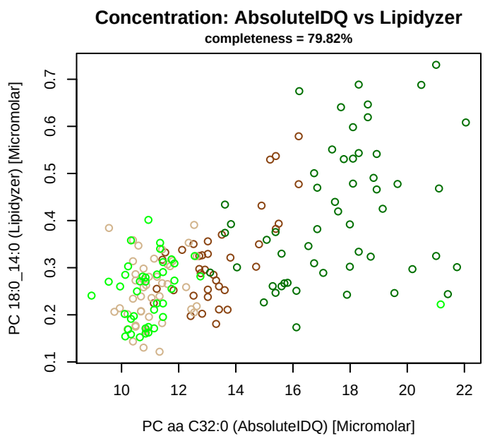
b = 0.49186

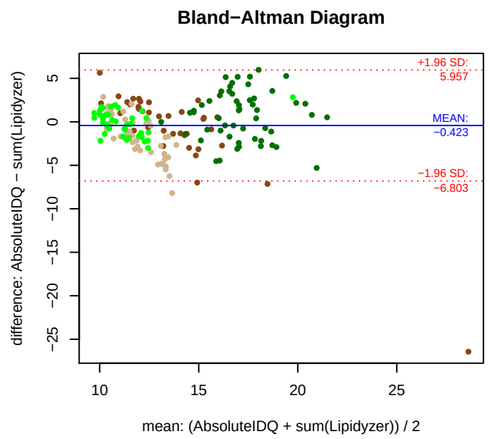
R^2 = 0.35292

Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	8.95	7.19	1.76
Max	22.05	41.83	19.78
Mean	13.18	14	0.83
Median	12.22	13.74	1.52
SD	3.03	3.74	0.71





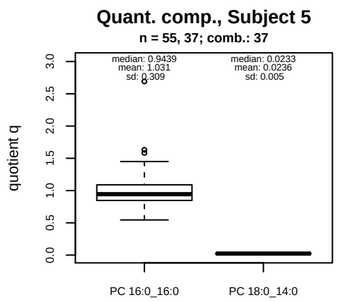


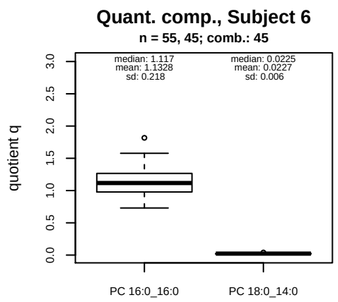
Stability of composition

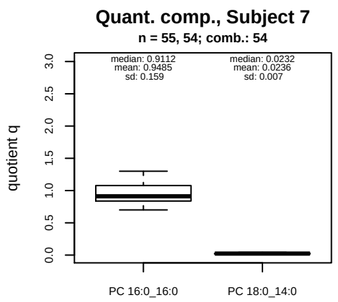
(PC 16:0_16:0 + PC 18:0_14:0) / PC aa C32:0
Shapiro−Wilk Test of log quotients, pv: 0.00013; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0.00011; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.75; sport: 0.125; OLTT: 1

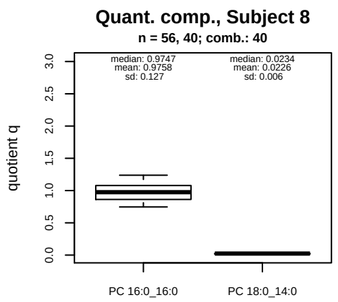
PC 18:0_14:0 / PC aa C32:0
Shapiro−Wilk Test of log quotients, pv: 0.02181; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.53573; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.625; OLTT: 0.5

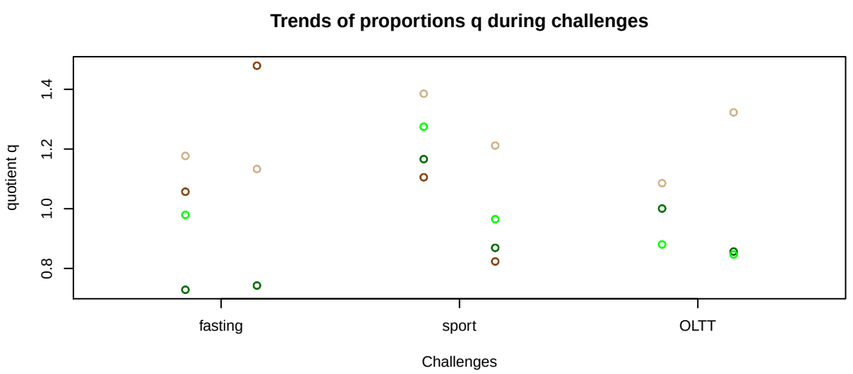
PC 16:0_16:0 / PC aa C32:0
Shapiro−Wilk Test of log quotients, pv: 3e−05; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 2e−05; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.875; sport: 0.125; OLTT: 0.875

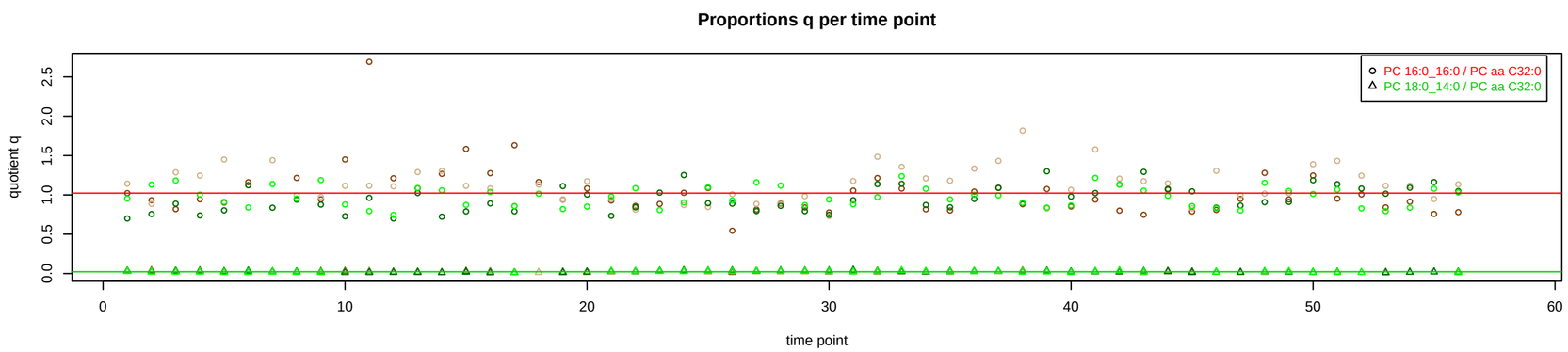




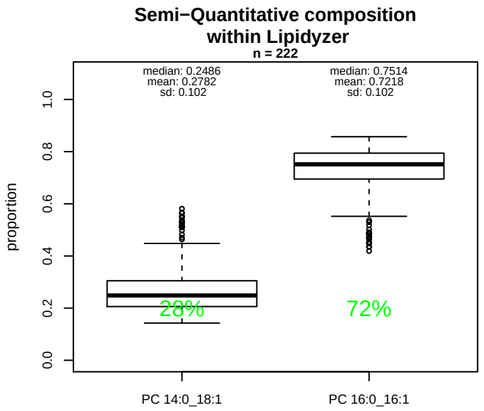


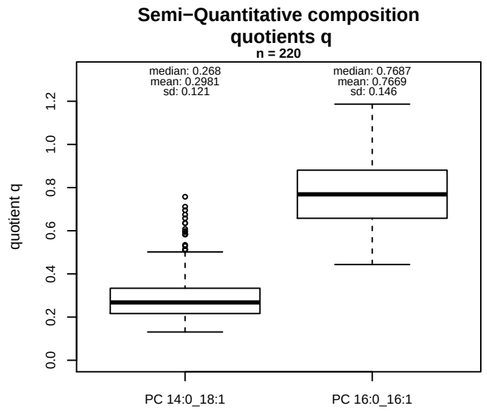






PC aa C32:1 = PC 14:0_18:1 + PC 16:0_16:1 + R





Semi−Quantitative composition: Lipidyzer

PC aa C32:1 consists of:
PC 14:0_18:1 27.8%
PC 16:0_16:1 72.2%
and of (not quantified):
PC 12:0_20:1, PC 13:0_19:1, PC 14:1_18:0, PC 15:0_17:1,
PC 15:1_17:0, PC O−16:0_17:1, PC O−18:0_15:1, PC O−16:
PC O−20:1_13:0
and further compounds

Composition: mean of proportions q

conc(PC aa C32:1) * 0.2981 = conc(PC 14:0_18:1) [var(q)=0.2981]
Percentiles: 5%−>0.1773, 25%−>0.2167, 75%−>0.3336, 95%−>0.5843
conc(PC aa C32:1) * 0.7669 = conc(PC 16:0_16:1) [var(q)=0.7669]
Percentiles: 5%−>0.5433, 25%−>0.6577, 75%−>0.8806, 95%−>0.9891

Linear model

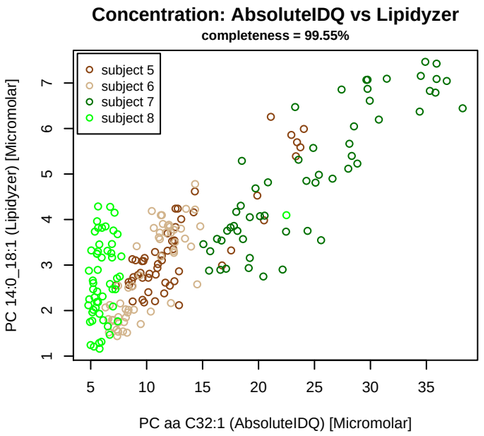
```
PC aa C32:1 ~ b * ( PC 14:0_18:1
   + PC 16:0_16:1 )
```

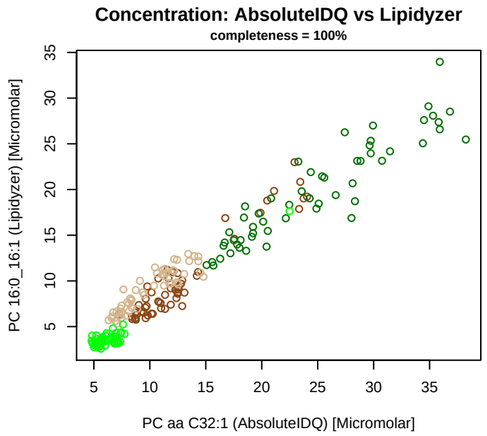
b = 0.97254

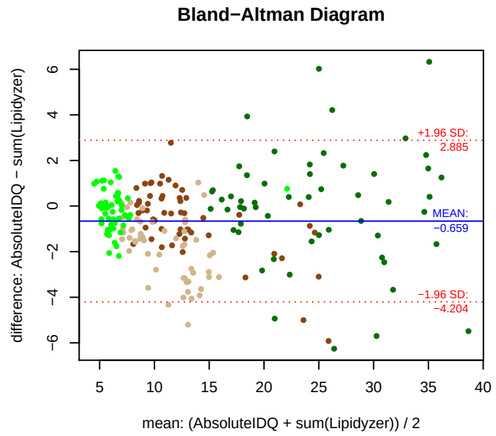
R^2 = 0.95086

Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	4.79	4.01	0.78
Max	38.24	41.4	3.16
Mean	13.42	14.16	0.74
Median	11.09	12.15	1.06
SD	8.15	8.14	0.01





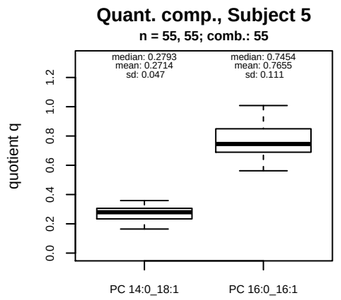


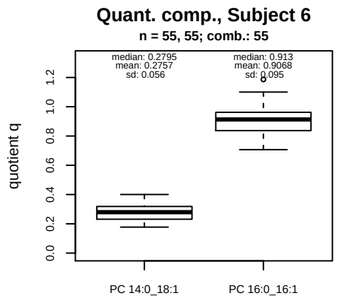
Stability of composition

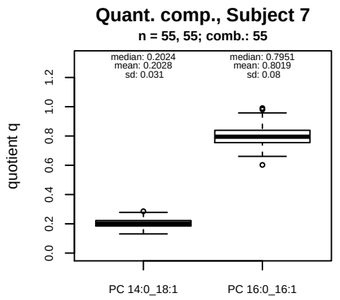
(PC 14:0_18:1 + PC 16:0_16:1) / PC aa C32:1
Shapiro−Wilk Test of log quotients, pv: 0.23341; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.02667; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.625; OLTT: 0.875

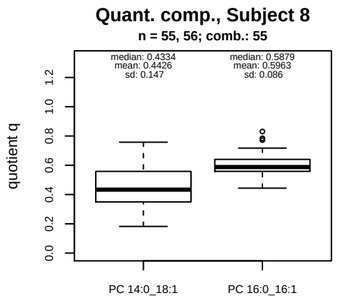
PC 16:0_16:1 / PC aa C32:1
Shapiro−Wilk Test of log quotients, pv: 0.00051; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 1; sport: 0.375; OLTT: 1

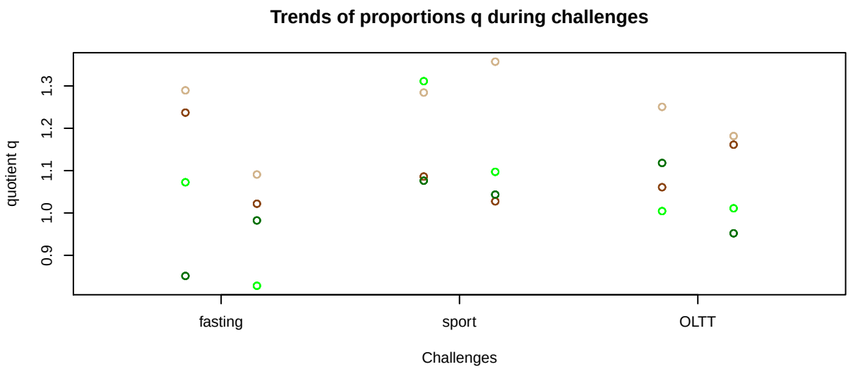
PC 14:0_18:1 / PC aa C32:1
Shapiro−Wilk Test of log quotients, pv: 1e−05; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.625; OLTT: 0.25

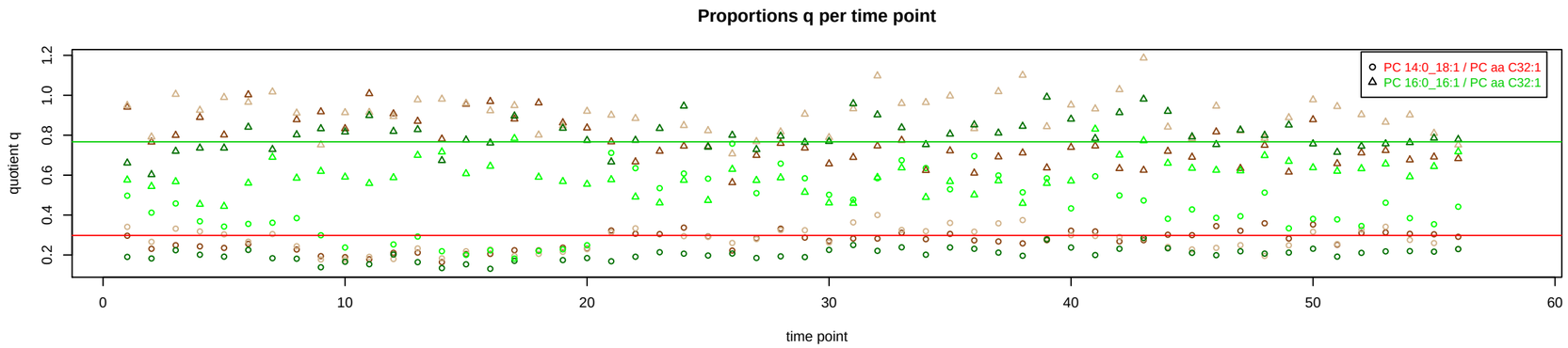




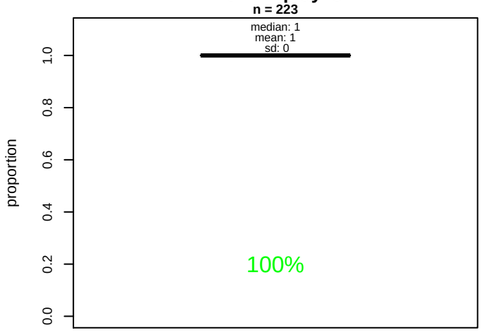


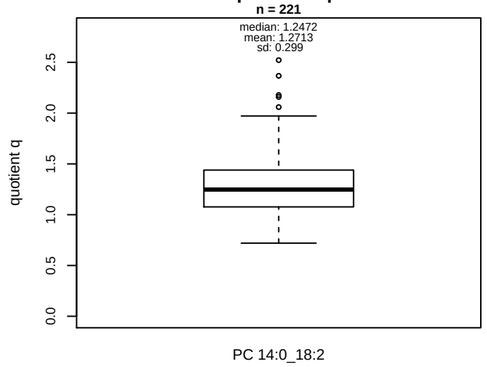






PC aa C32:2 = PC 14:0_18:2 + R





Semi−Quantitative composition: Lipidyzer

PC aa C32:2 consists of:
PC 14:0_18:2 100%
and of (not quantified):
PC 12:0_20:2, PC 14:1_18:1, PC 15:0_17:2, PC 16:1_16:1, PC 15:1_17:1, PC O−16:0_17:2, PC O−16:1_17:1, PC O−18: and further compounds

Composition: mean of proportions q

conc(PC aa C32:2) * 1.2713 = conc(PC 14:0_18:2) [var(q)=1.2713]
Percentiles: 5%−>0.8229, 25%−>1.0768, 75%−>1.439, 95%−>1.7371

Linear model

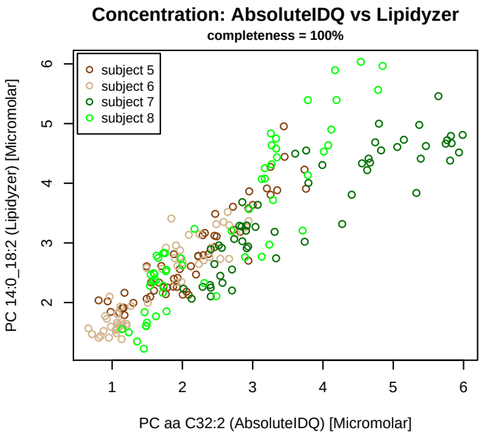
```
PC aa C32:2 ~ b * ( PC 14:0_18:2 )
```

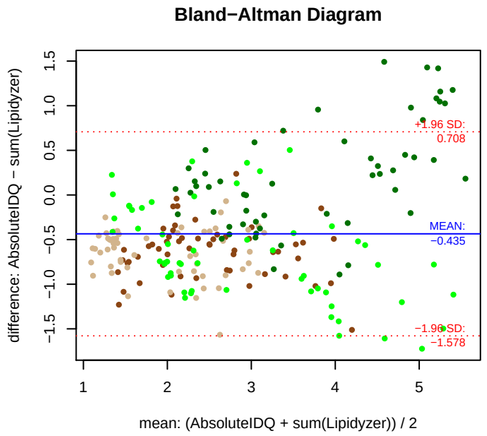
b = 1.03115

R^2 = 0.78893

Ranges

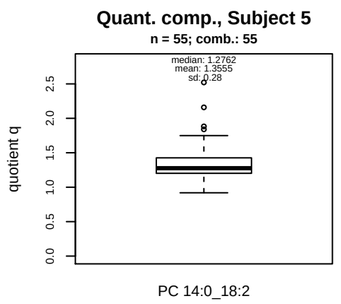
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	0.66	1.23	0.56
Max	5.99	6.04	0.05
Mean	2.55	2.99	0.43
Median	2.32	2.77	0.45
SD	1.27	1.09	0.18

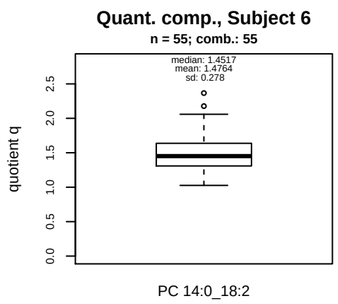


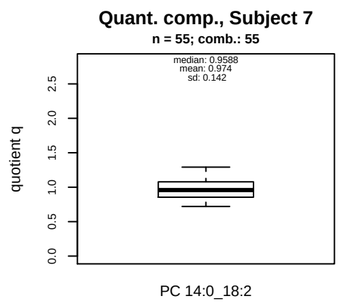


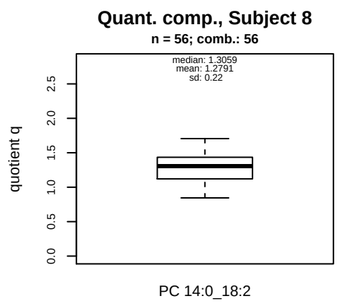
Stability of composition

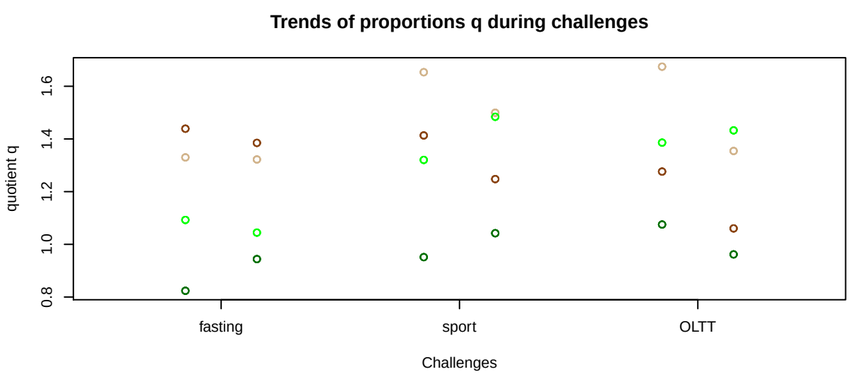
PC 14:0_18:2 / PC aa C32:2
Shapiro−Wilk Test of log quotients, pv: 0.28199; OK
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.875; sport: 0.875; OLTT: 0.25

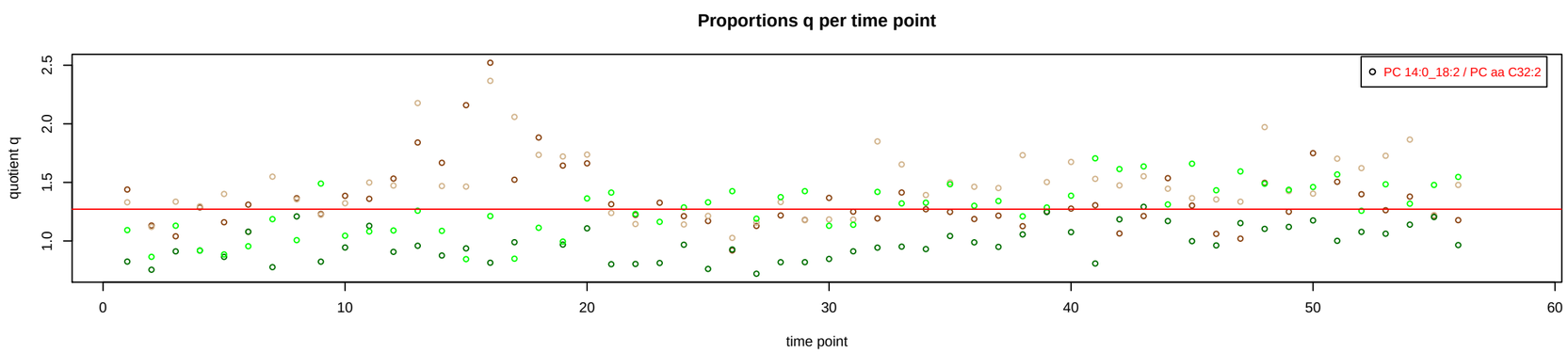












PC aa C32:3 = PC 14:0_18:3 + R

PC 14:0_18:3 excluded because of missingness > 75%

No independent Variable with coverage >0.25 out of PC 14:0_18:3

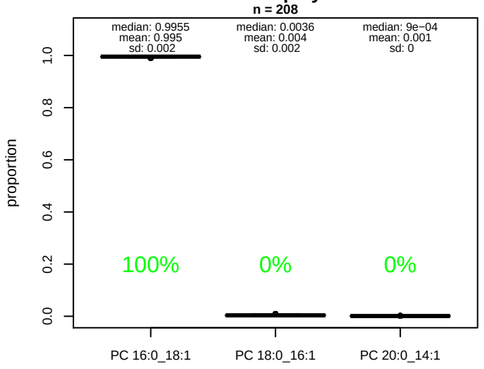
Qualitative composition

PC aa C32:3 consists of:
PC 14:0_18:3, PC 12:0_20:3, PC 14:1_18:2, PC 15:1_17:2, [13C1]SM 36:3
and further compounds

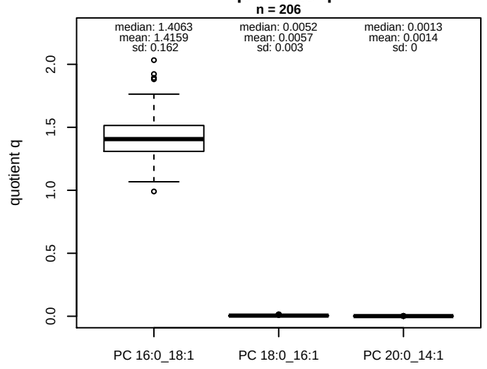
PC aa C34:1 = PC 14:0_20:1 + PC 16:0_18:1 + PC 18:0_16:1 + PC 20:0_14:1 + R

PC 14:0_20:1 excluded because of missingness > 75%

Semi−Quantitative composition within Lipidyzer



Semi−Quantitative composition quotients q



Semi−Quantitative composition: Lipidyzer

PC aa C34:1 consists of:
PC 16:0_18:1 99.5%
PC 18:0_16:1 0.4%
PC 20:0_14:1 0.1%
and of (not quantified):
PC 14:0_20:1, PC 12:0_22:1, PC 14:1_20:0, PC 15:0_19:1, PC 15:1_19:0, PC 17:0_17:1, PC O−17:0_18:1, PC O−16:0_1 PC O−18:0_17:1, PC O−20:0_15:1, PC O−16:1_19:0, PC O−[13C1]SM 38:1
and further compounds

Composition: mean of proportions q

conc(PC aa C34:1) * 1.4159 = conc(PC 16:0_18:1) [var(q)=1.4159]
Percentiles: 5%−>1.1793, 25%−>1.3089, 75%−>1.5146, 95%−>1.6821
conc(PC aa C34:1) * 0.0057 = conc(PC 18:0_16:1) [var(q)=0.0057]
Percentiles: 5%−>0.0028, 25%−>0.0036, 75%−>0.0067, 95%−>0.012
conc(PC aa C34:1) * 0.0014 = conc(PC 20:0_14:1) [var(q)=0.0014]
Percentiles: 5%−>9e−04, 25%−>0.0011, 75%−>0.0016, 95%−>0.0022

Linear model

```
PC aa C34:1 ~ b * ( PC 16:0_18:1
   + PC 18:0_16:1
   + PC 20:0_14:1 )
```

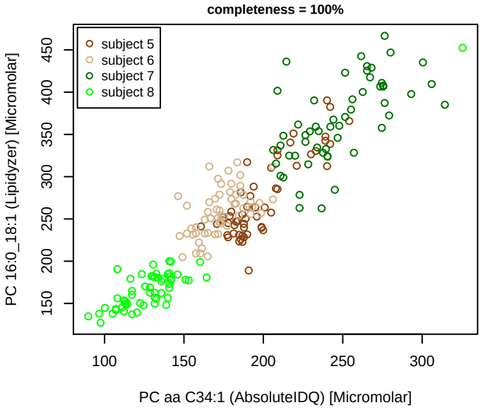
b = 0.55441

R^2 = 0.86597

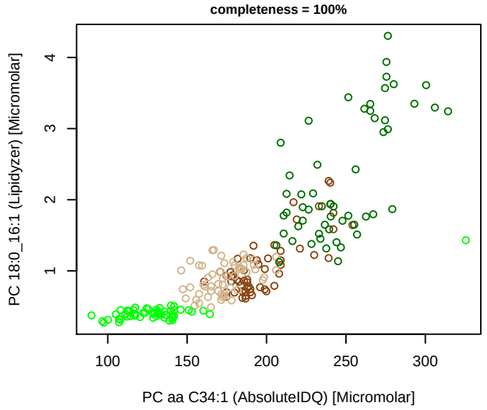
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	89.8	127.65	37.85
Max	325.5	471.26	145.76
Mean	187.14	268.99	81.85
Median	183.6	261.66	78.06
SD	49.04	84.03	35

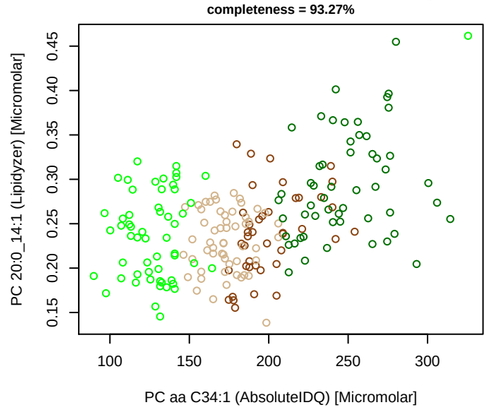
Concentration: AbsoluteIDQ vs Lipidyzer



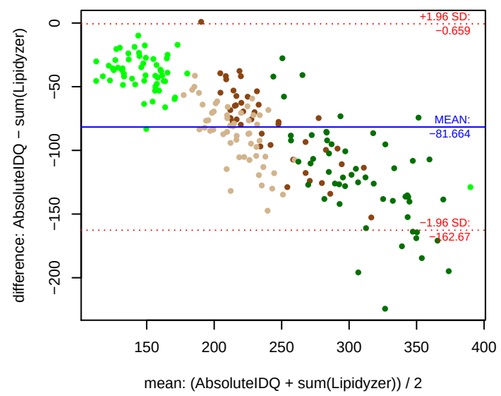
Concentration: AbsoluteIDQ vs Lipidyzer



Concentration: AbsoluteIDQ vs Lipidyzer



Bland−Altman Diagram



Stability of composition

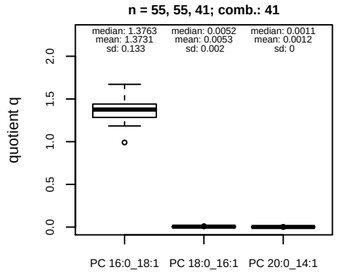
(PC 16:0_18:1 + PC 18:0_16:1 + PC 20:0_14:1) / PC aa C34:1
Shapiro−Wilk Test of log quotients, pv: 0.82819; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00213; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.75; sport: 0.125; OLTT: 1

PC 18:0_16:1 / PC aa C34:1
Shapiro−Wilk Test of log quotients, pv: 0.00069; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00029; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.25; OLTT: 0.125

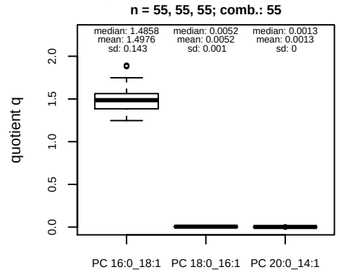
PC 16:0_18:1 / PC aa C34:1
Shapiro−Wilk Test of log quotients, pv: 0.85563; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.02562; EQUAL
Wilcoxon: Challenge; fasting: 0.625; sport: 0.125; OLTT: 1

PC 20:0_14:1 / PC aa C34:1
Shapiro−Wilk Test of log quotients, pv: 0.01446; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.75; sport: 0.625; OLTT: 1

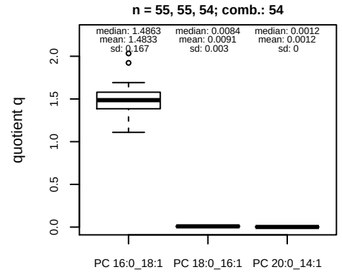
Quant. comp., Subject 5



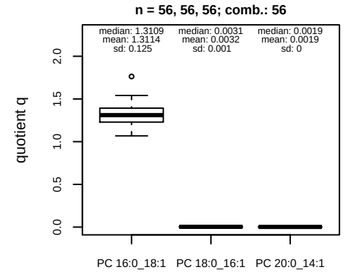
Quant. comp., Subject 6



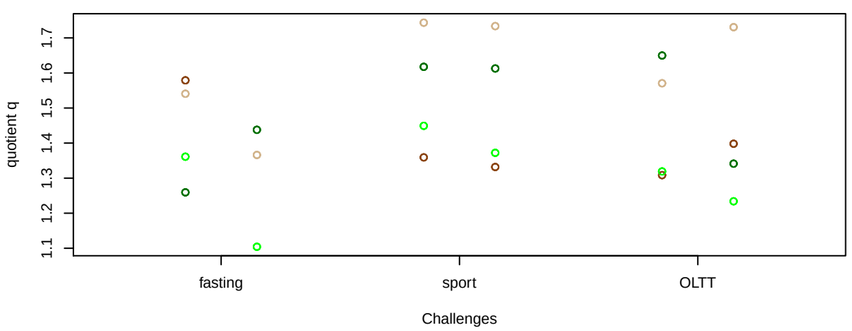
Quant. comp., Subject 7



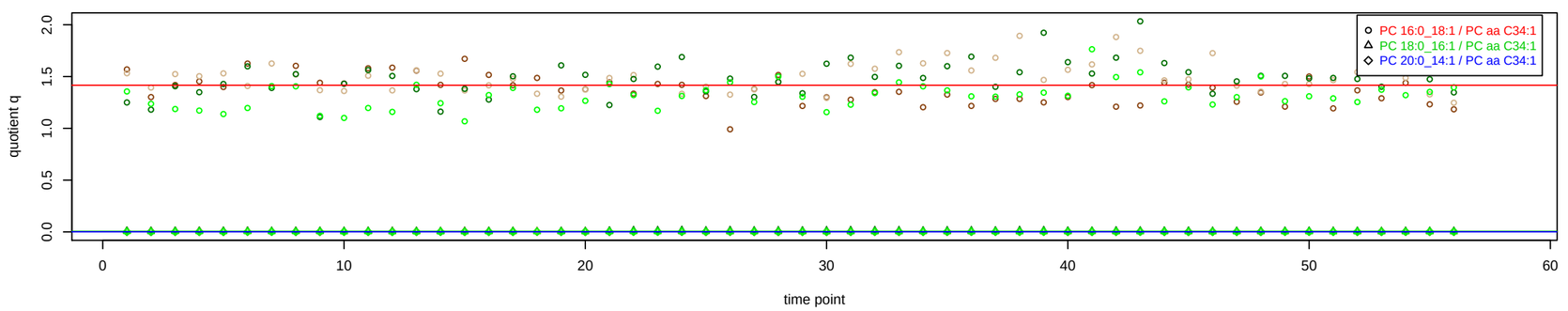
Quant. comp., Subject 8



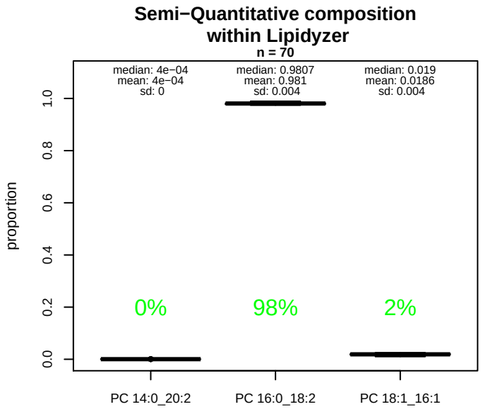
Trends of proportions q during challenges

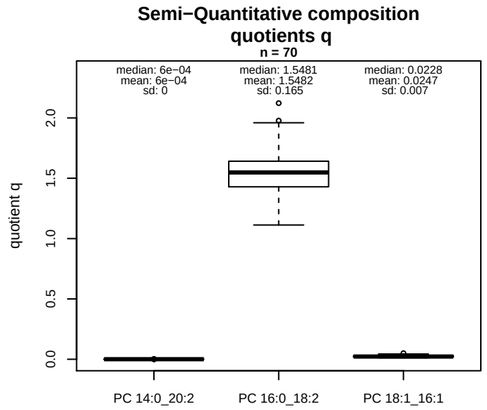


Proportions q per time point



PC aa C34:2 = PC 14:0_20:2 + PC 16:0_18:2 + PC 18:1_16:1 + R





Semi−Quantitative composition: Lipidyzer

PC aa C34:2 consists of:
PC 14:0_20:2 <0.05%
PC 16:0_18:2 98.1%
PC 18:1_16:1 1.9%
and of (not quantified):
PC 12:0_22:2, PC 14:1_20:1, PC 15:1_19:1, PC 17:0_17:2, PC 17:1_17:1, PC 18:0_16:2, PC O−18:0_17:2, PC O−16:1_1
[13C1]SM 38:2
and further compounds

Composition: mean of proportions q

conc(PC aa C34:2) * 6e−04 = conc(PC 14:0_20:2) [var(q)=6e−04]
Percentiles: 5%−>4e−04, 25%−>5e−04, 75%−>7e−04, 95%−>0.001
conc(PC aa C34:2) * 1.5482 = conc(PC 16:0_18:2) [var(q)=1.5482]
Percentiles: 5%−>1.2968, 25%−>1.4291, 75%−>1.6414, 95%−>1.8214
conc(PC aa C34:2) * 0.0247 = conc(PC 18:1_16:1) [var(q)=0.0247]
Percentiles: 5%−>0.0155, 25%−>0.0188, 75%−>0.0299, 95%−>0.0371

Linear model

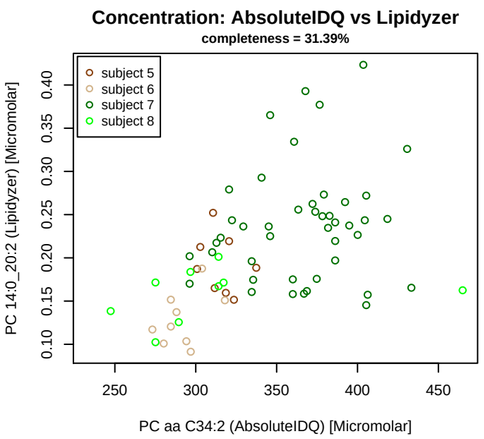
```
PC aa C34:2 ~ b * ( PC 14:0_20:2
   + PC 16:0_18:2
   + PC 18:1_16:1 )
```

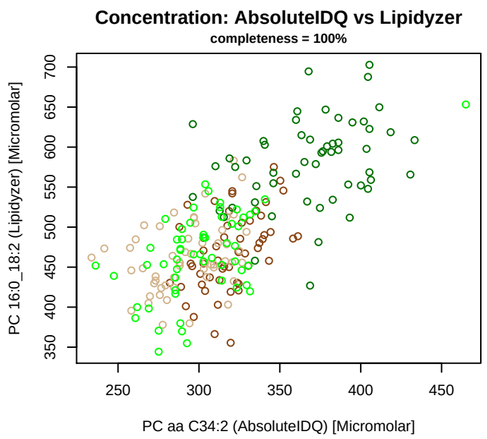
b = 0.39293

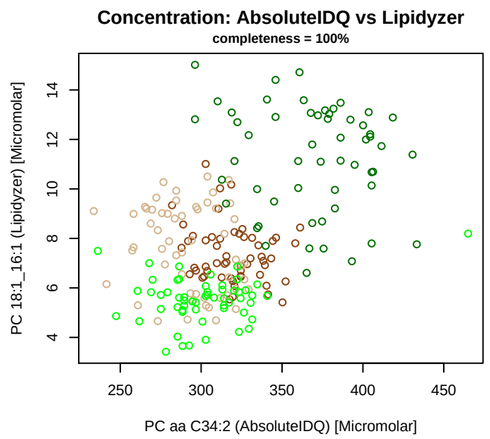
R^2 = 0.49433

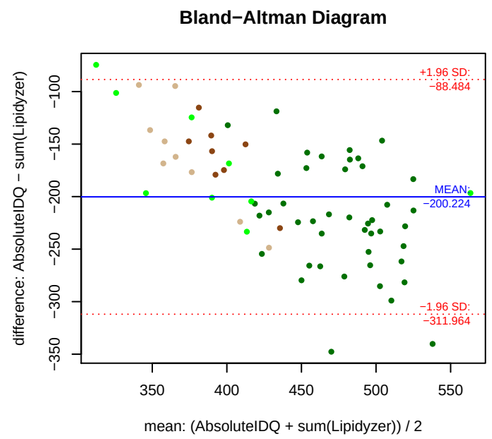
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	233.6	349.63	116.03
Max	465	708.04	243.04
Mean	320.57	543.8	223.23
Median	315.6	551.65	236.05
SD	40.33	79.51	39.18









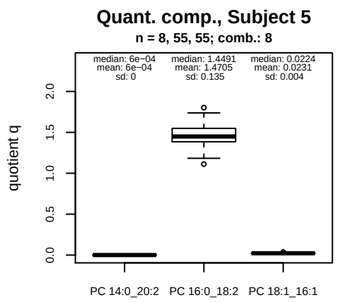
Stability of composition

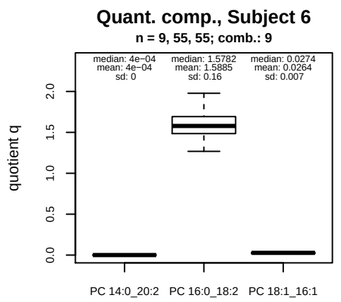
(PC 14:0_20:2 + PC 16:0_18:2 + PC 18:1_16:1) / PC aa C34:2
Shapiro−Wilk Test of log quotients, pv: 0.55528; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.38377; EQUAL
Wilcoxon: Challenge; fasting: 1; sport: 1; OLTT: 1

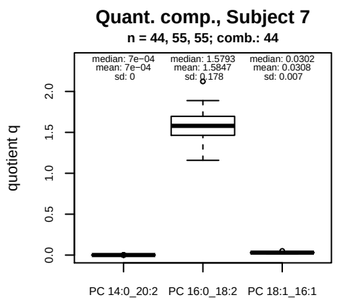
PC 16:0_18:2 / PC aa C34:2
Shapiro−Wilk Test of log quotients, pv: 0.95815; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.021; EQUAL
Wilcoxon: Challenge; fasting: 0.375; sport: 0.875; OLTT: 0.625

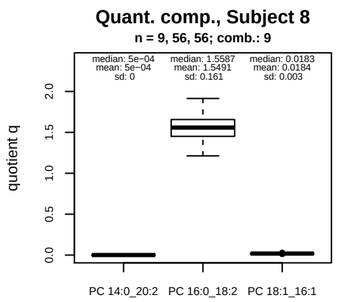
PC 14:0_20:2 / PC aa C34:2
Shapiro−Wilk Test of log quotients, pv: 0.38507; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.61799; EQUAL
Wilcoxon: Challenge; fasting: 1; sport: 1; OLTT: 1

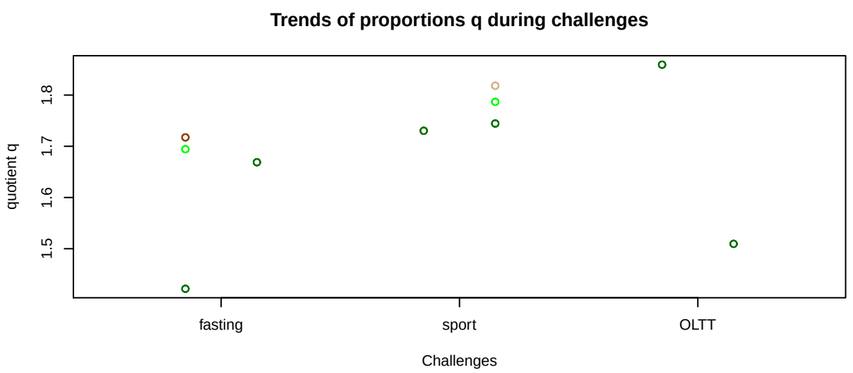
PC 18:1_16:1 / PC aa C34:2
Shapiro−Wilk Test of log quotients, pv: 0.00691; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.375; OLTT: 0.125

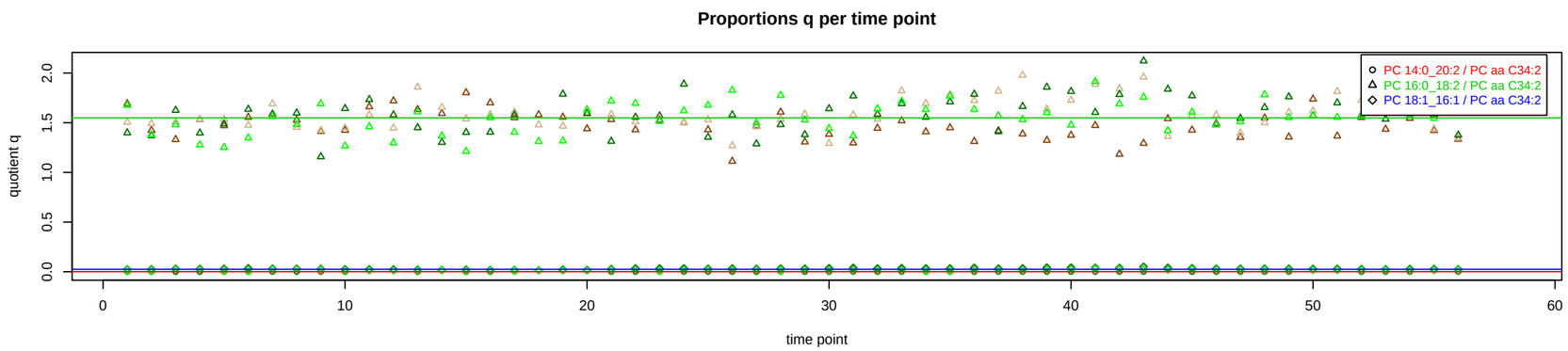




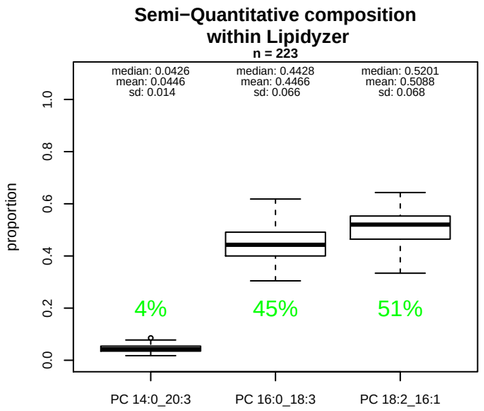


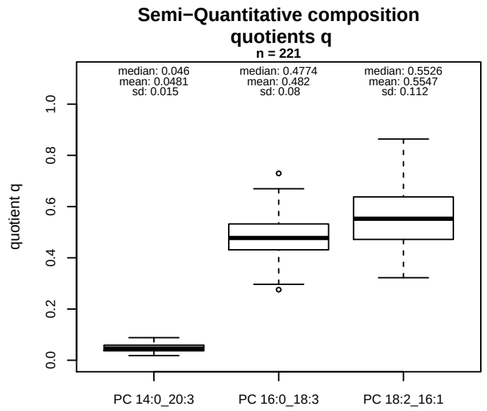






PC aa C34:3 = PC 14:0_20:3 + PC 16:0_18:3 + PC 18:2_16:1 + R





Semi−Quantitative composition: Lipidyzer

PC aa C34:3 consists of:
PC 14:0_20:3 4.5%
PC 16:0_18:3 44.7%
PC 18:2_16:1 50.9%
and of (not quantified):
PC 14:1_20:2, PC 16:1_18:2, PC 17:1_17:2, PC O−18:1_17:2
and further compounds

Composition: mean of proportions q

conc(PC aa C34:3) * 0.0481 = conc(PC 14:0_20:3) [var(q)=0.0481]
Percentiles: 5%−>0.0252, 25%−>0.0369, 75%−>0.0588, 95%−>0.0729
conc(PC aa C34:3) * 0.482 = conc(PC 16:0_18:3) [var(q)=0.482]
Percentiles: 5%−>0.3539, 25%−>0.4312, 75%−>0.5322, 95%−>0.6165
conc(PC aa C34:3) * 0.5547 = conc(PC 18:2_16:1) [var(q)=0.5547]
Percentiles: 5%−>0.3811, 25%−>0.4718, 75%−>0.6377, 95%−>0.7406

Linear model

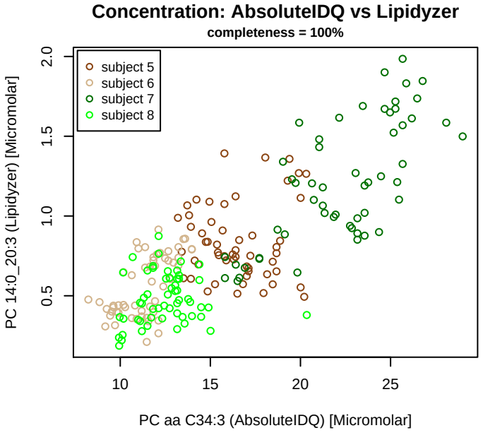
```
PC aa C34:3 ~ b * ( PC 14:0_20:3
   + PC 16:0_18:3
   + PC 18:2_16:1 )
```

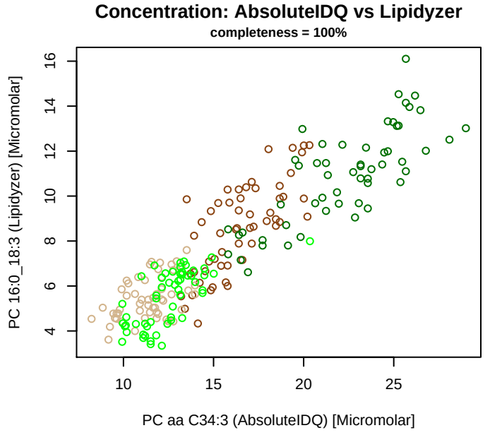
b = 1.0004

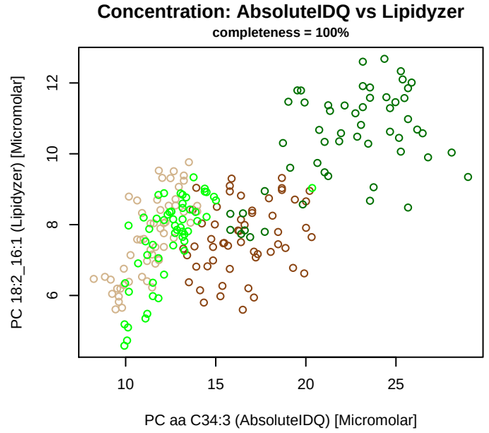
R^2 = 0.85431

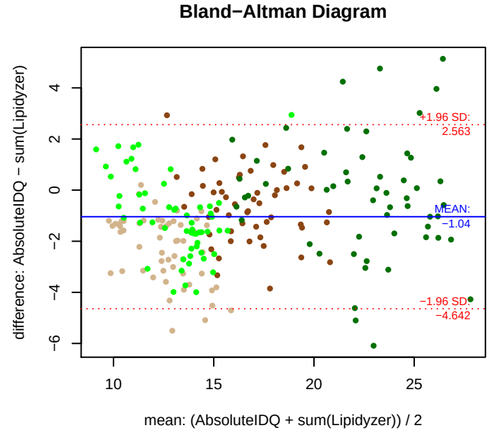
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	8.23	8.34	0.11
Max	29	29.94	0.94
Mean	15.67	16.72	1.05
Median	13.98	15.66	1.68
SD	4.82	4.43	0.39









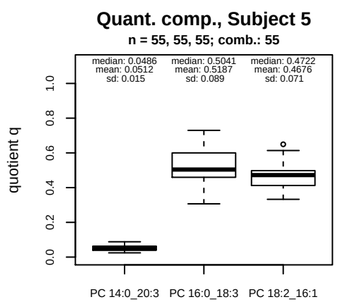
Stability of composition

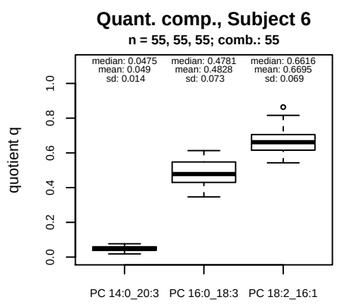
(PC 14:0_20:3 + PC 16:0_18:3 + PC 18:2_16:1) / PC aa C34:3
Shapiro−Wilk Test of log quotients, pv: 0.6127; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.52902; EQUAL
Wilcoxon: Challenge; fasting: 0.375; sport: 0.25; OLTT: 0.375

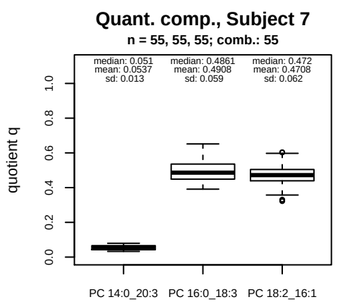
PC 16:0_18:3 / PC aa C34:3
Shapiro−Wilk Test of log quotients, pv: 0.13301; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 1; OLTT: 0.375

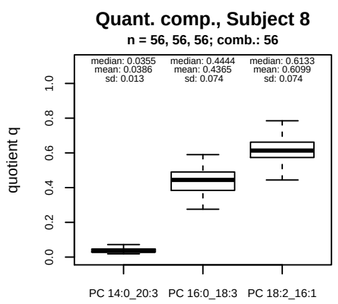
PC 14:0_20:3 / PC aa C34:3
Shapiro−Wilk Test of log quotients, pv: 0.00108; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 4e−05; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.25; OLTT: 0.25

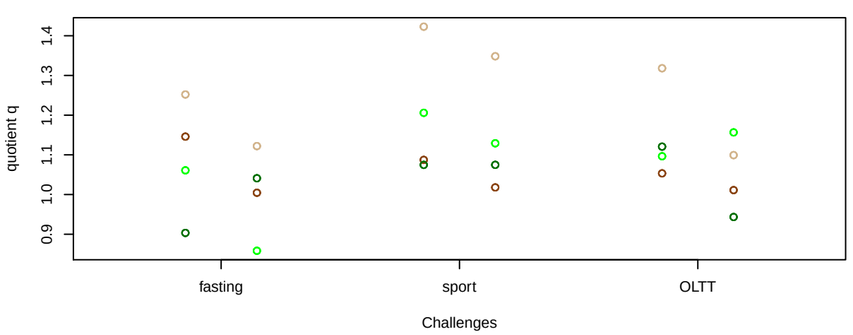
PC 18:2_16:1 / PC aa C34:3
Shapiro−Wilk Test of log quotients, pv: 0.0115; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 2e−04; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.625; sport: 0.25; OLTT: 0.625

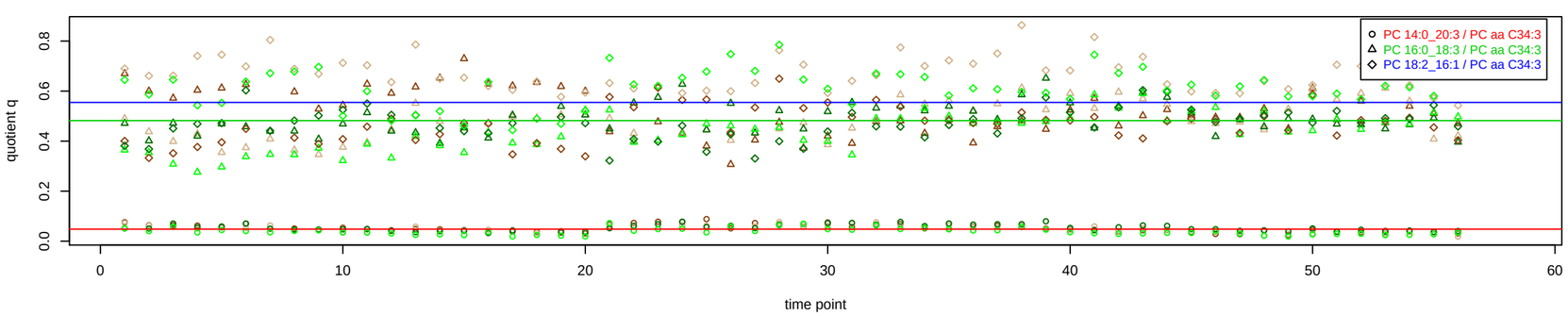






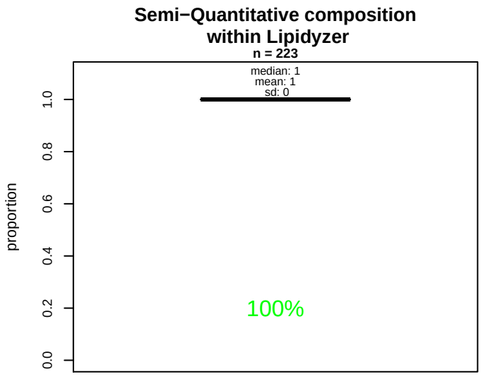


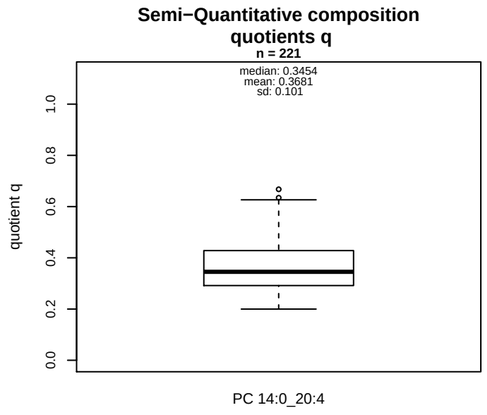




PC aa C34:4 = PC 14:0_20:4 + PC 16:0_18:4 + R

PC 16:0_18:4 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C34:4 consists of:
PC 14:0_20:4 100%
and of (not quantified):
PC 16:0_18:4, PC 12:0_22:4, PC 14:1_20:3, PC 16:1_18:3, PC O−15:0_20:4
and further compounds

Composition: mean of proportions q

conc(PC aa C34:4) * 0.3681 = conc(PC 14:0_20:4) [var(q)=0.3681]
Percentiles: 5%−>0.2438, 25%−>0.2917, 75%−>0.4282, 95%−>0.565

Linear model

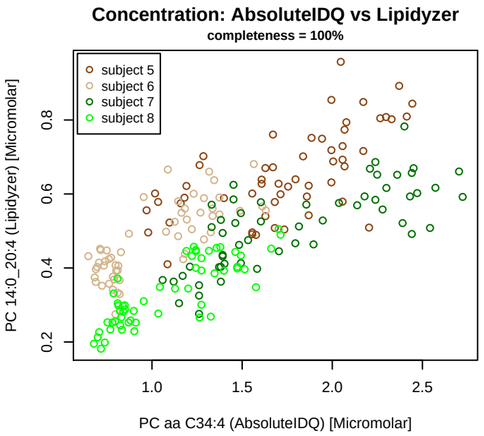
```
PC aa C34:4 ~ b * ( PC 14:0_20:4 )
```

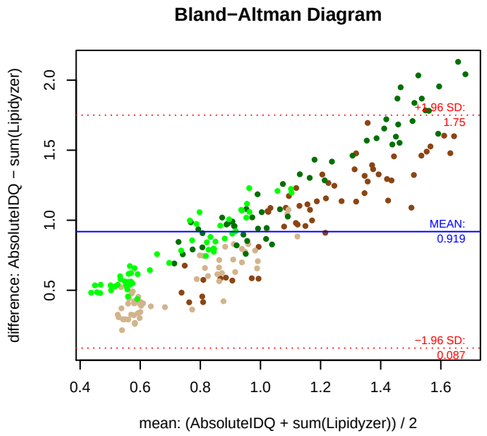
b = 2.47409

R^2 = 0.53623

Ranges

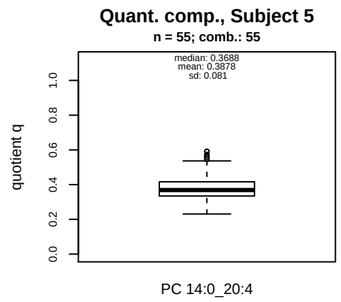
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	0.65	0.18	0.47
Max	2.72	0.96	1.77
Mean	1.41	0.49	0.92
Median	1.34	0.49	0.84
SD	0.52	0.16	0.37

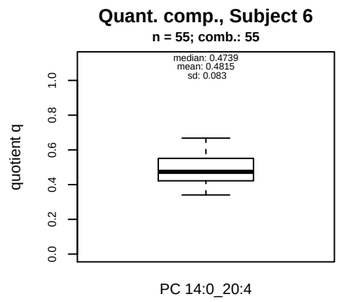


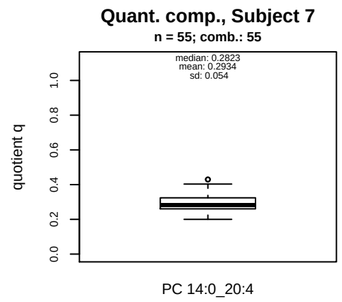


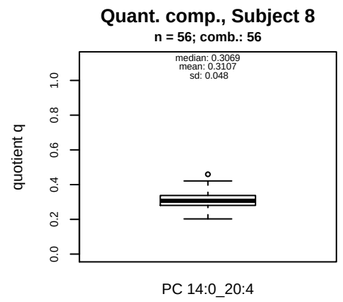
Stability of composition

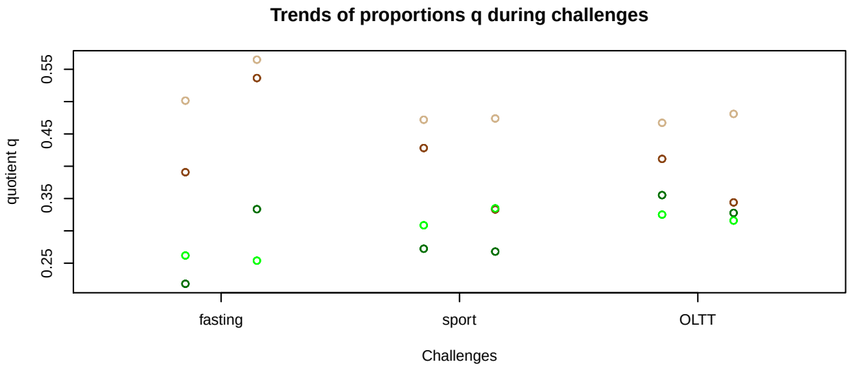
PC 14:0_20:4 / PC aa C34:4
Shapiro−Wilk Test of log quotients, pv: 0.01137; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.875; OLTT: 0.375

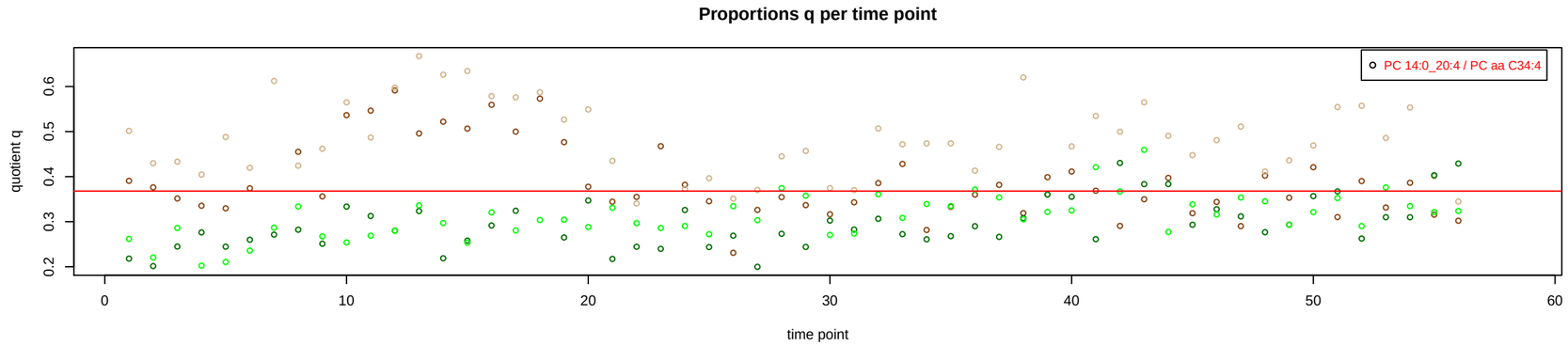




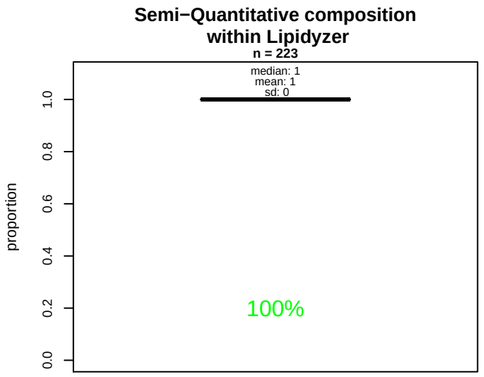


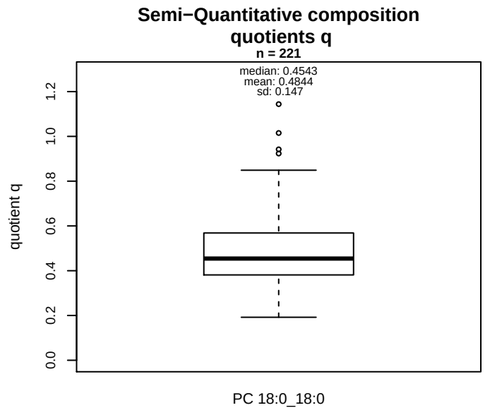






PC aa C36:0 = PC 18:0_18:0 + R





Semi−Quantitative composition: Lipidyzer

PC aa C36:0 consists of:
PC 18:0_18:0 100%
and of (not quantified):
PC 11:0_25:0, PC 12:0_24:0, PC 13:0_23:0, PC 14:0_22:0, PC 15:0_21:0, PC 16:0_20:0, PC 17:0_19:0, PC 15:1_22:6, PC 17:2_20:5, PC O−17:0_20:0, PC O−16:0_21:0, PC O−18:[13C1]SM 40:0
and further compounds

Composition: mean of proportions q

conc(PC aa C36:0) * 0.4844 = conc(PC 18:0_18:0) [var(q)=0.4844]
Percentiles: 5%−>0.3066, 25%−>0.3812, 75%−>0.5685, 95%−>0.747

Linear model

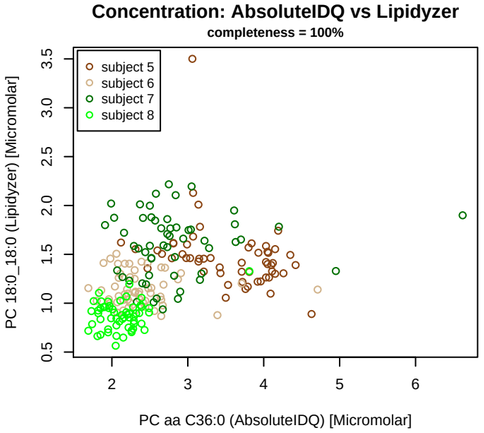
```
PC aa C36:0 ~ b * ( PC 18:0_18:0 )
```

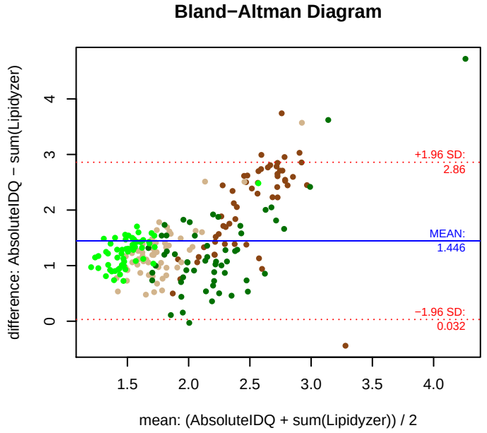
b = 0.75569

R^2 = 0.14288

Ranges

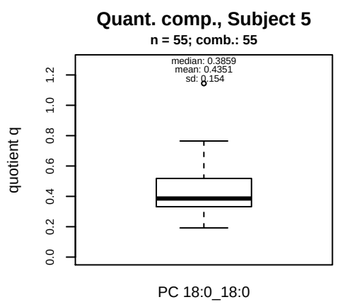
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	1.69	0.56	1.12
Max	6.62	3.5	3.12
Mean	2.72	1.27	1.44
Median	2.48	1.24	1.24
SD	0.77	0.39	0.39

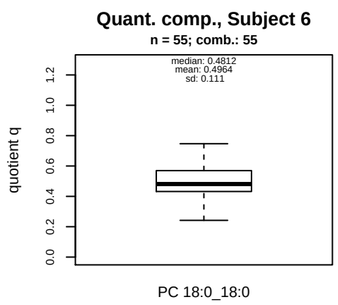


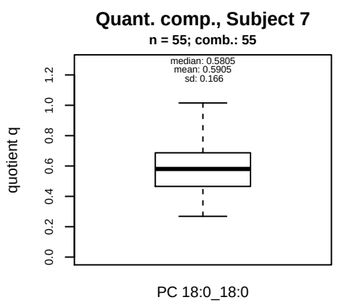


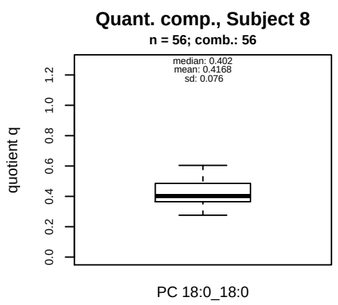
Stability of composition

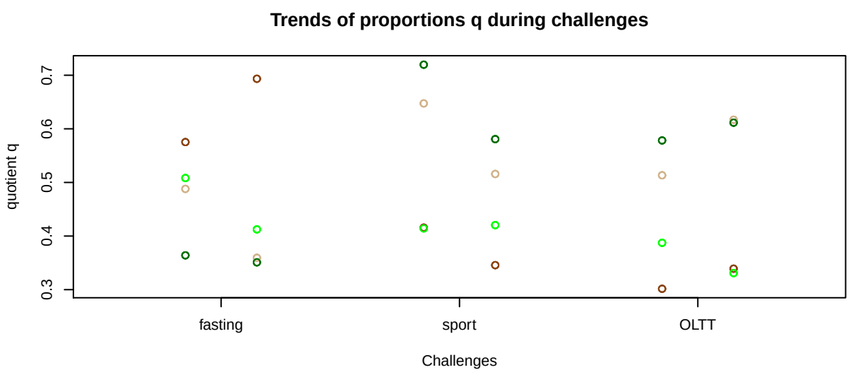
PC 18:0_18:0 / PC aa C36:0
Shapiro−Wilk Test of log quotients, pv: 0.64583; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.477; EQUAL
Wilcoxon: Challenge; fasting: 0.625; sport: 0.25; OLTT: 0.625

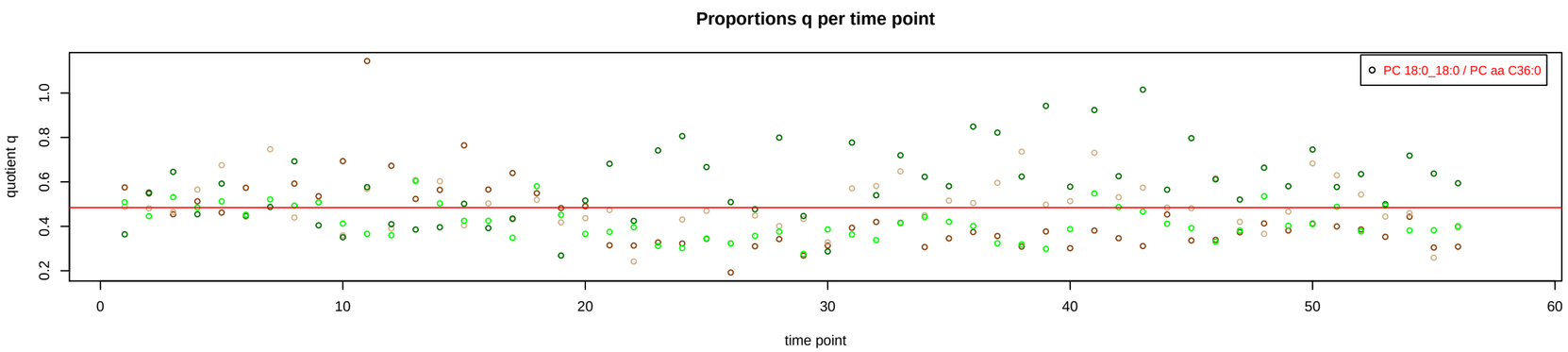






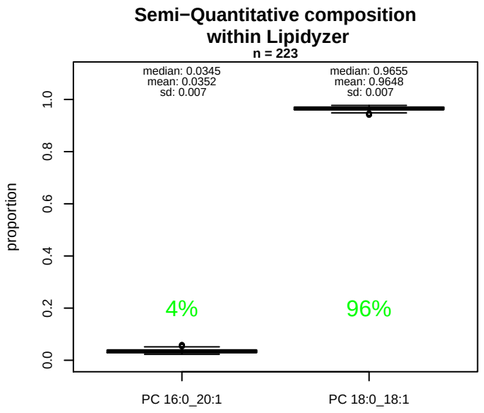


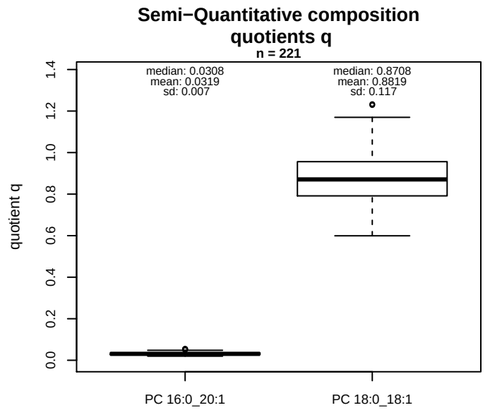




PC aa C36:1 = PC 16:0_20:1 + PC 18:0_18:1 + PC 20:0_16:1 + R

PC 20:0_16:1 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C36:1 consists of:
PC 16:0_20:1 3.5%
PC 18:0_18:1 96.5%
and of (not quantified):
PC 20:0_16:1, PC 14:0_22:1, PC 14:1_22:0, PC 15:1_21:0, PC 16:1_20:0, PC 17:0_19:1, PC 17:1_19:0, PC O−18:0_19:1, PC O−20:0_17:1, PC O−16:1_21:0, PC O−18:1_19:0, PC O−[13C1]SM 40:1
and further compounds

Composition: mean of proportions q

conc(PC aa C36:1) * 0.0319 = conc(PC 16:0_20:1) [var(q)=0.0319]
Percentiles: 5%−>0.0231, 25%−>0.027, 75%−>0.0359, 95%−>0.0447
conc(PC aa C36:1) * 0.8819 = conc(PC 18:0_18:1) [var(q)=0.8819]
Percentiles: 5%−>0.7171, 25%−>0.7916, 75%−>0.9562, 95%−>1.0794

Linear model

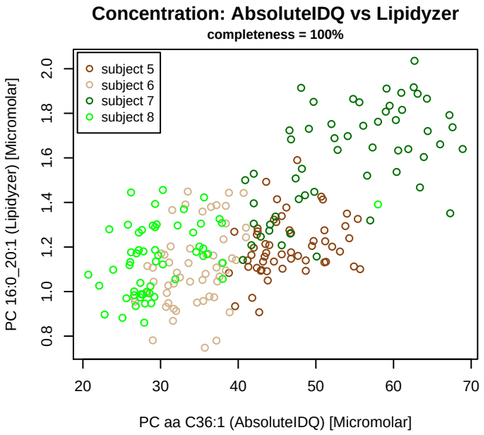
```
PC aa C36:1 ~ b * ( PC 16:0_20:1
   + PC 18:0_18:1 )
```

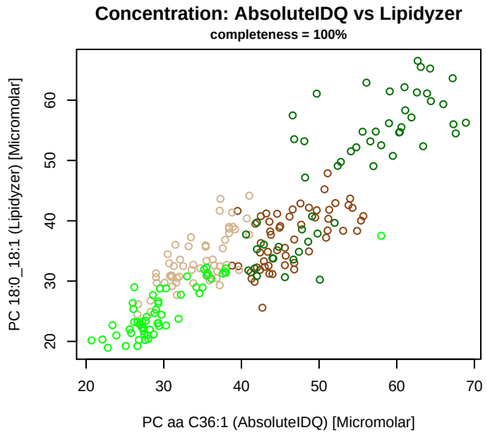
b = 0.89548

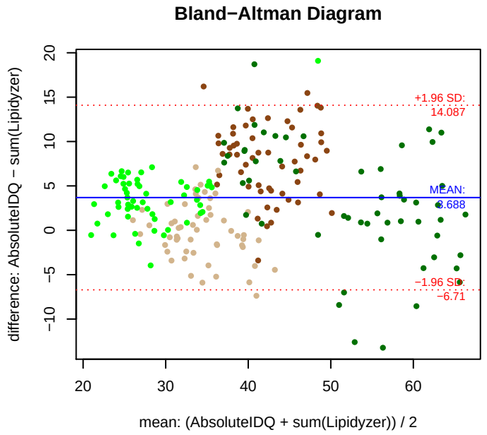
R^2 = 0.7898

Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	20.7	19.85	0.85
Max	68.9	68.55	0.35
Mean	41.15	37.5	3.66
Median	40.6	34.64	5.96
SD	11.29	11.16	0.13





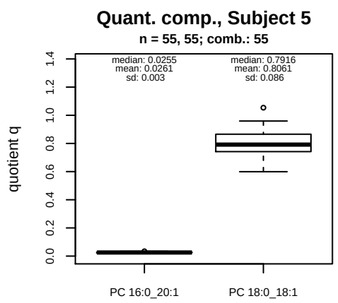


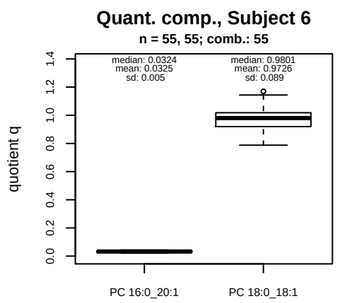
Stability of composition

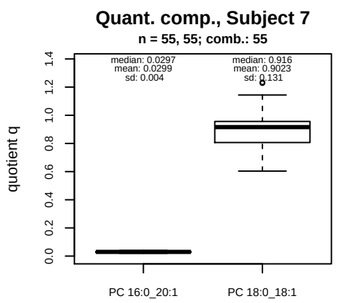
(PC 16:0_20:1 + PC 18:0_18:1) / PC aa C36:1
Shapiro−Wilk Test of log quotients, pv: 0.7629; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.16842; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.875

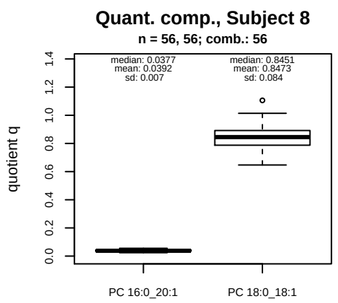
PC 18:0_18:1 / PC aa C36:1
Shapiro−Wilk Test of log quotients, pv: 0.66034; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.39144; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.875

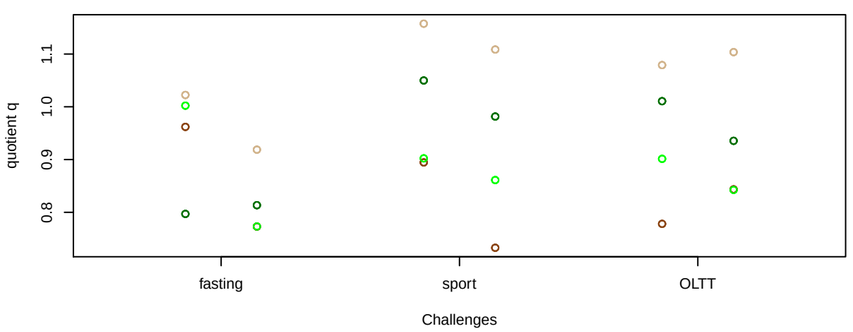
PC 16:0_20:1 / PC aa C36:1
Shapiro−Wilk Test of log quotients, pv: 0.27012; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.625

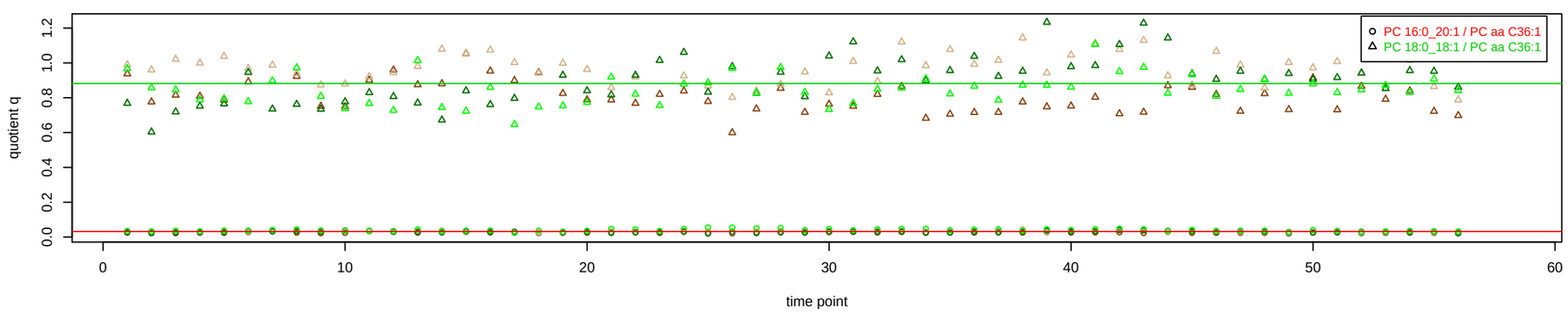




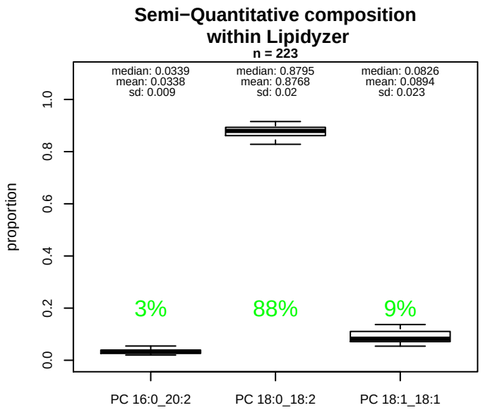


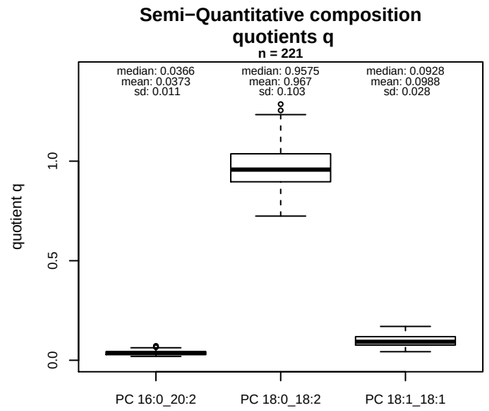






PC aa C36:2 = PC 16:0_20:2 + PC 18:0_18:2 + PC 18:1_18:1 + R





Semi−Quantitative composition: Lipidyzer

PC aa C36:2 consists of:
PC 16:0_20:2 3.4%
PC 18:0_18:2 87.7%
PC 18:1_18:1 8.9%
and of (not quantified):
PC14 0 22:2, PC14 1 22:1, PC16 1 20:1, PC17 1 19:1, PC17 2 19:0, PCO−20 0 17:2, PCO−18 1 19:1, PCO−20 1 17 [13C1]SM 40:2
and further compounds

Composition: mean of proportions q

conc(PC aa C36:2) * 0.0373 = conc(PC 16:0_20:2) [var(q)=0.0373]
Percentiles: 5%−>0.0226, 25%−>0.0285, 75%−>0.0432, 95%−>0.0581
conc(PC aa C36:2) * 0.967 = conc(PC 18:0_18:2) [var(q)=0.967]
Percentiles: 5%−>0.8172, 25%−>0.8964, 75%−>1.037, 95%−>1.1362
conc(PC aa C36:2) * 0.0988 = conc(PC 18:1_18:1) [var(q)=0.0988]
Percentiles: 5%−>0.0601, 25%−>0.0762, 75%−>0.1186, 95%−>0.1467

Linear model

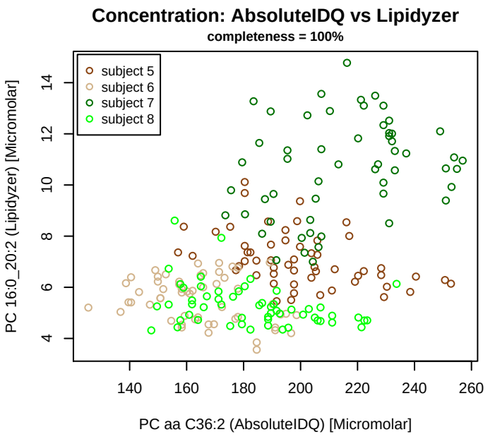
```
PC aa C36:2 ~ b * ( PC 16:0_20:2
   + PC 18:0_18:2
   + PC 18:1_18:1 )
```

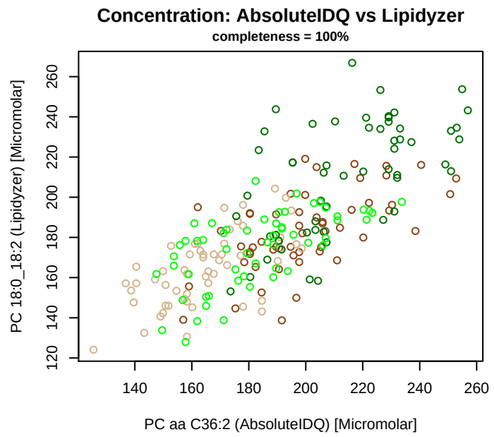
b = 0.6305

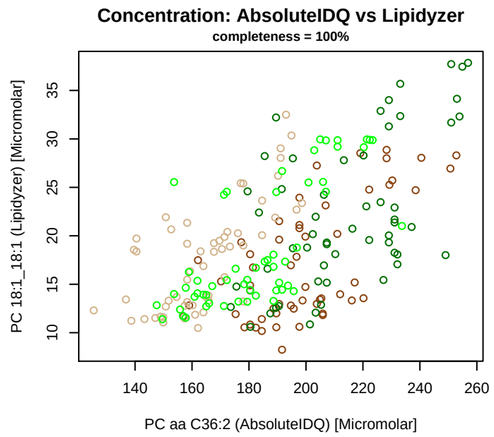
R^2 = 0.57943

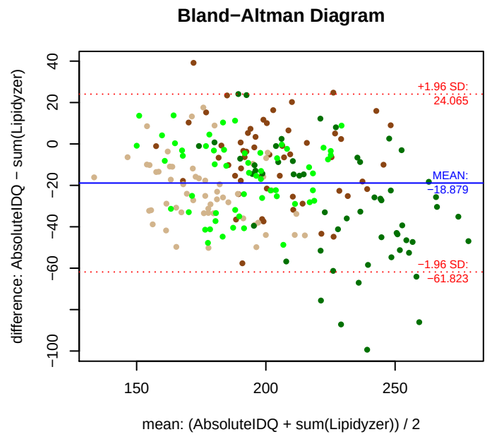
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	125.5	141.63	16.13
Max	256.9	302.37	45.47
Mean	190.68	209.51	18.83
Median	189.6	204.41	14.81
SD	27.84	33.51	5.67









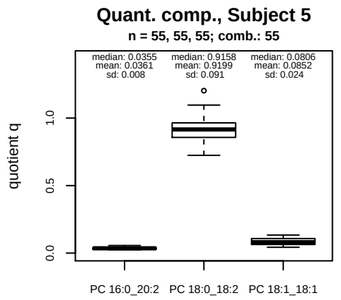
Stability of composition

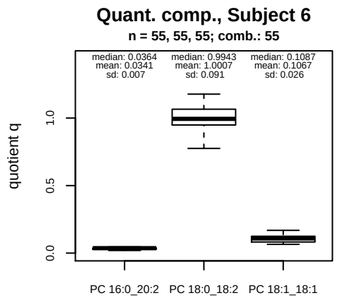
(PC 16:0_20:2 + PC 18:0_18:2 + PC 18:1_18:1) / PC aa C36:2
Shapiro−Wilk Test of log quotients, pv: 0.68759; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.03886; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.375

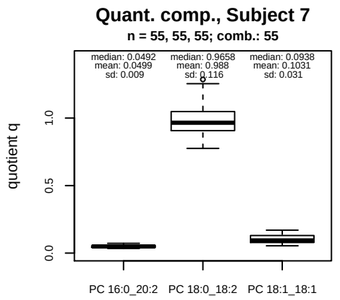
PC 16:0_20:2 / PC aa C36:2
Shapiro−Wilk Test of log quotients, pv: 0.06915; OK
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.375; sport: 0.125; OLTT: 0.125

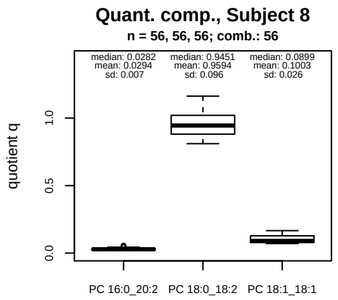
PC 18:0_18:2 / PC aa C36:2
Shapiro−Wilk Test of log quotients, pv: 0.72516; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.08316; EQUAL
Wilcoxon: Challenge; fasting: 0.125; sport: 0.125; OLTT: 0.375

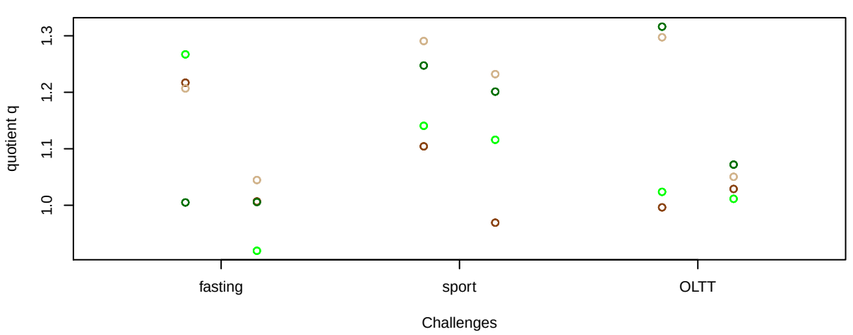
PC 18:1_18:1 / PC aa C36:2
Shapiro−Wilk Test of log quotients, pv: 0.00285; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0.00031; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.875; sport: 0.125; OLTT: 0.375

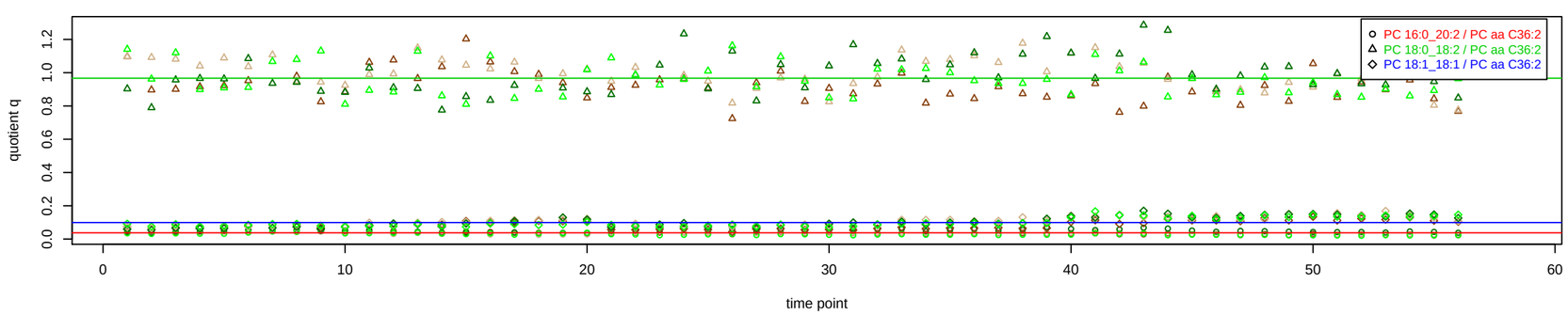




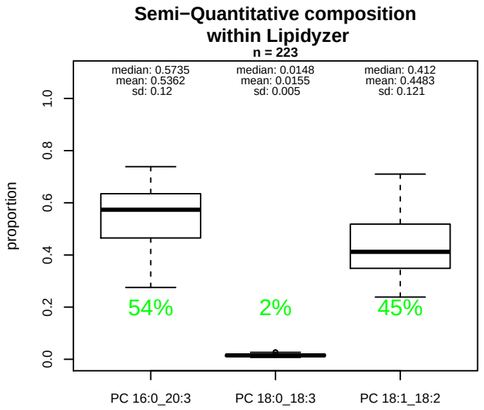


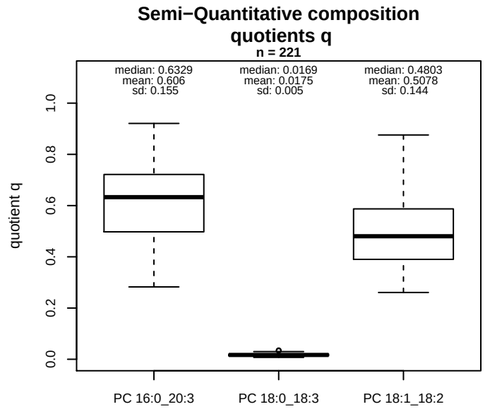






PC aa C36:3 = PC 16:0_20:3 + PC 18:0_18:3 + PC 18:1_18:2 + R





Semi−Quantitative composition: Lipidyzer

PC aa C36:3 consists of:
PC 16:0_20:3 53.6%
PC 18:0_18:3 1.5%
PC 18:1_18:2 44.8%
and of (not quantified):
PC14 1 22:2, PC16 1 20:2, PC17 2 19:1, PCO−20 1 17:2, SM40.3
and further compounds

Composition: mean of proportions q

conc(PC aa C36:3) * 0.606 = conc(PC 16:0_20:3) [var(q)=0.606]
Percentiles: 5%−>0.3434, 25%−>0.4975, 75%−>0.7216, 95%−>0.8409
conc(PC aa C36:3) * 0.0175 = conc(PC 18:0_18:3) [var(q)=0.0175]
Percentiles: 5%−>0.01, 25%−>0.0137, 75%−>0.0203, 95%−>0.0279
conc(PC aa C36:3) * 0.5078 = conc(PC 18:1_18:2) [var(q)=0.5078]
Percentiles: 5%−>0.3177, 25%−>0.3901, 75%−>0.5871, 95%−>0.7643

Linear model

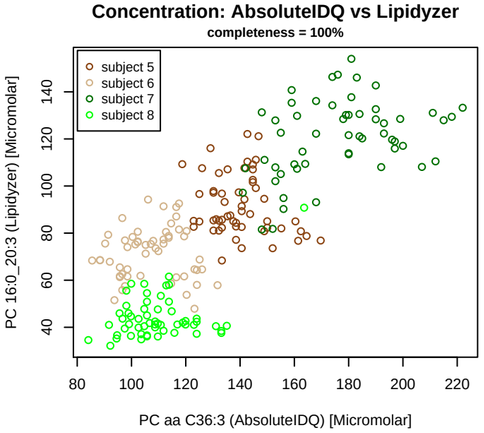
```
PC aa C36:3 ~ b * ( PC 16:0_20:3
   + PC 18:0_18:3
   + PC 18:1_18:2 )
```

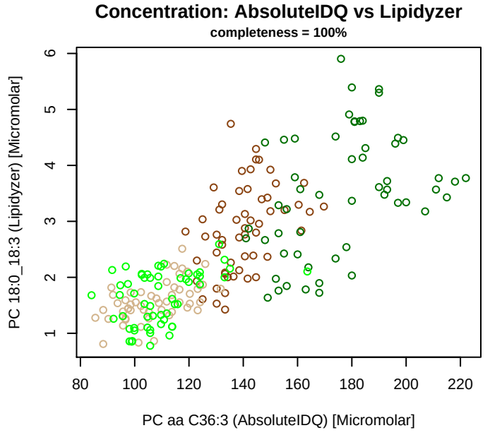
b = 0.79714

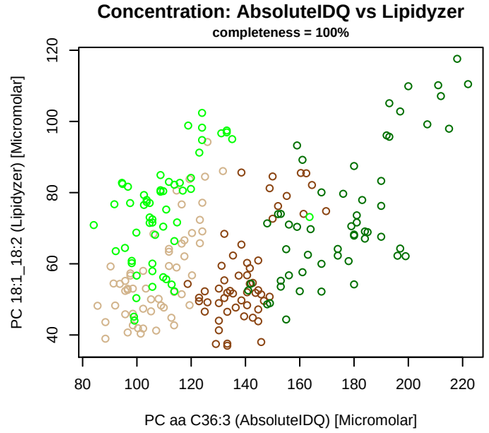
R^2 = 0.80444

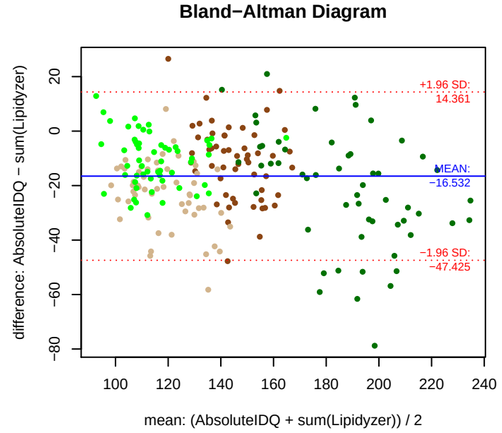
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	84.1	86.21	2.11
Max	222	250.69	28.69
Mean	133.31	150	16.69
Median	126	141.27	15.27
SD	31.67	35.54	3.87









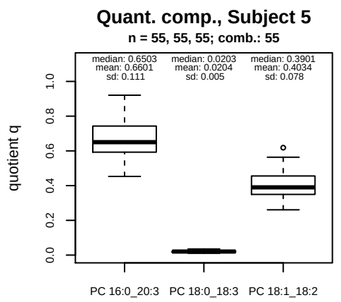
Stability of composition

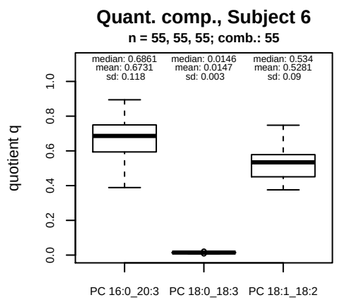
(PC 16:0_20:3 + PC 18:0_18:3 + PC 18:1_18:2) / PC aa C36:3
Shapiro−Wilk Test of log quotients, pv: 0.43192; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.6275; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.25

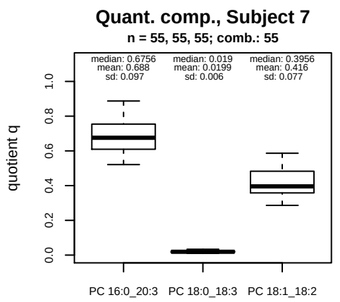
PC 16:0_20:3 / PC aa C36:3
Shapiro−Wilk Test of log quotients, pv: 0; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.375; sport: 0.125; OLTT: 0.125

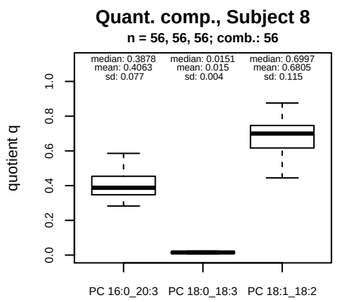
PC 18:0_18:3 / PC aa C36:3
Shapiro−Wilk Test of log quotients, pv: 0.6707; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00016; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.625; OLTT: 0.625

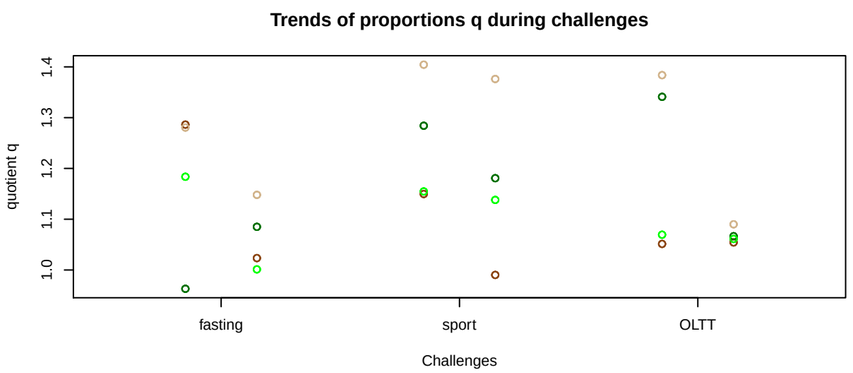
PC 18:1_18:2 / PC aa C36:3
Shapiro−Wilk Test of log quotients, pv: 0.00353; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.125; OLTT: 1

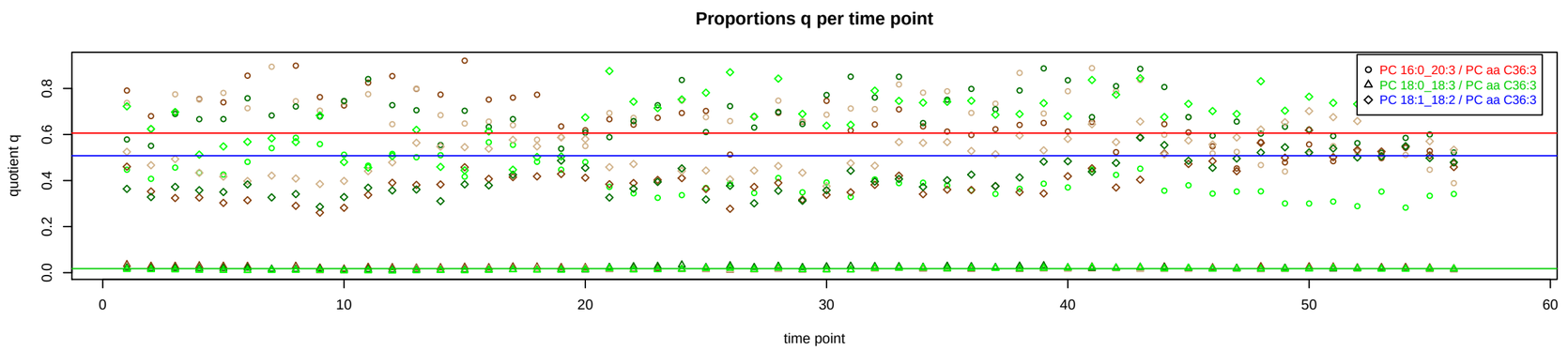






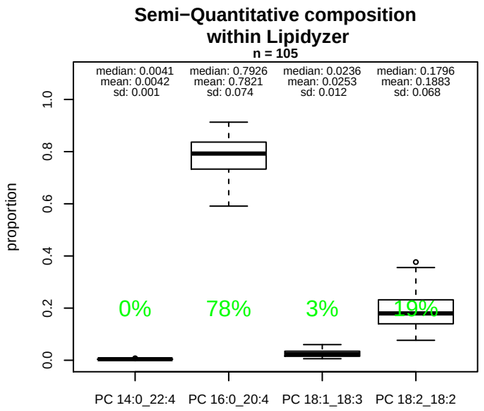


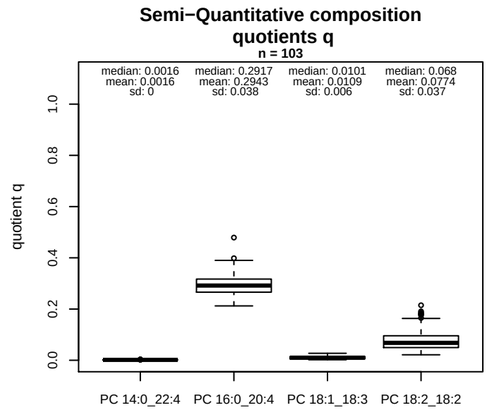




PC aa C36:4 = PC 14:0_22:4 + PC 16:0_20:4 + PC 18:0_18:4 + PC 18:1_18:3 + PC 18:2_18:2 + R

PC 18:0_18:4 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C36:4 consists of:
PC 14:0_22:4 0.4%
PC 16:0_20:4 78.2%
PC 18:1_18:3 2.5%
PC 18:2_18:2 18.8%
and of (not quantified):
PC O−17:0_20:4
and further compounds

Linear model

```
PC aa C36:4 ~ b * ( PC 14:0_22:4
   + PC 16:0_20:4
   + PC 18:1_18:3
   + PC 18:2_18:2 )
```

b = 2.55262

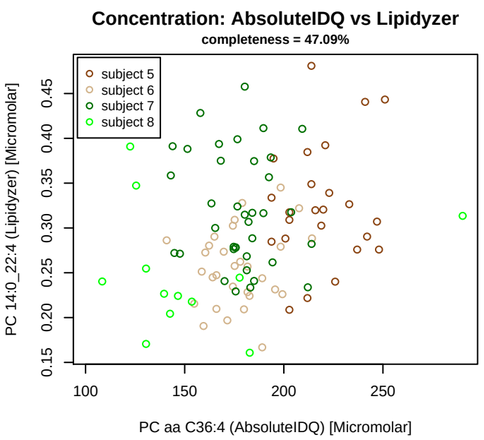
R^2 = 0.65155

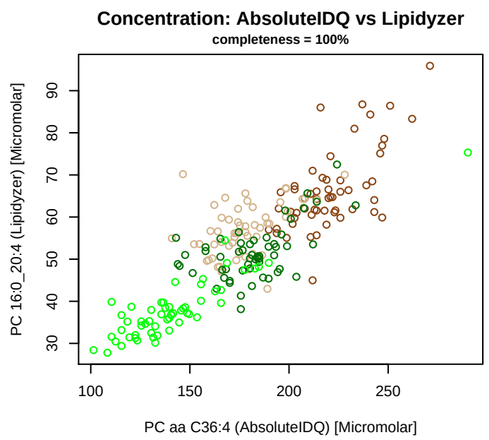
Ranges

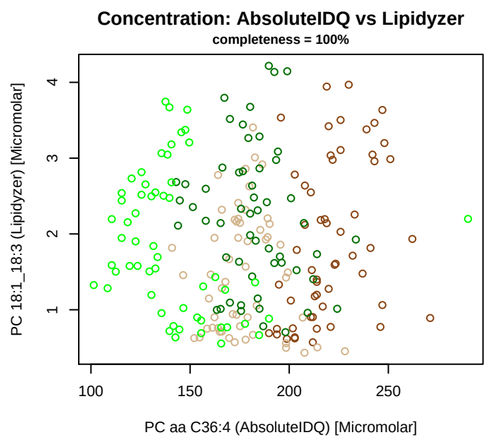
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	101.4	47.02	54.38
Max	290.2	98.75	191.45
Mean	180.31	70.22	110.09
Median	179.9	69.92	109.98
SD	35.18	10.41	24.76

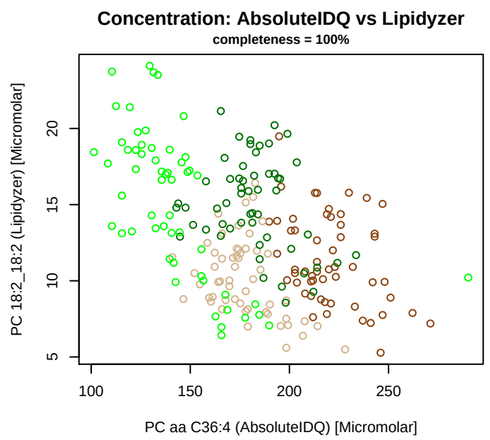
Composition: mean of proportions q

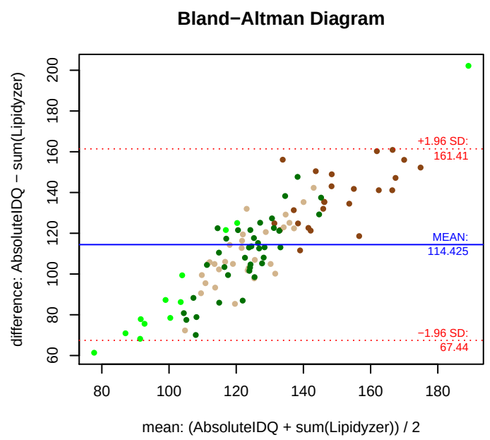
conc(PC aa C36:4) * 0.0016 = conc(PC 14:0_22:4) [var(q)=0.0016]
Percentiles: 5%−>0.0011, 25%−>0.0013, 75%−>0.0018, 95%−>0.0025
conc(PC aa C36:4) * 0.2943 = conc(PC 16:0_20:4) [var(q)=0.2943]
Percentiles: 5%−>0.2393, 25%−>0.2658, 75%−>0.317, 95%−>0.3555
conc(PC aa C36:4) * 0.0109 = conc(PC 18:1_18:3) [var(q)=0.0109]
Percentiles: 5%−>0.0033, 25%−>0.0056, 75%−>0.0147, 95%−>0.022
conc(PC aa C36:4) * 0.0774 = conc(PC 18:2_18:2) [var(q)=0.0774]
Percentiles: 5%−>0.0354, 25%−>0.0496, 75%−>0.0957, 95%−>0.1558











Stability of composition

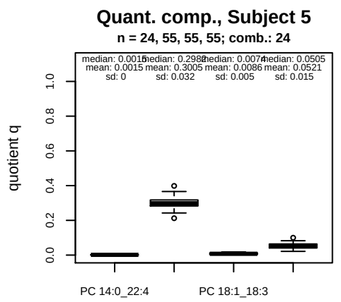
(PC 14:0_22:4 + PC 16:0_20:4 + PC 18:1_18:3 + PC 18:2_18:2) / PC aa C36:4
Shapiro−Wilk Test of log quotients, pv: 0.91369; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.21225; EQUAL
Wilcoxon: Challenge; sport: 0.5; OLTT: 1

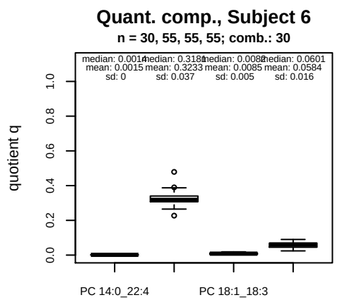
PC 14:0_22:4 / PC aa C36:4
Shapiro−Wilk Test of log quotients, pv: 0.48012; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00455; DIFFERENCE
Wilcoxon: Challenge; sport: 0.5; OLTT: 1

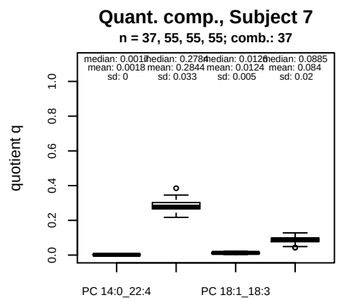
PC 16:0_20:4 / PC aa C36:4
Shapiro−Wilk Test of log quotients, pv: 0.22093; OK
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.875; sport: 0.25; OLTT: 0.25

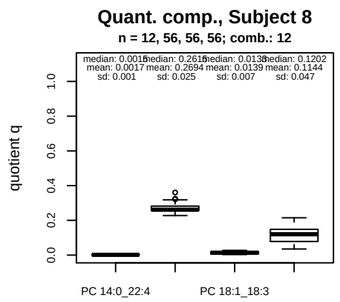
PC 18:1_18:3 / PC aa C36:4
Shapiro−Wilk Test of log quotients, pv: 2e−05; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 1; OLTT: 0.625

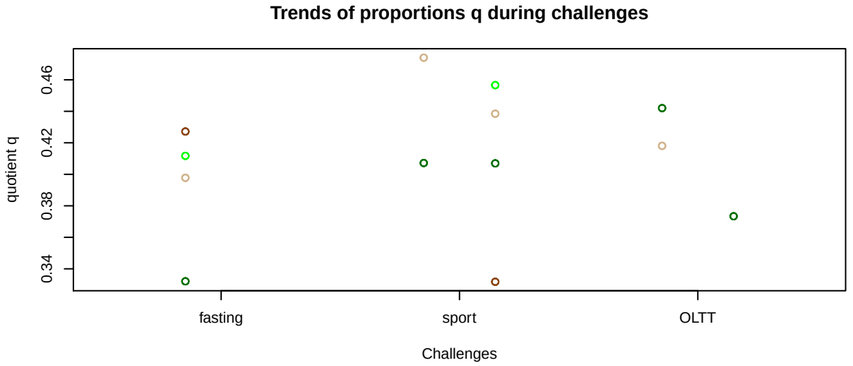
PC 18:2_18:2 / PC aa C36:4
Shapiro−Wilk Test of log quotients, pv: 0.52175; OK
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.125; OLTT: 0.625

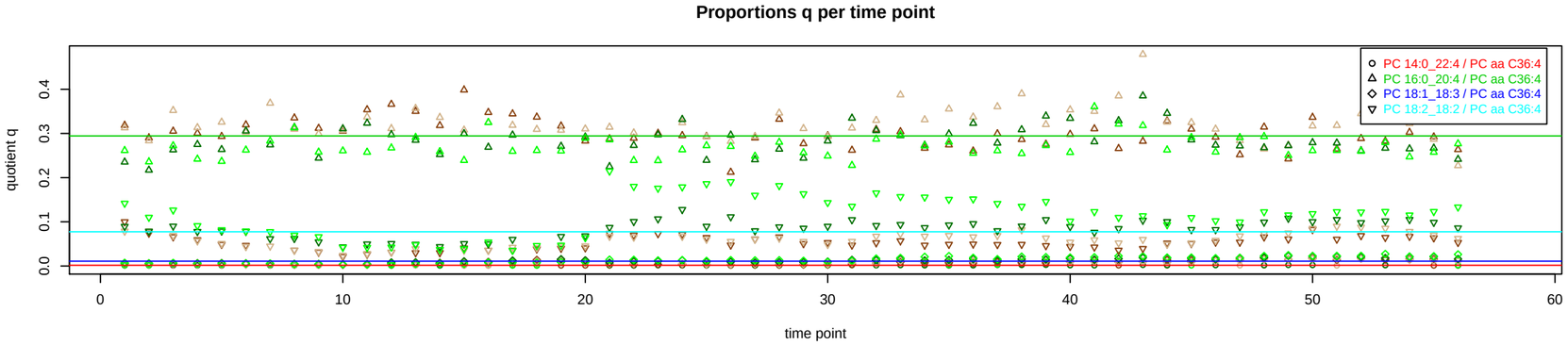






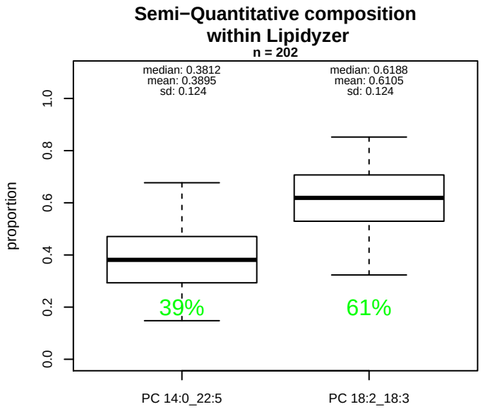


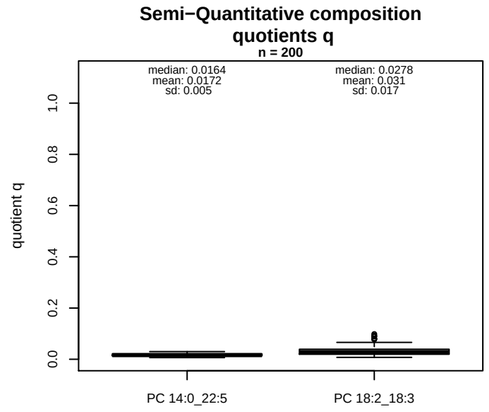




PC aa C36:5 = PC 14:0_22:5 + PC 16:0_20:5 + PC 18:2_18:3 + R

PC 16:0_20:5 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C36:5 consists of:
PC 14:0_22:5 39%
PC 18:2_18:3 61%
and of (not quantified):
PC 16:0_20:5, PC 14 1_22:4, PC 16 1_20:4, PC 18 1_18:4,
and further compounds

Linear model

```
PC aa C36:5 ~ b * ( PC 14:0_22:5
   + PC 18:2_18:3 )
```

b = 9.52537

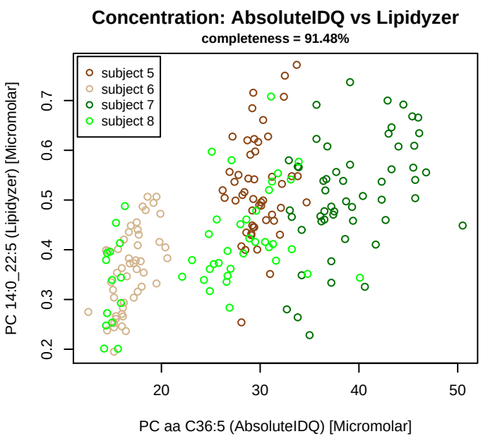
R^2 = 0.17224

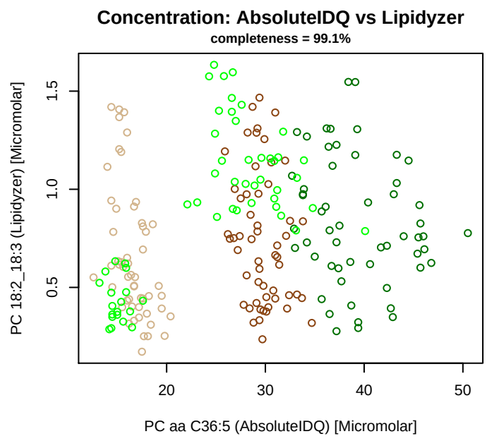
Ranges

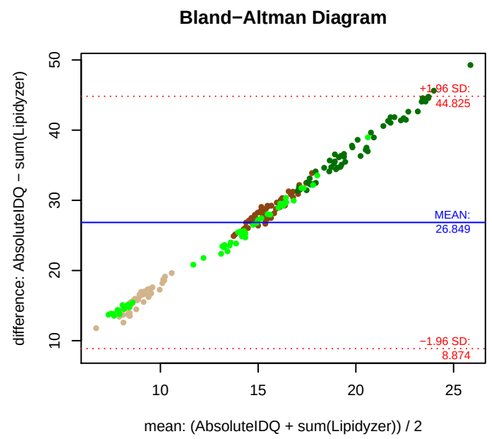
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	12.6	0.49	12.11
Max	50.5	2.12	48.38
Mean	27.44	1.24	26.2
Median	28.7	1.24	27.46
SD	9.37	0.38	8.99

Composition: mean of proportions q

conc(PC aa C36:5) * 0.0172 = conc(PC 14:0_22:5) [var(q)=0.0172]
Percentiles: 5%−>0.0101, 25%−>0.0138, 75%−>0.0206, 95%−>0.0262
conc(PC aa C36:5) * 0.031 = conc(PC 18:2_18:3) [var(q)=0.031]
Percentiles: 5%−>0.0113, 25%−>0.0196, 75%−>0.0391, 95%−>0.0615





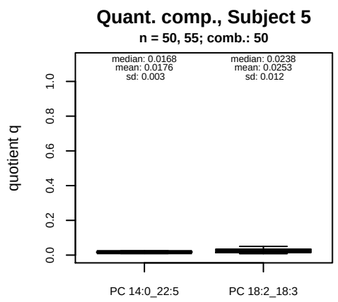


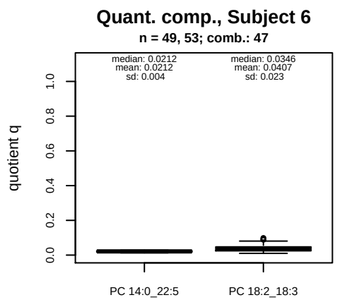
Stability of composition

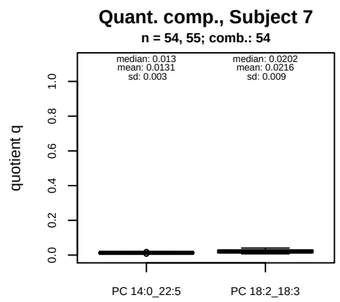
(PC 14:0_22:5 + PC 18:2_18:3) / PC aa C36:5
Shapiro−Wilk Test of log quotients, pv: 0.49031; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.43298; EQUAL
Wilcoxon: Challenge; fasting: 1; sport: 0.125; OLTT: 0.5

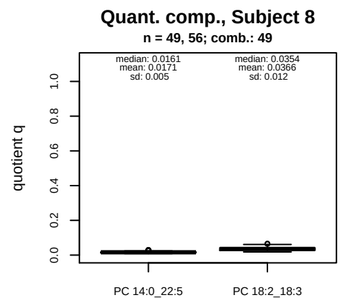
PC 18:2_18:3 / PC aa C36:5
Shapiro−Wilk Test of log quotients, pv: 0.25945; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.0212; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.125

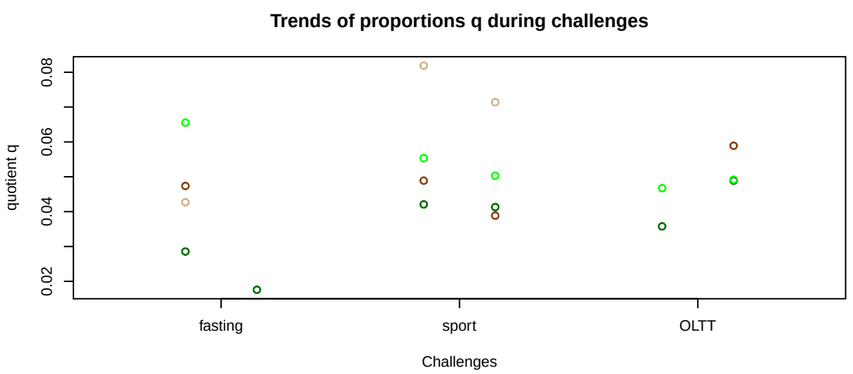
PC 14:0_22:5 / PC aa C36:5
Shapiro−Wilk Test of log quotients, pv: 0.03493; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 2e−04; DIFFERENCE
Wilcoxon: Challenge; fasting: 1; sport: 0.625; OLTT: 1

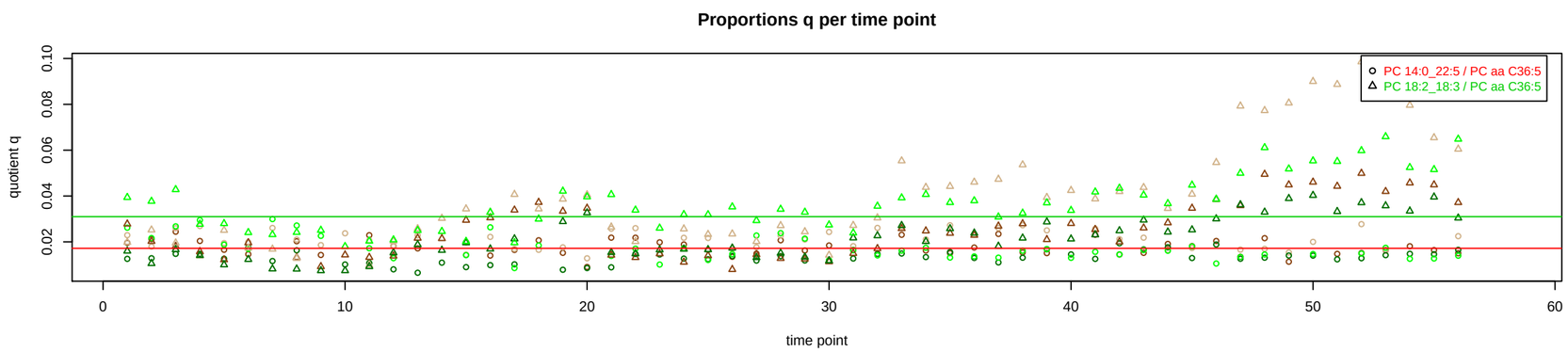




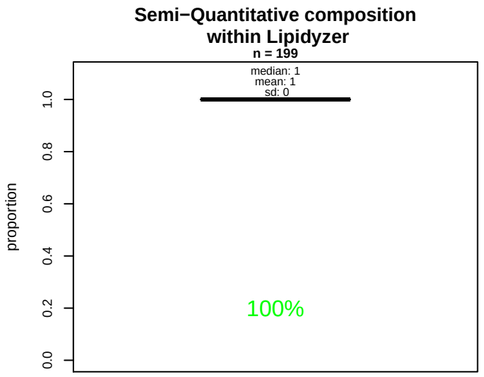


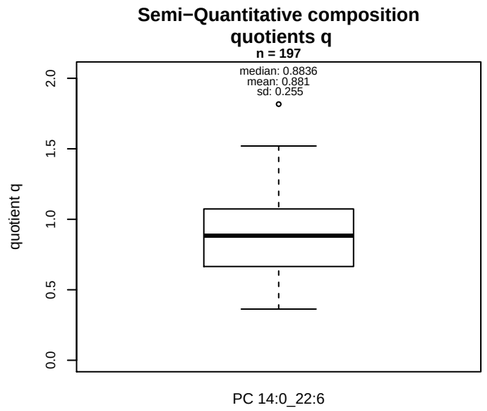






PC aa C36:6 = PC 14:0_22:6 + R





Semi−Quantitative composition: Lipidyzer

PC aa C36:6 consists of:
PC 14:0_22:6 100%
and of (not quantified):
PC 14:1_22:5, PC 16:1_20:5, PC 18:3_18:3, PC 18:4_18:2,
and further compounds

Composition: mean of proportions q

conc(PC aa C36:6) * 0.881 = conc(PC 14:0_22:6) [var(q)=0.881]
Percentiles: 5%−>0.4947, 25%−>0.6651, 75%−>1.0732, 95%−>1.2925

Linear model

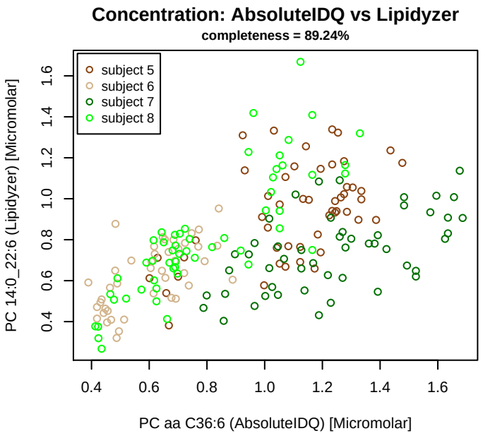
```
PC aa C36:6 ~ b * ( PC 14:0_22:6 )
```

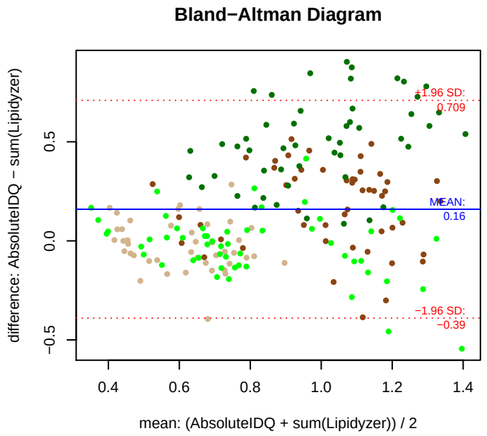
b = 0.74555

R^2 = 0.32274

Ranges

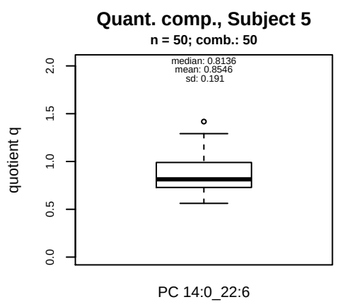
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	0.39	0.27	0.12
Max	1.69	1.67	0.02
Mean	0.91	0.79	0.13
Median	0.9	0.76	0.14
SD	0.33	0.26	0.08

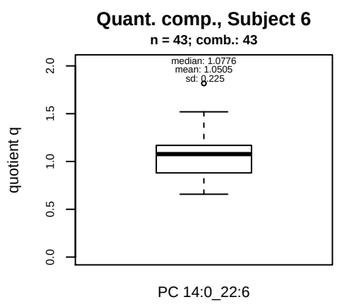


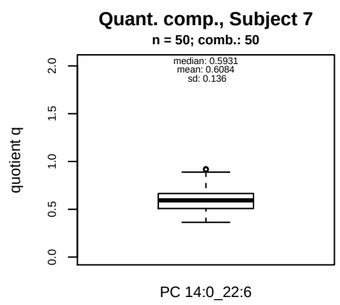


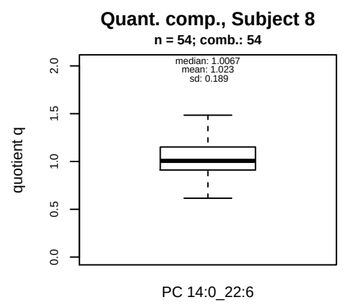
Stability of composition

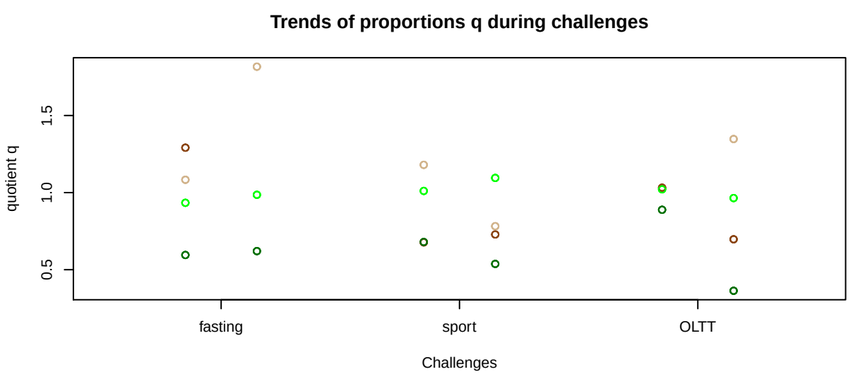
PC 14:0_22:6 / PC aa C36:6
Shapiro−Wilk Test of log quotients, pv: 0.00996; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.68751; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.625; OLTT: 0.25

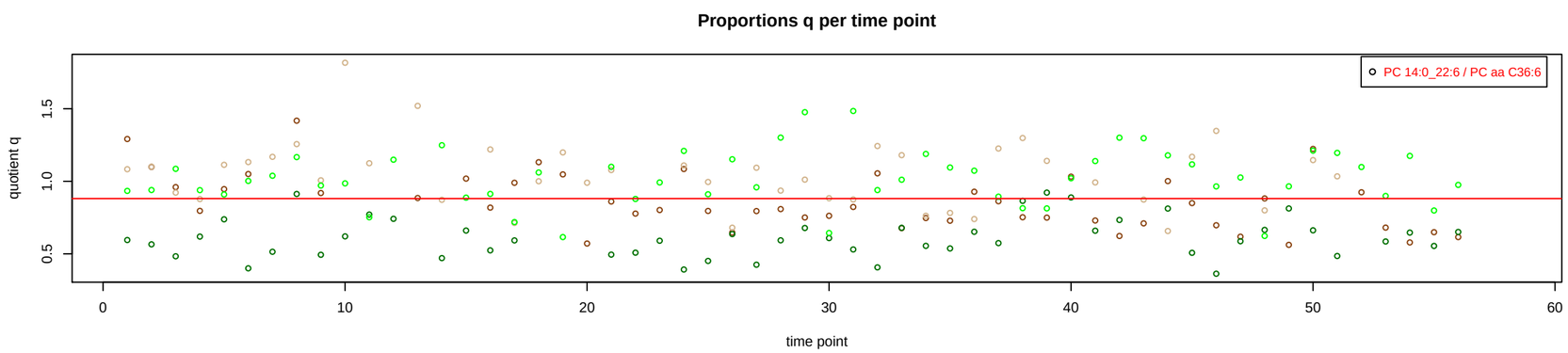




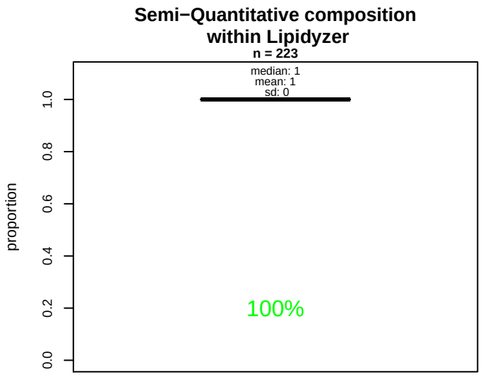


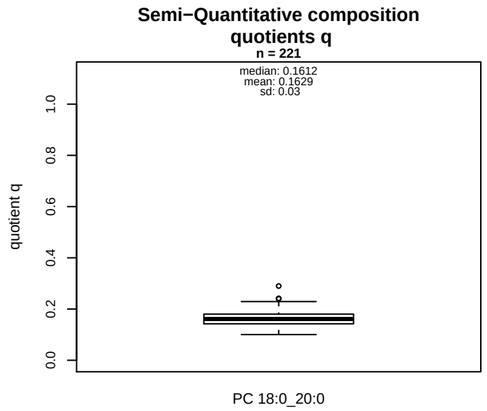






PC aa C38:0 = PC 18:0_20:0 + R





Semi−Quantitative composition: Lipidyzer

PC aa C38:0 consists of:
PC 18:0_20:0 100%
and of (not quantified):
PC 12:0_26:0, PC 13:0_25:0, PC 14:0_24:0, PC 16:0_22:0,
PC 17:0_21:0, PC 17:1_22:6, PC 19:0_19:0, PC O−17:0_22:(
PC O−18:0_21:0, PC O−20:0_19:0, PC O−18:1_22:6, SM42.(
and further compounds

Composition: mean of proportions q

conc(PC aa C38:0) * 0.1629 = conc(PC 18:0_20:0) [var(q)=0.1629]
Percentiles: 5%−>0.1193, 25%−>0.1424, 75%−>0.18, 95%−>0.2153

Linear model

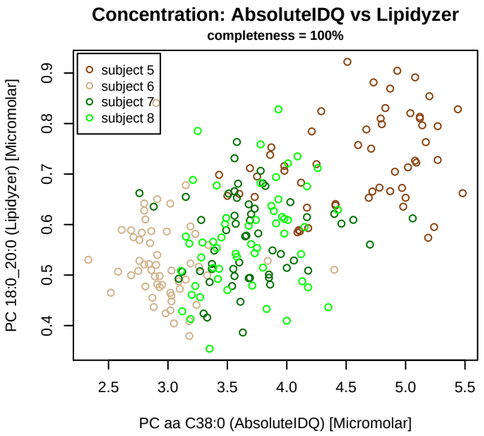
```
PC aa C38:0 ~ b * ( PC 18:0_20:0 )
```

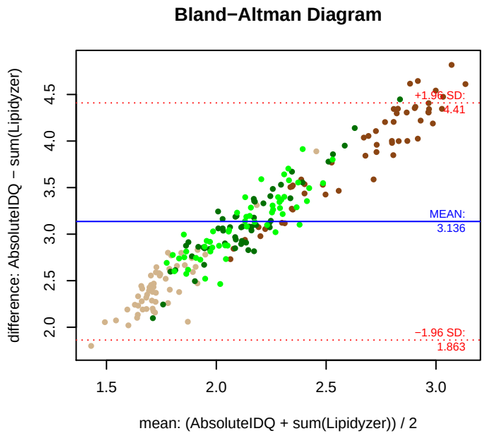
b = 3.58022

R^2 = 0.34478

Ranges

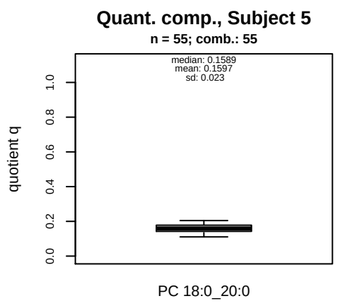
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	2.33	0.35	1.98
Max	5.48	0.92	4.56
Mean	3.74	0.6	3.14
Median	3.66	0.59	3.07
SD	0.71	0.12	0.6

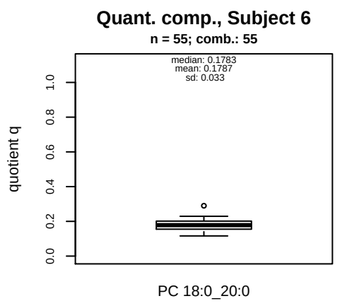


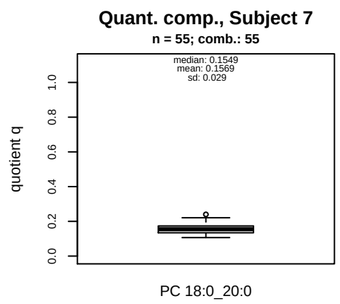


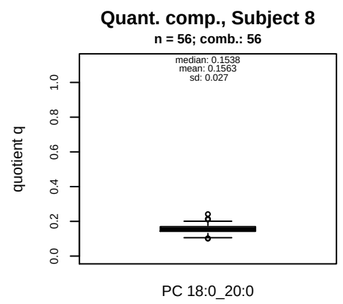
Stability of composition

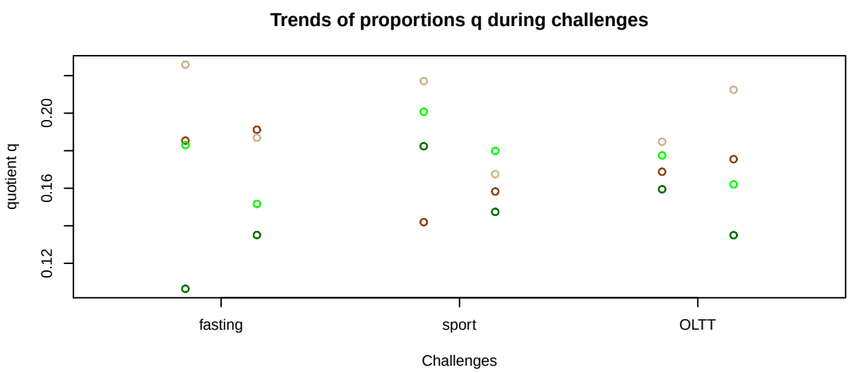
PC 18:0_20:0 / PC aa C38:0
Shapiro−Wilk Test of log quotients, pv: 0.94774; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.05256; EQUAL
Wilcoxon: Challenge; fasting: 0.625; sport: 0.25; OLTT: 1

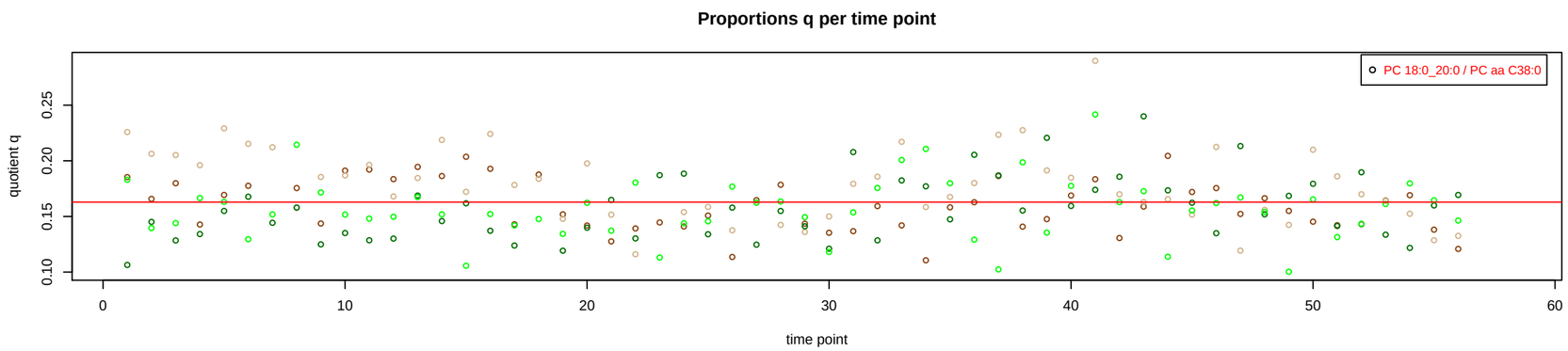






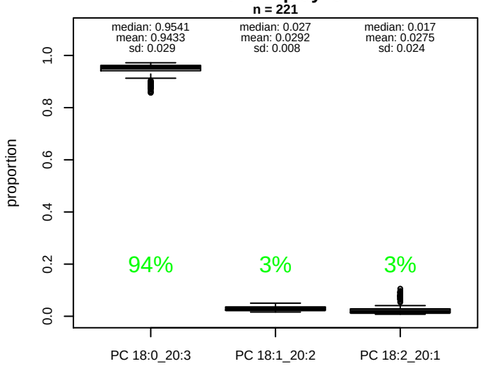


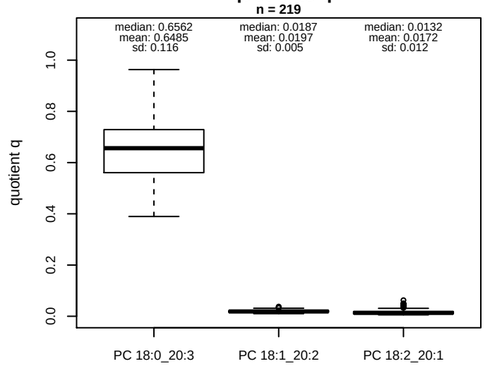




PC aa C38:3 = PC 18:0_20:3 + PC 18:1_20:2 + PC 18:2_20:1 + PC 20:0_18:3 + R

PC 20:0_18:3 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C38:3 consists of:
PC 18:0_20:3 94.3%
PC 18:1_20:2 2.9%
PC 18:2_20:1 2.7%
and of (not quantified):
PC 20:0_18:3, PC 16:1_22:2, PC 18:3_20:0, [13C1]SM 42:3,
and further compounds

Composition: mean of proportions q

conc(PC aa C38:3) * 0.6485 = conc(PC 18:0_20:3) [var(q)=0.6485]
Percentiles: 5%−>0.4476, 25%−>0.5606, 75%−>0.7287, 95%−>0.8496
conc(PC aa C38:3) * 0.0197 = conc(PC 18:1_20:2) [var(q)=0.0197]
Percentiles: 5%−>0.0126, 25%−>0.0161, 75%−>0.0224, 95%−>0.0299
conc(PC aa C38:3) * 0.0172 = conc(PC 18:2_20:1) [var(q)=0.0172]
Percentiles: 5%−>0.007, 25%−>0.0096, 75%−>0.0184, 95%−>0.0436

Linear model

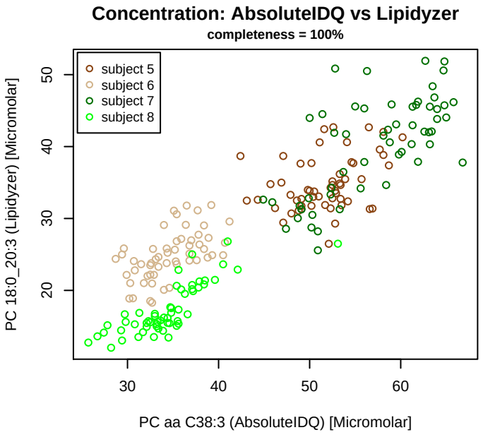
```
PC aa C38:3 ~ b * ( PC 18:0_20:3
   + PC 18:1_20:2
   + PC 18:2_20:1 )
```

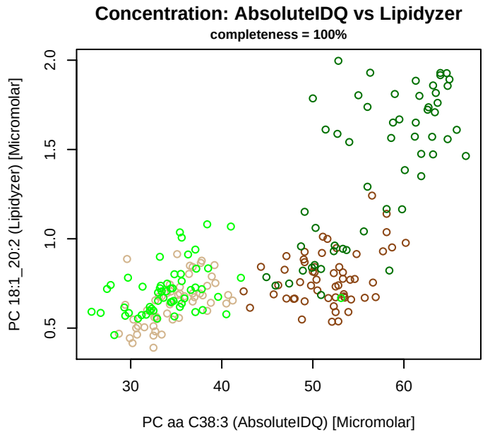
b = 0.98751

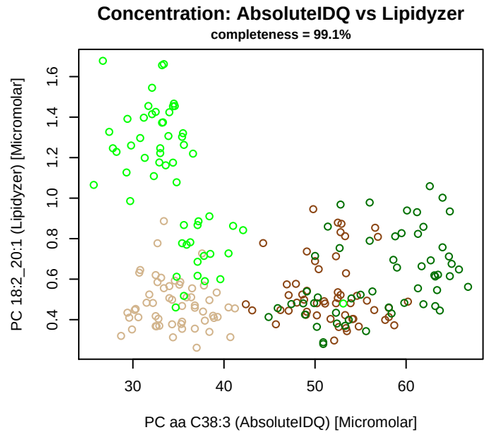
R^2 = 0.80663

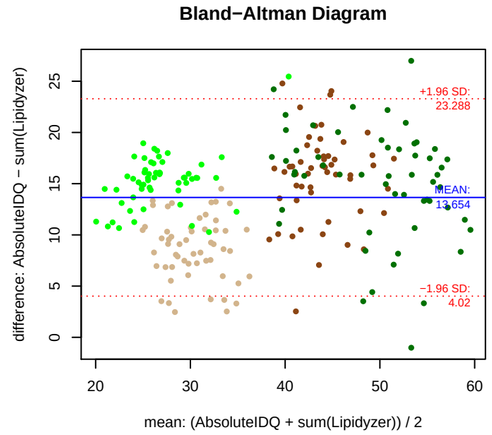
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	25.7	13.72	11.98
Max	66.8	54.35	12.45
Mean	44.46	30.82	13.64
Median	42.4	30.43	11.97
SD	11.16	10.15	1.01









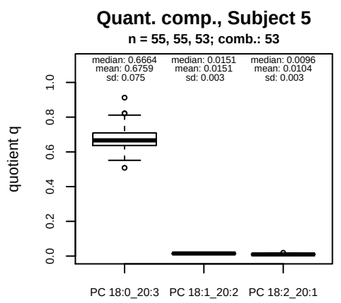
Stability of composition

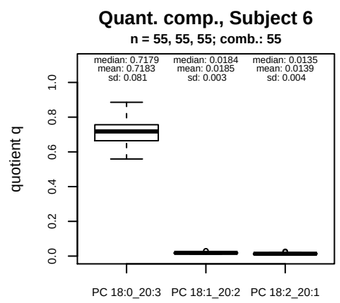
(PC 18:0_20:3 + PC 18:1_20:2 + PC 18:2_20:1) / PC aa C38:3
Shapiro−Wilk Test of log quotients, pv: 0.06972; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.5; sport: 0.125; OLTT: 0.25

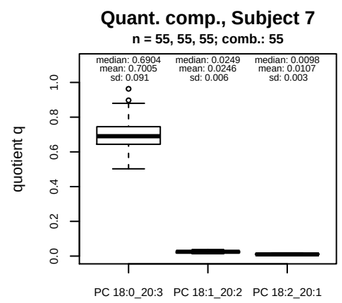
PC 18:1_20:2 / PC aa C38:3
Shapiro−Wilk Test of log quotients, pv: 0.11436; OK
SW: ok; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 1; OLTT: 0.375

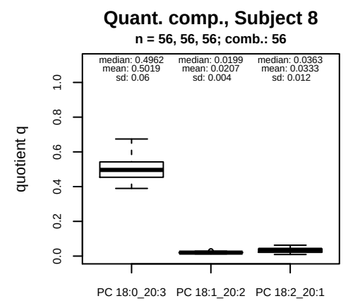
PC 18:0_20:3 / PC aa C38:3
Shapiro−Wilk Test of log quotients, pv: 2e−04; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.25

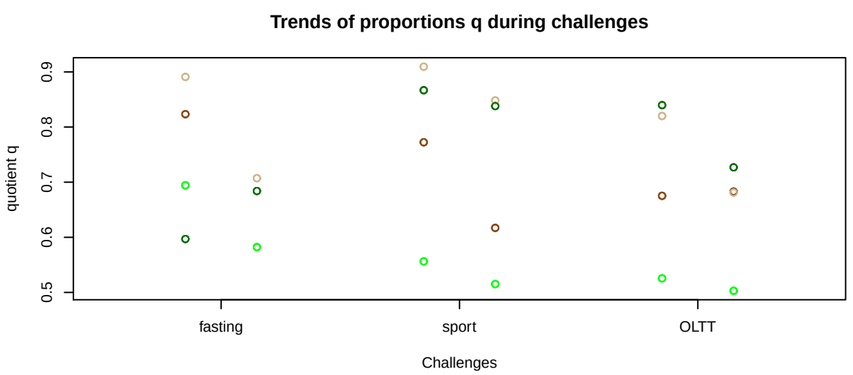
PC 18:2_20:1 / PC aa C38:3
Shapiro−Wilk Test of log quotients, pv: 0; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.5; sport: 0.25; OLTT: 0.875

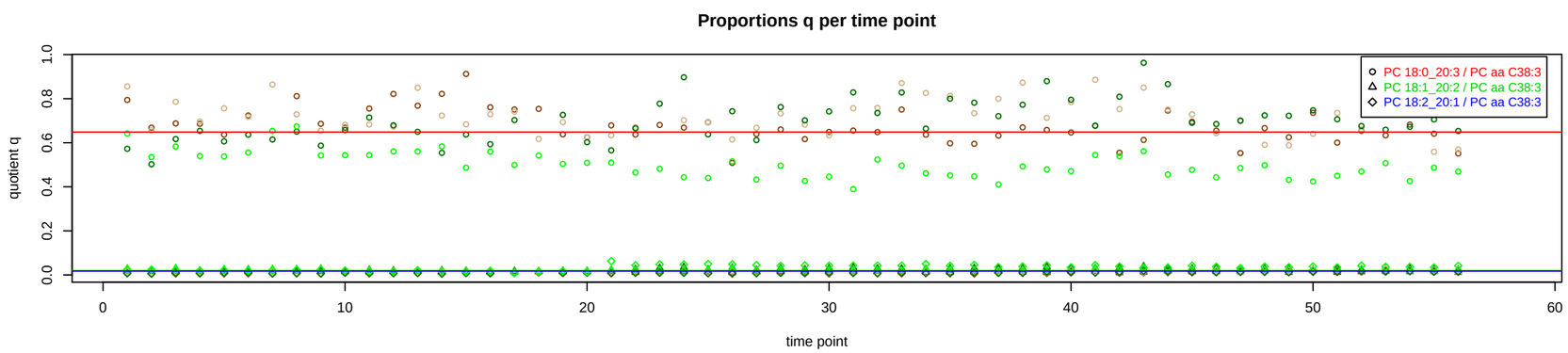




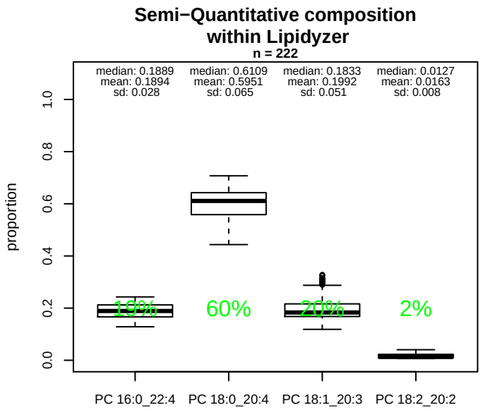


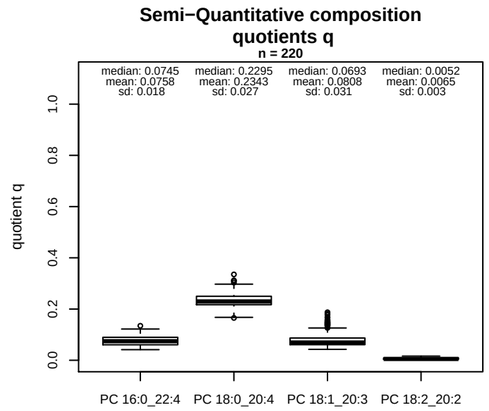






PC aa C38:4 = PC 16:0_22:4 + PC 18:0_20:4 + PC 18:1_20:3 + PC 18:2_20:2 + R





Semi−Quantitative composition: Lipidyzer

PC aa C38:4 consists of:
PC 16:0_22:4 18.9%
PC 18:0_20:4 59.5%
PC 18:1_20:3 19.9%
PC 18:2_20:2 1.6%
and of (not quantified):
PC 18:4_20:0
and further compounds

Linear model

```
PC aa C38:4 ~ b * ( PC 16:0_22:4
   + PC 18:0_20:4
   + PC 18:1_20:3
   + PC 18:2_20:2 )
```

b = 1.99845

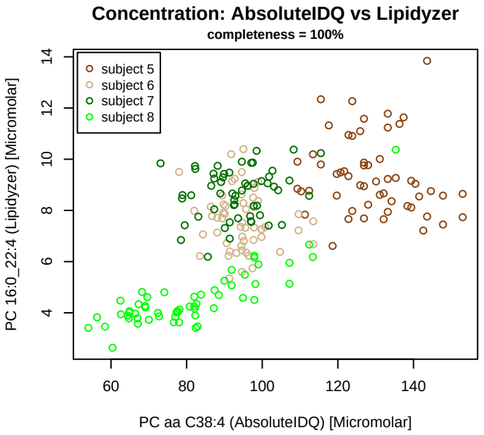
R^2 = 0.58796

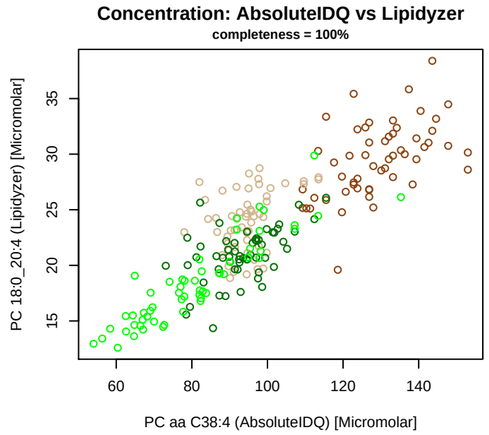
Ranges

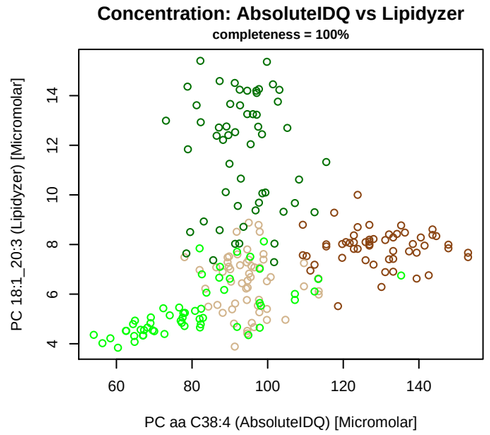
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	54	19.61	34.39
Max	153	61.31	91.69
Mean	99.43	39.14	60.29
Median	95.5	40.09	55.41
SD	21.26	8.1	13.16

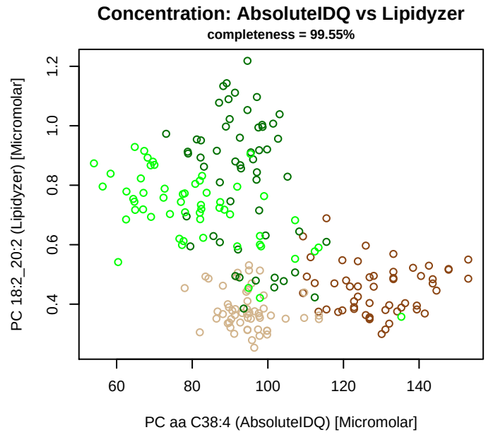
Composition: mean of proportions q

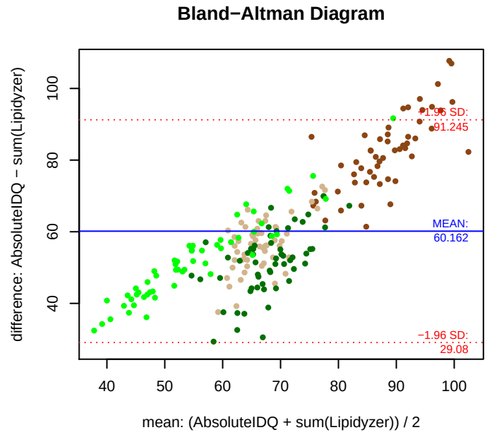
conc(PC aa C38:4) * 0.0758 = conc(PC 16:0_22:4) [var(q)=0.0758]
Percentiles: 5%−>0.0504, 25%−>0.0605, 75%−>0.0897, 95%−>0.1059
conc(PC aa C38:4) * 0.2343 = conc(PC 18:0_20:4) [var(q)=0.2343]
Percentiles: 5%−>0.1971, 25%−>0.217, 75%−>0.2499, 95%−>0.2867
conc(PC aa C38:4) * 0.0808 = conc(PC 18:1_20:3) [var(q)=0.0808]
Percentiles: 5%−>0.049, 25%−>0.0608, 75%−>0.0869, 95%−>0.15
conc(PC aa C38:4) * 0.0065 = conc(PC 18:2_20:2) [var(q)=0.0065]
Percentiles: 5%−>0.0028, 25%−>0.0037, 75%−>0.0094, 95%−>0.0126











Stability of composition

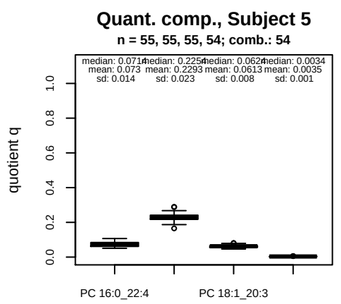
(PC 16:0_22:4 + PC 18:0_20:4 + PC 18:1_20:3 + PC 18:2_20:2) / PC aa C38:4
Shapiro−Wilk Test of log quotients, pv: 0.00246; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.52376; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.625

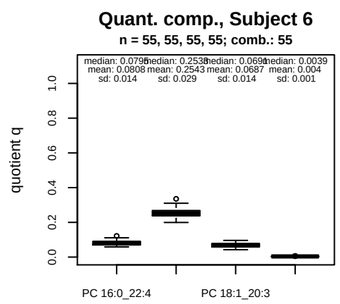
PC 16:0_22:4 / PC aa C38:4
Shapiro−Wilk Test of log quotients, pv: 0.01057; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 2e−05; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.625; sport: 0.875; OLTT: 0.375

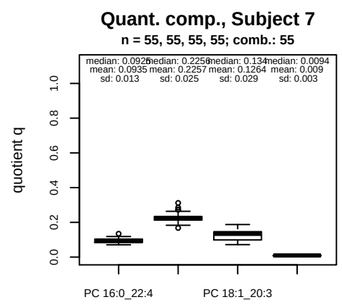
PC 18:0_20:4 / PC aa C38:4
Shapiro−Wilk Test of log quotients, pv: 0.04492; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.05199; EQUAL
Wilcoxon: Challenge; fasting: 0.375; sport: 0.125; OLTT: 0.625

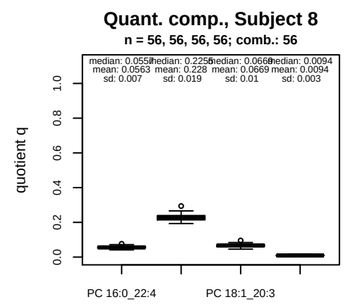
PC 18:1_20:3 / PC aa C38:4
Shapiro−Wilk Test of log quotients, pv: 0; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 2e−05; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.25; OLTT: 0.125

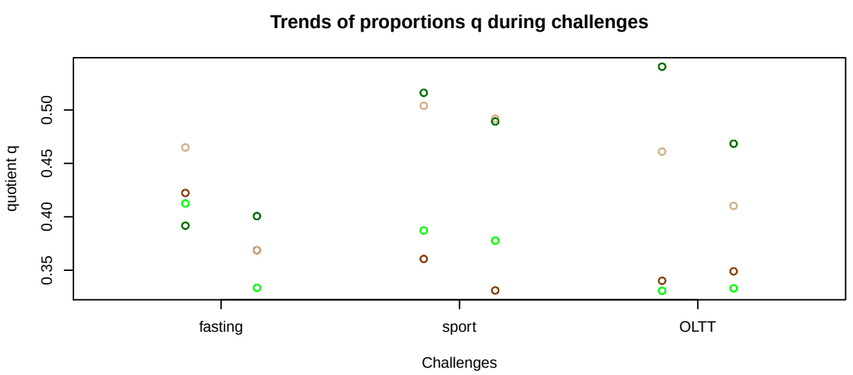
PC 18:2_20:2 / PC aa C38:4
Shapiro−Wilk Test of log quotients, pv: 0; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.625; OLTT: 0.875

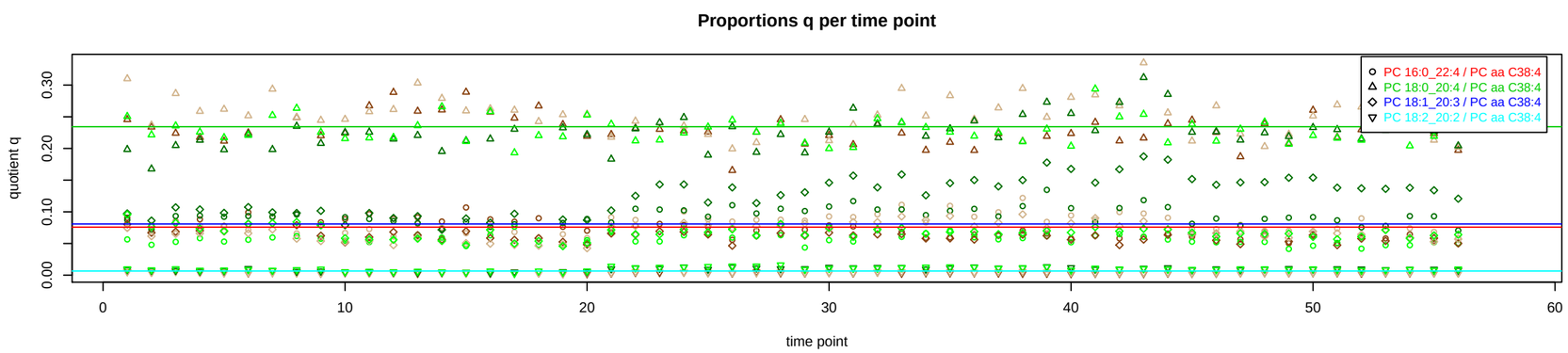






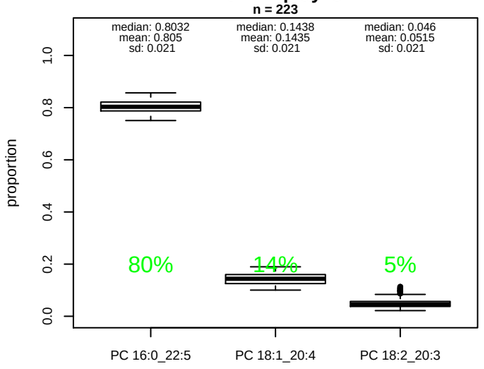


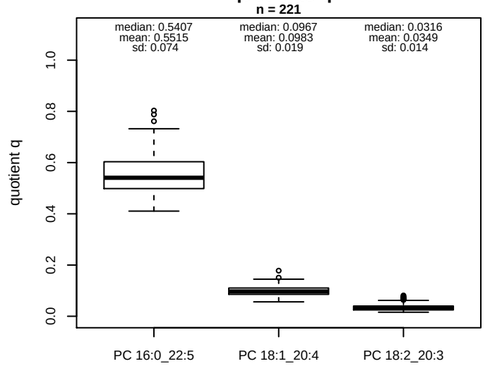




PC aa C38:5 = PC 16:0_22:5 + PC 18:0_20:5 + PC 18:1_20:4 + PC 18:2_20:3 + R

PC 18:0_20:5 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C38:5 consists of:
PC 16:0_22:5 80.5%
PC 18:1_20:4 14.4%
PC 18:2_20:3 5.1%
and of (not quantified):
PC 18:0_20:5, PC 16:1_22:4, PC 18:3_20:2, PC 18:4_20:1,
and further compounds

Composition: mean of proportions q

conc(PC aa C38:5) * 0.5515 = conc(PC 16:0_22:5) [var(q)=0.5515]
Percentiles: 5%−>0.438, 25%−>0.4985, 75%−>0.6034, 95%−>0.6725
conc(PC aa C38:5) * 0.0983 = conc(PC 18:1_20:4) [var(q)=0.0983]
Percentiles: 5%−>0.0687, 25%−>0.0856, 75%−>0.1103, 95%−>0.1286
conc(PC aa C38:5) * 0.0349 = conc(PC 18:2_20:3) [var(q)=0.0349]
Percentiles: 5%−>0.0201, 25%−>0.0248, 75%−>0.0399, 95%−>0.0647

Linear model

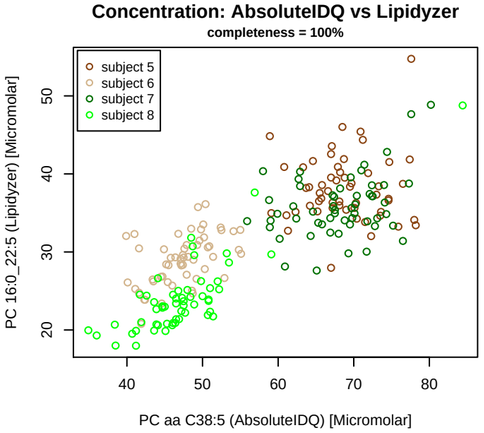
```
PC aa C38:5 ~ b * ( PC 16:0_22:5
   + PC 18:1_20:4
   + PC 18:2_20:3 )
```

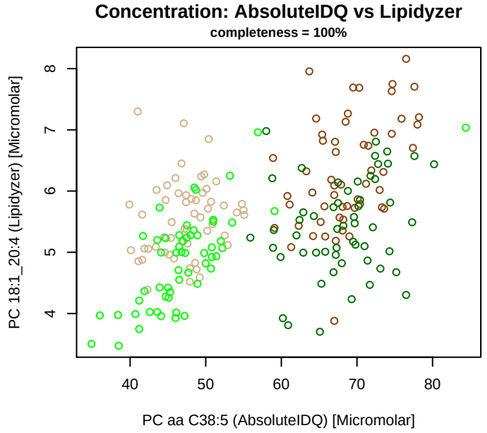
b = 1.21475

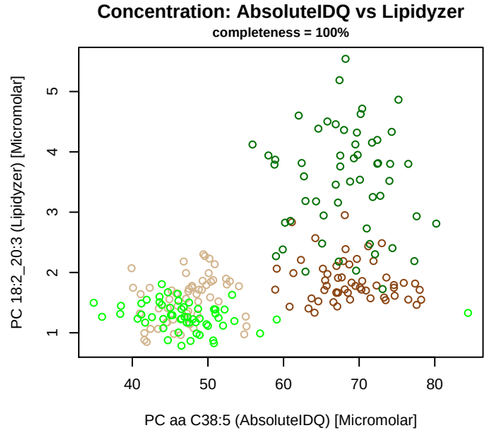
R^2 = 0.677

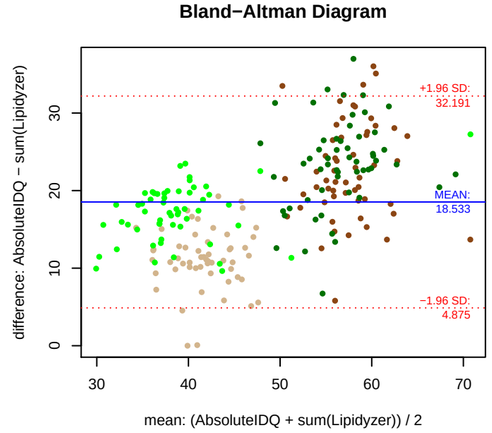
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	34.9	22.92	11.98
Max	84.4	63.92	20.48
Mean	57.86	39.37	18.49
Median	58	40.77	17.23
SD	11.88	8.02	3.85









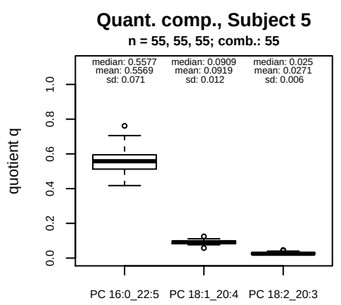
Stability of composition

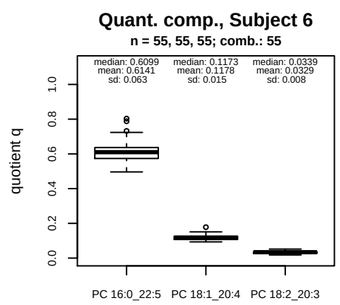
(PC 16:0_22:5 + PC 18:1_20:4 + PC 18:2_20:3) / PC aa C38:5
Shapiro−Wilk Test of log quotients, pv: 0.37049; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 2e−05; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.625; sport: 0.25; OLTT: 0.25

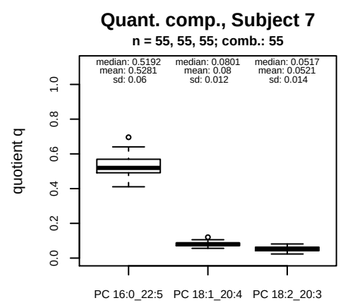
PC 18:1_20:4 / PC aa C38:5
Shapiro−Wilk Test of log quotients, pv: 0.41624; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.82498; EQUAL
Wilcoxon: Challenge; fasting: 0.375; sport: 0.25; OLTT: 0.375

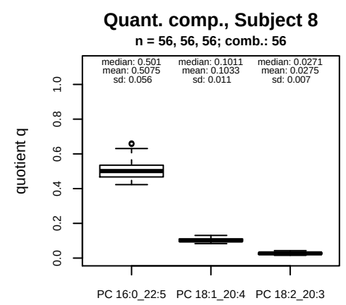
PC 16:0_22:5 / PC aa C38:5
Shapiro−Wilk Test of log quotients, pv: 0.26347; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.875; sport: 0.25; OLTT: 0.25

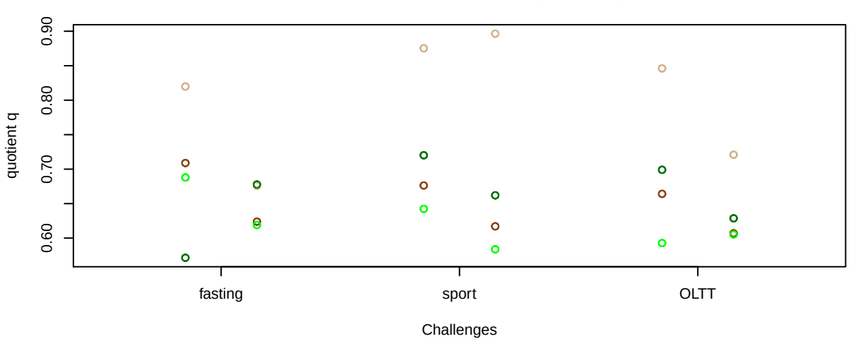
PC 18:2_20:3 / PC aa C38:5
Shapiro−Wilk Test of log quotients, pv: 0.00026; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.03257; EQUAL
Wilcoxon: Challenge; fasting: 0.125; sport: 0.125; OLTT: 0.125

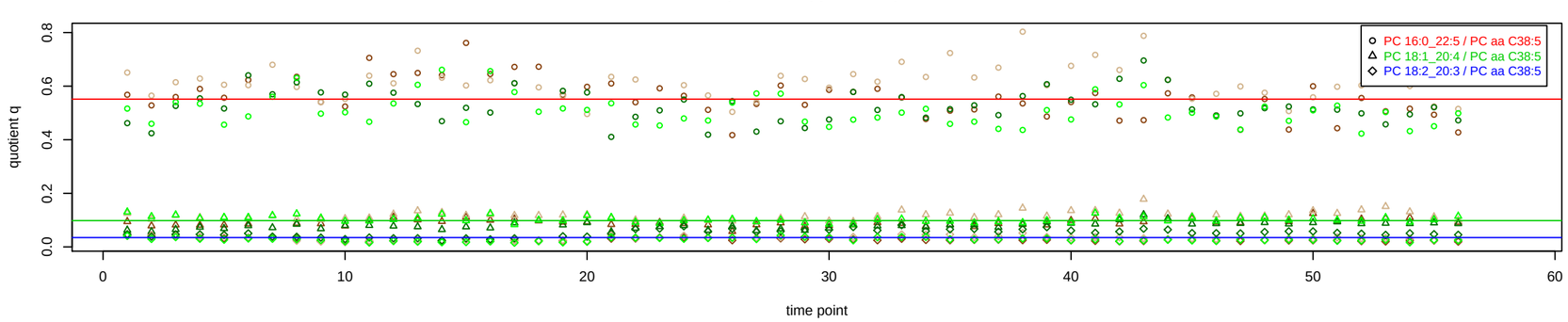






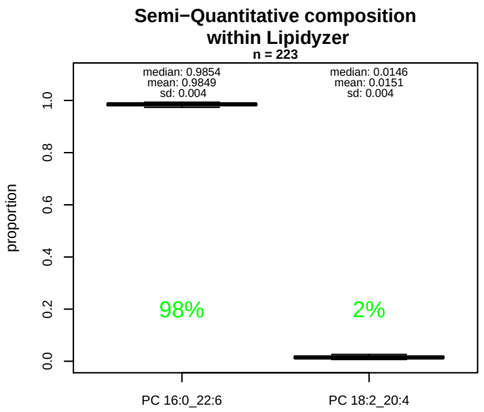


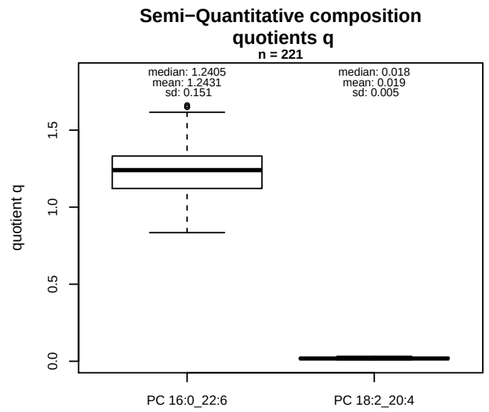




PC aa C38:6 = PC 16:0_22:6 + PC 18:1_20:5 + PC 18:2_20:4 + R

PC 18:1_20:5 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C38:6 consists of:
PC 16:0_22:6 98.5%
PC 18:2_20:4 1.5%
and of (not quantified):
PC 18:1_20:5, PC 16:1_22:5, PC 18:3_20:3, PC 18:4_20:2,
and further compounds

Linear model

```
PC aa C38:6 ~ b * ( PC 16:0_22:6
   + PC 18:2_20:4 )
```

b = 0.71118

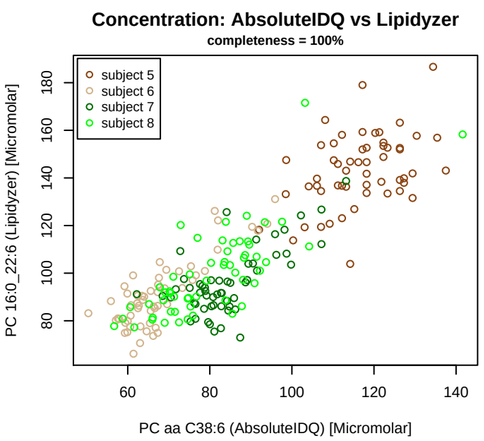
R^2 = 0.77057

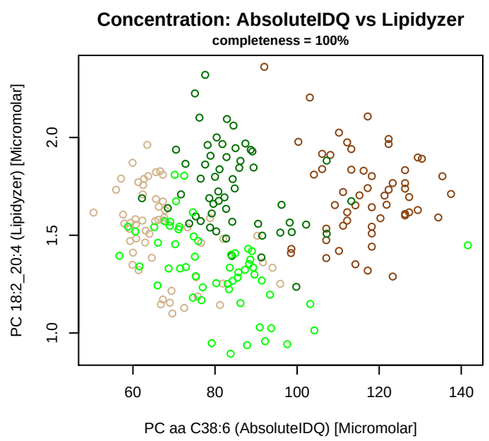
Ranges

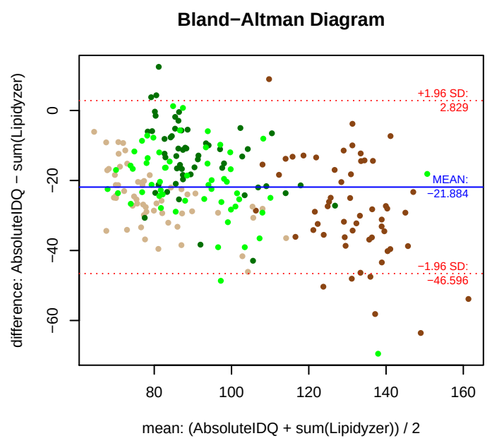
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	50.4	67.49	17.09
Max	141.6	188.25	46.65
Mean	87.19	109.18	21.99
Median	82.9	100.57	17.67
SD	21.12	26.01	4.89

Composition: mean of proportions q

conc(PC aa C38:6) * 1.2431 = conc(PC 16:0_22:6) [var(q)=1.2431]
Percentiles: 5%−>1.0168, 25%−>1.1214, 75%−>1.3321, 95%−>1.5009
conc(PC aa C38:6) * 0.019 = conc(PC 18:2_20:4) [var(q)=0.019]
Percentiles: 5%−>0.0118, 25%−>0.0148, 75%−>0.0234, 95%−>0.0279





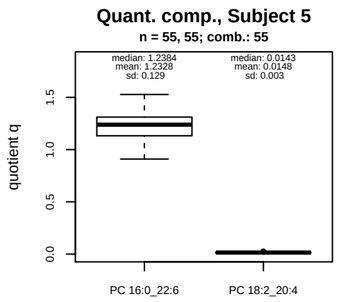


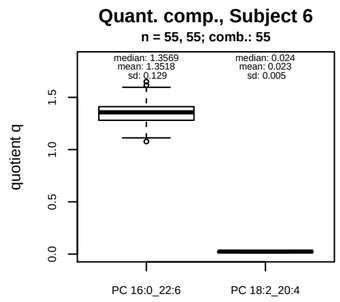
Stability of composition

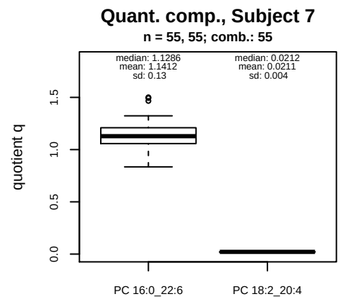
(PC 16:0_22:6 + PC 18:2_20:4) / PC aa C38:6
Shapiro−Wilk Test of log quotients, pv: 0.86063; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.06938; EQUAL
Wilcoxon: Challenge; fasting: 0.625; sport: 0.625; OLTT: 0.25

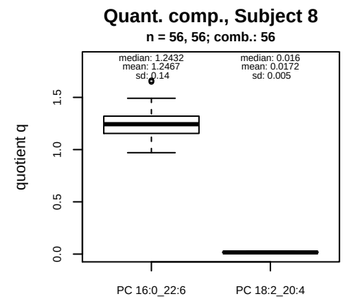
PC 18:2_20:4 / PC aa C38:6
Shapiro−Wilk Test of log quotients, pv: 0.00068; NO
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.125; OLTT: 0.625

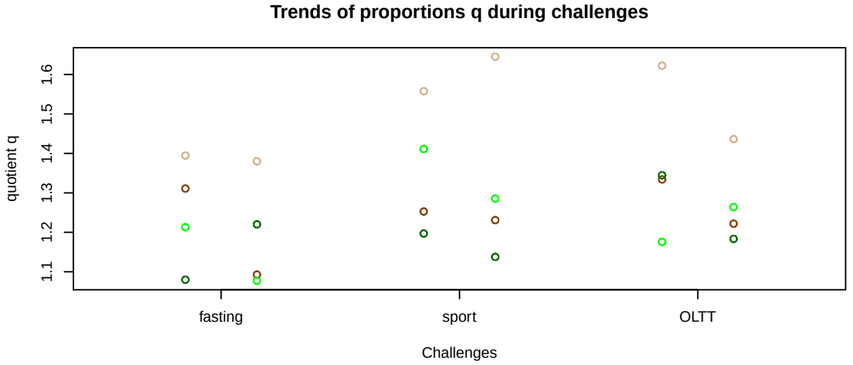
PC 16:0_22:6 / PC aa C38:6
Shapiro−Wilk Test of log quotients, pv: 0.79949; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.05839; EQUAL
Wilcoxon: Challenge; fasting: 0.625; sport: 0.625; OLTT: 0.25

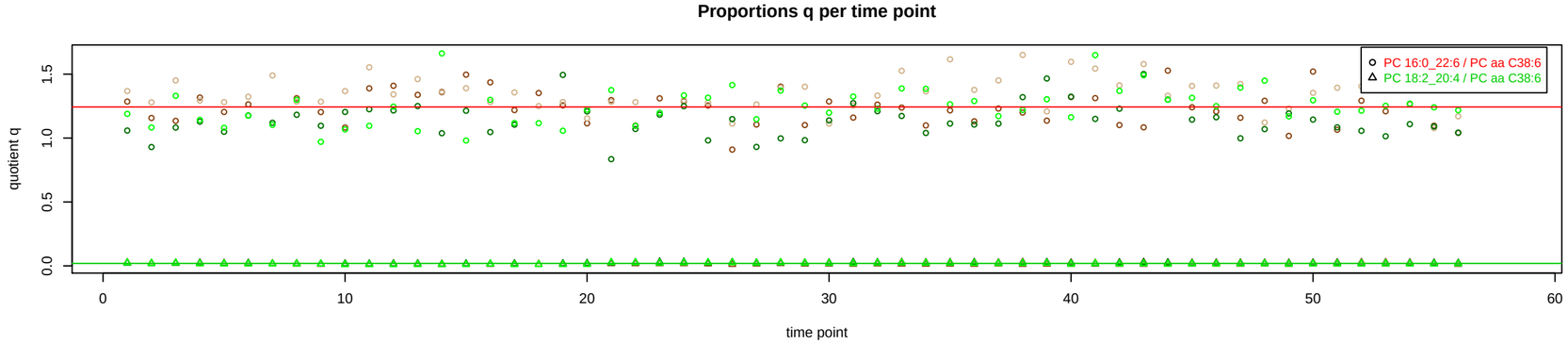












PC aa C40:1 = R

No independent Variable measured.

Qualitative composition

PC aa C40:1 consists of:
PC 16:0_24:1, PC 18:0_22:1, PC 18:1_22:0, PC 19:1_21:0, PC O−20:1_21:0
and further compounds

PC aa C40:2 = PC 18:0_22:2 + PC 18:1_22:1 + R

PC 18:0_22:2, PC 18:1_22:1 excluded because of missingness > 75%

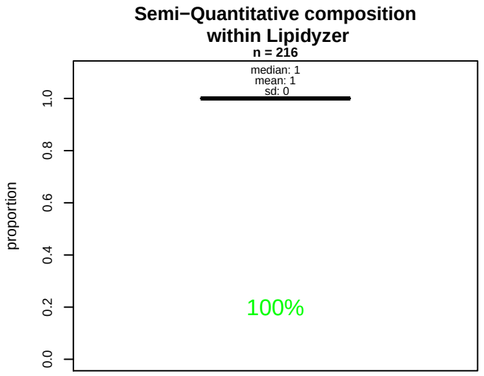
No independent Variable with coverage >0.25 out of PC 18:0_22:2, PC 18:1_22:1

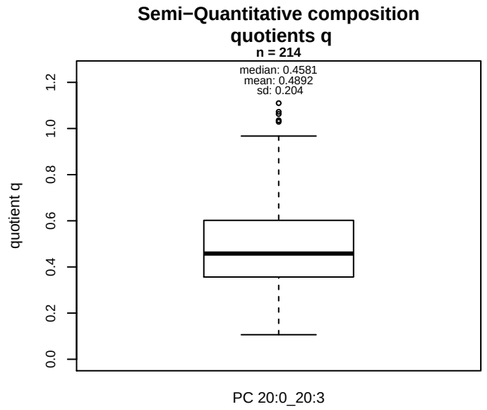
Qualitative composition

PC aa C40:2 consists of:
PC 18:0_22:2, PC 18:1_22:1, PC 16:1_24:1, PC 18:2_22:0, PC 20:1_20:1
and further compounds

PC aa C40:3 = PC 18:2_22:1 + PC 20:0_20:3 + R

PC 18:2_22:1 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC aa C40:3 consists of:
PC 20:0_20:3 100%
and of (not quantified):
PC 18:2_22:1, PC 18:0_22:3, PC 18:1_22:2, PC 18:3_22:0, PC 20:1_20:2
and further compounds

Linear model

```
PC aa C40:3 ~ b * ( PC 20:0_20:3 )
```

b = −0.06122

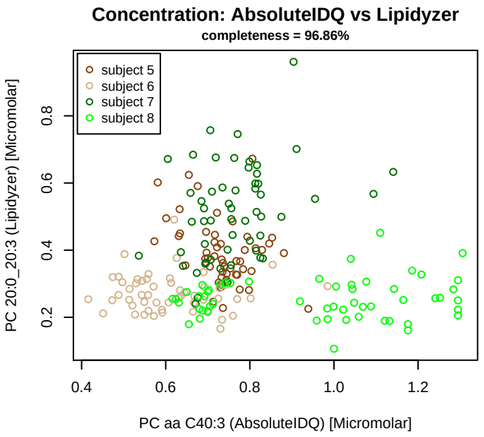
R^2 = 0.00209

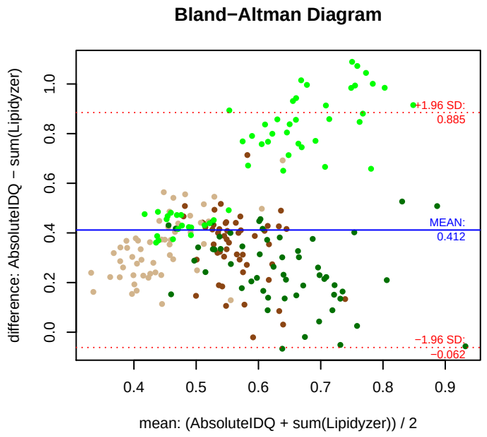
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	0.42	0.11	0.31
Max	1.31	0.96	0.35
Mean	0.77	0.36	0.41
Median	0.73	0.32	0.41
SD	0.19	0.14	0.05

Composition: mean of proportions q

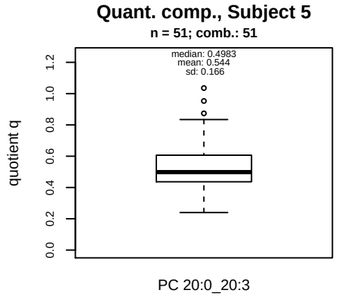
conc(PC aa C40:3) * 0.4892 = conc(PC 20:0_20:3) [var(q)=0.4892]
Percentiles: 5%−>0.198, 25%−>0.3568, 75%−>0.5993, 95%−>0.8453

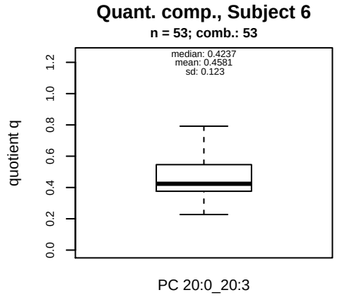


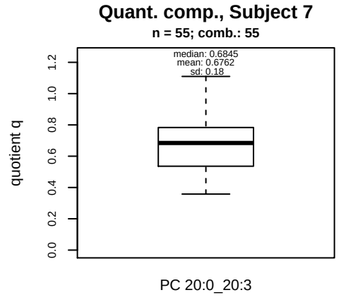


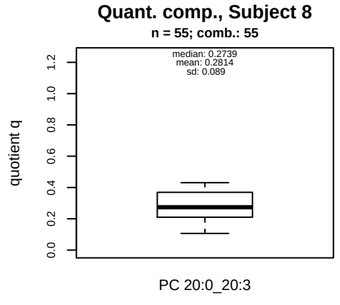
Stability of composition

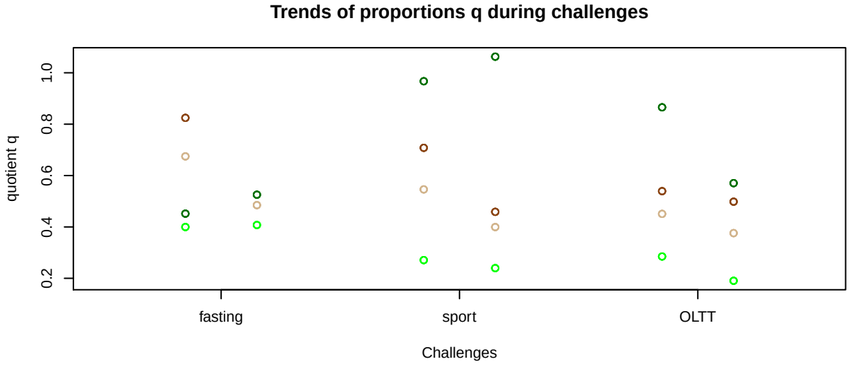
PC 20:0_20:3 / PC aa C40:3
Shapiro−Wilk Test of log quotients, pv: 0.0089; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 1; sport: 0.375; OLTT: 0.125

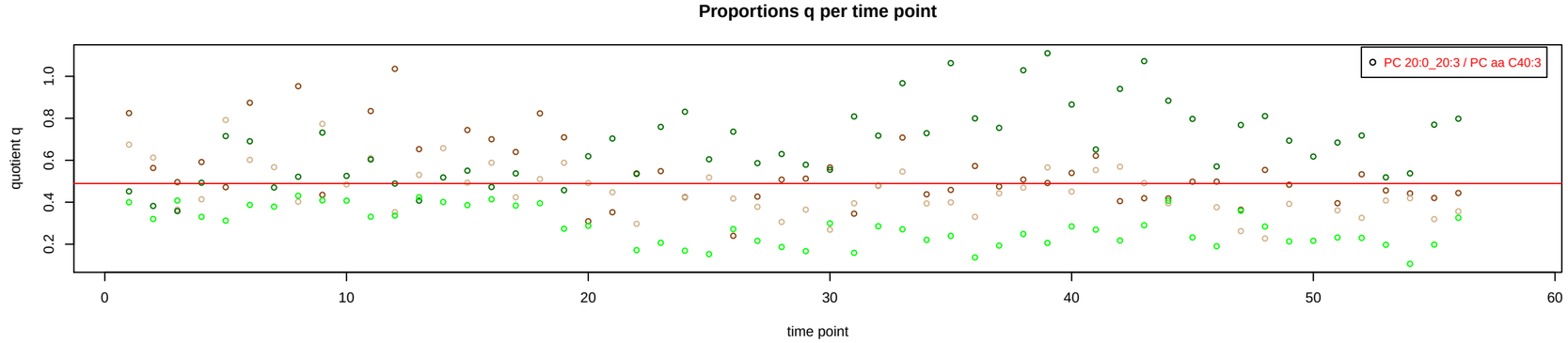




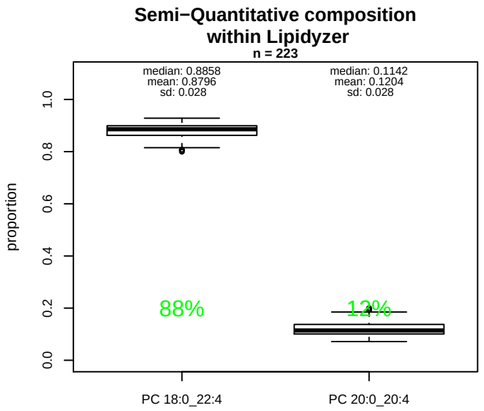


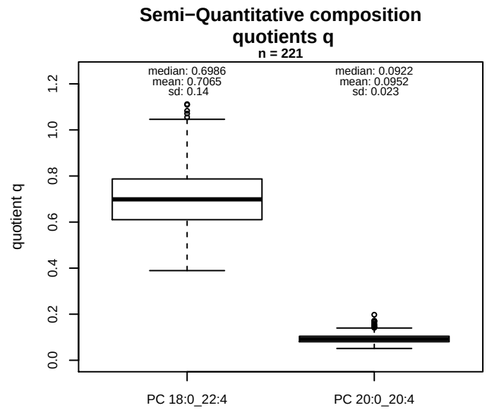






PC aa C40:4 = PC 18:0_22:4 + PC 20:0_20:4 + R





Semi−Quantitative composition: Lipidyzer

PC aa C40:4 consists of:
PC 18:0_22:4 88%
PC 20:0_20:4 12%
and of (not quantified):
PC 18:2_22:2, PC 18:3_22:1, PC 18:4_22:0, PC 20:1_20:3, PC 20:2_20:2
and further compounds

Linear model

```
PC aa C40:4 ~ b * ( PC 18:0_22:4
   + PC 20:0_20:4 )
```

b = 0.82589

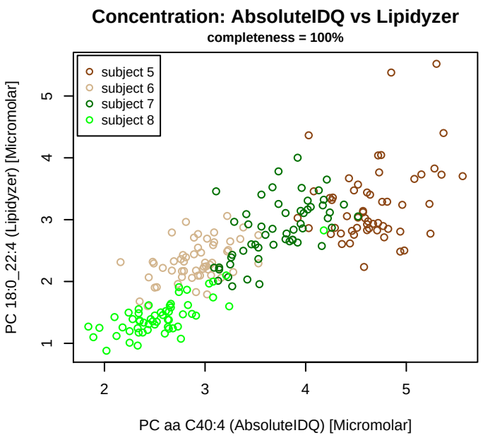
R^2 = 0.67225

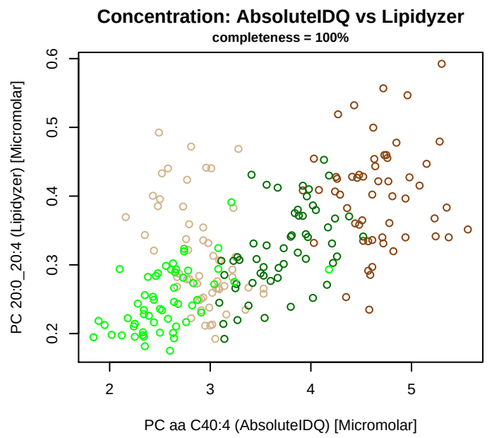
Ranges

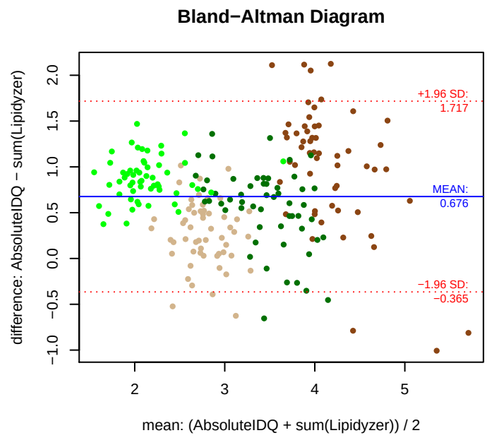
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	1.84	1.08	0.76
Max	5.56	6.11	0.55
Mean	3.46	2.79	0.67
Median	3.25	2.85	0.4
SD	0.89	0.88	0

Composition: mean of proportions q

conc(PC aa C40:4) * 0.7065 = conc(PC 18:0_22:4) [var(q)=0.7065]
Percentiles: 5%−>0.4936, 25%−>0.6103, 75%−>0.7872, 95%−>0.9503
conc(PC aa C40:4) * 0.0952 = conc(PC 20:0_20:4) [var(q)=0.0952]
Percentiles: 5%−>0.0644, 25%−>0.0803, 75%−>0.1044, 95%−>0.1461





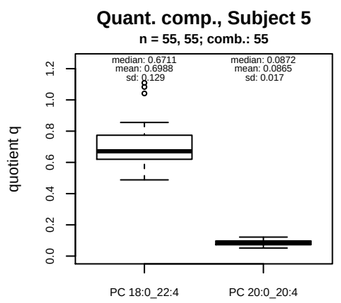


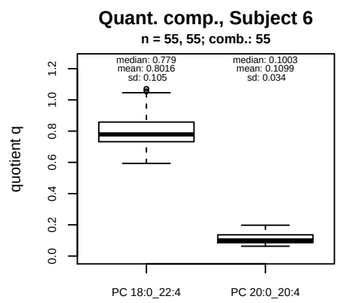
Stability of composition

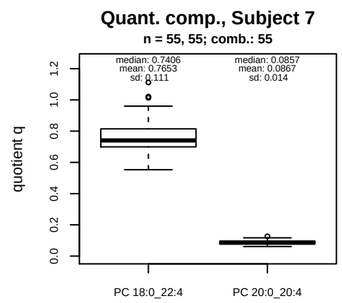
(PC 18:0_22:4 + PC 20:0_20:4) / PC aa C40:4
Shapiro−Wilk Test of log quotients, pv: 0.92811; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.875; OLTT: 0.125

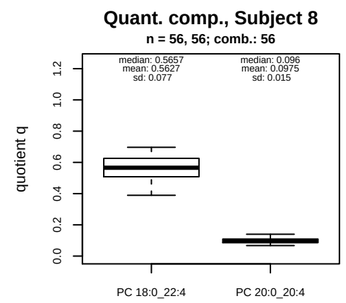
PC 20:0_20:4 / PC aa C40:4
Shapiro−Wilk Test of log quotients, pv: 0.00125; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.19594; EQUAL
Wilcoxon: Challenge; fasting: 0.375; sport: 1; OLTT: 0.25

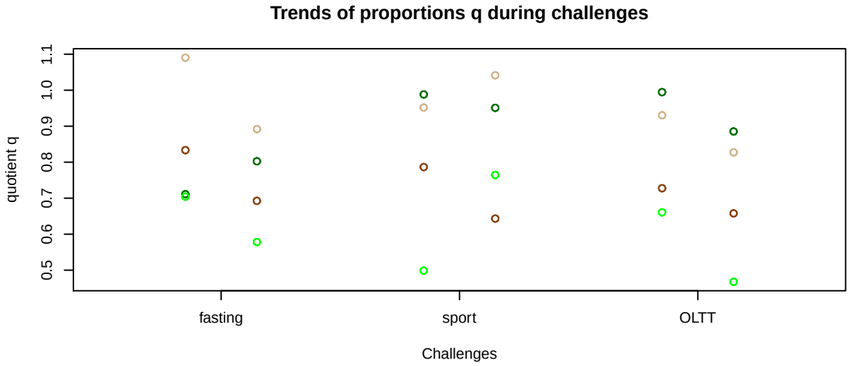
PC 18:0_22:4 / PC aa C40:4
Shapiro−Wilk Test of log quotients, pv: 0.64098; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.875; OLTT: 0.125

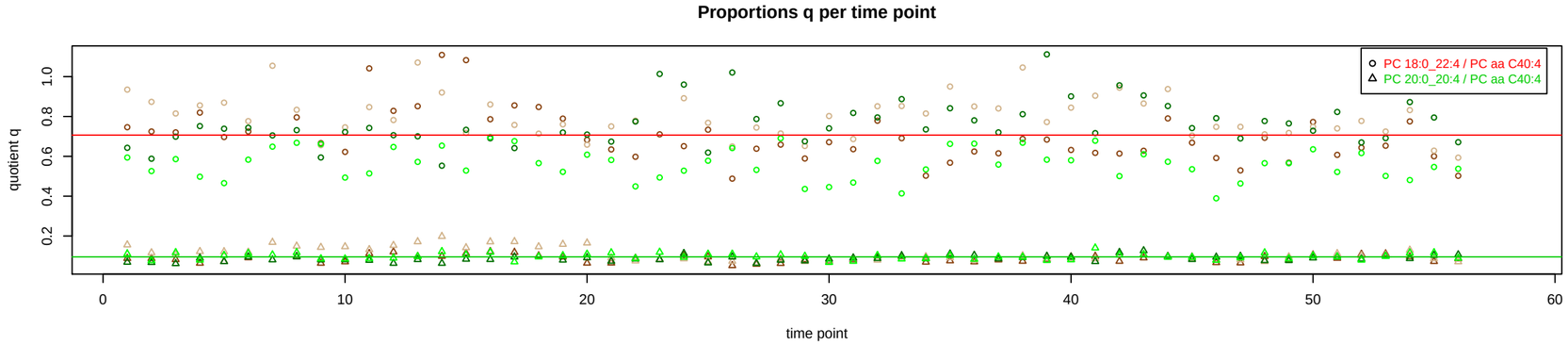




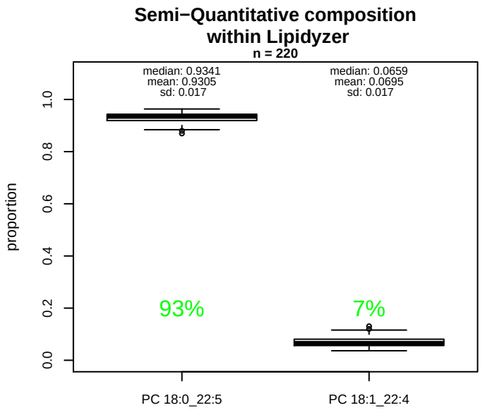


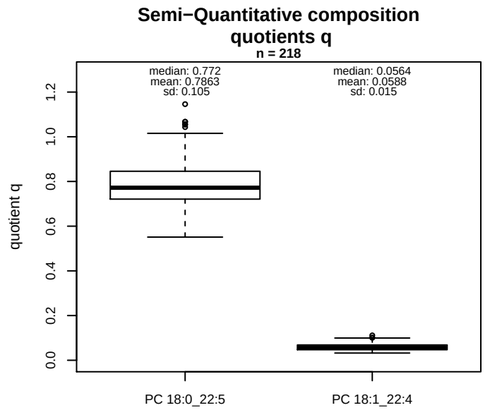






PC aa C40:5 = PC 18:0_22:5 + PC 18:1_22:4 + R





Semi−Quantitative composition: Lipidyzer

PC aa C40:5 consists of:
PC 18:0_22:5 93%
PC 18:1_22:4 7%
and of (not quantified):
PC 18:3_22:2, PC 18:4_22:1, PC 20:0_20:5, PC 20:1_20:4, PC 20:2_20:3
and further compounds

Composition: mean of proportions q

conc(PC aa C40:5) * 0.7863 = conc(PC 18:0_22:5) [var(q)=0.7863]
Percentiles: 5%−>0.6343, 25%−>0.721, 75%−>0.8457, 95%−>0.9819
conc(PC aa C40:5) * 0.0588 = conc(PC 18:1_22:4) [var(q)=0.0588]
Percentiles: 5%−>0.0373, 25%−>0.0473, 75%−>0.0684, 95%−>0.084

Linear model

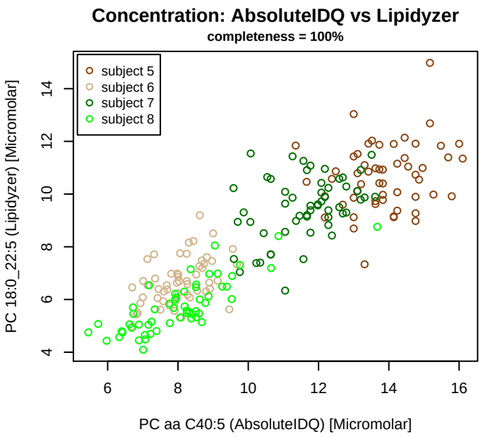
```
PC aa C40:5 ~ b * ( PC 18:0_22:5
   + PC 18:1_22:4 )
```

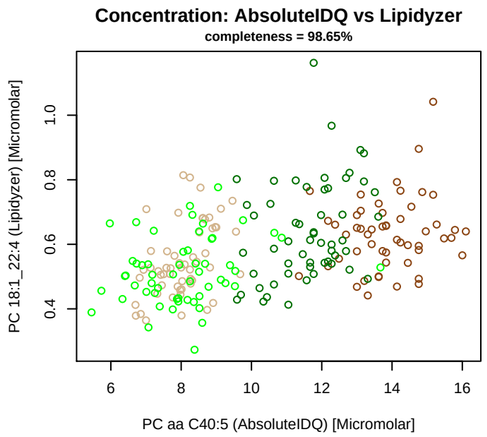
b = 1.00995

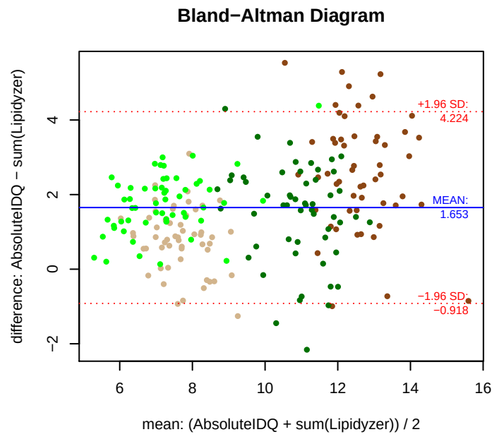
R^2 = 0.76522

Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	5.45	4.55	0.9
Max	16.1	16.02	0.08
Mean	10.39	8.74	1.65
Median	9.76	8.55	1.21
SD	2.72	2.34	0.37





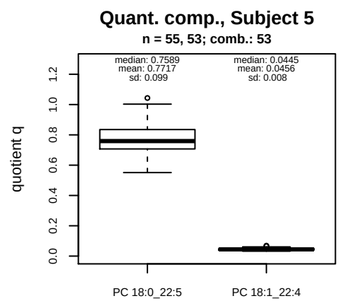


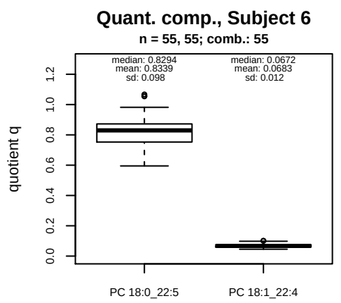
Stability of composition

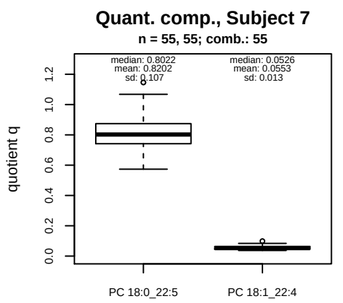
(PC 18:0_22:5 + PC 18:1_22:4) / PC aa C40:5
Shapiro−Wilk Test of log quotients, pv: 0.55079; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.06767; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.25

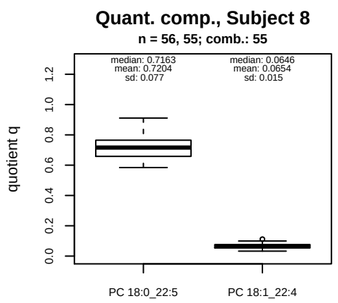
PC 18:1_22:4 / PC aa C40:5
Shapiro−Wilk Test of log quotients, pv: 0.30263; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.125; sport: 0.625; OLTT: 1

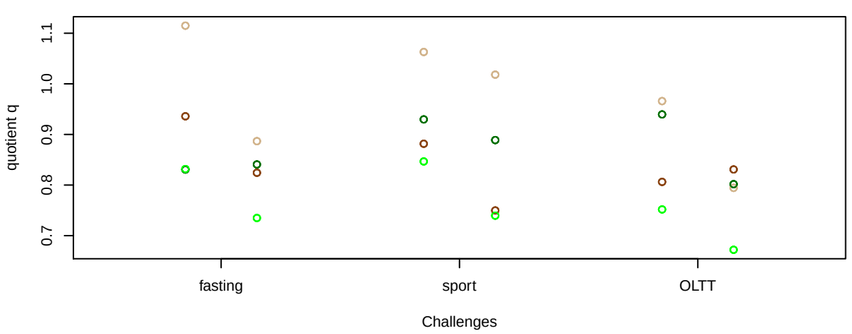
PC 18:0_22:5 / PC aa C40:5
Shapiro−Wilk Test of log quotients, pv: 0.63789; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00534; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.125; OLTT: 0.25

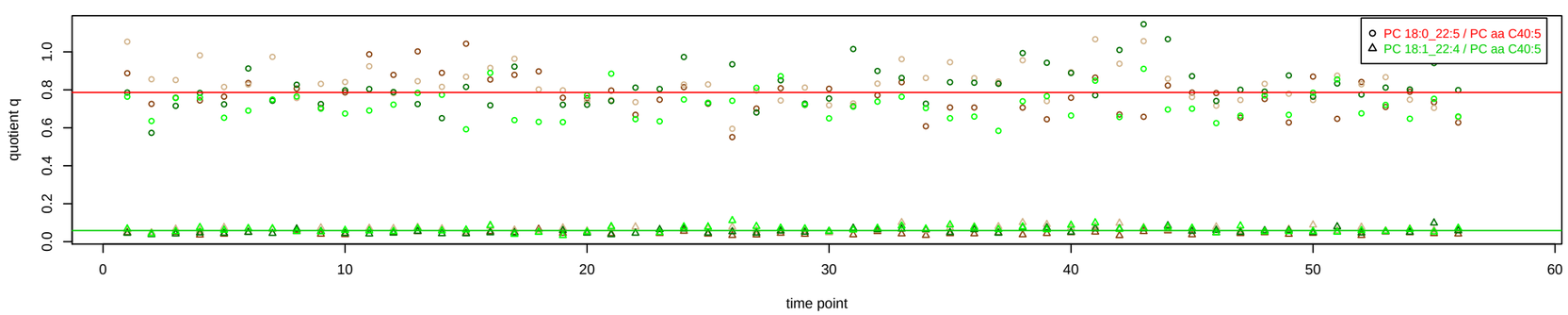




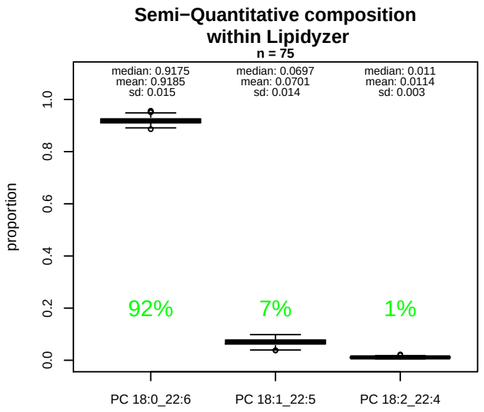


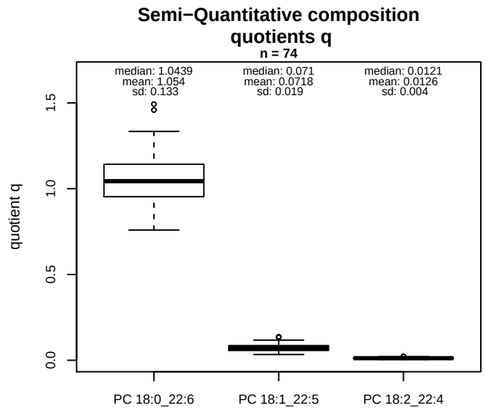






PC aa C40:6 = PC 18:0_22:6 + PC 18:1_22:5 + PC 18:2_22:4 + R





Semi−Quantitative composition: Lipidyzer

PC aa C40:6 consists of:
PC 18:0_22:6 91.8%
PC 18:1_22:5 7%
PC 18:2_22:4 1.1%
and of (not quantified):
PC 18:4_22:2, PC 20:1_20:5, PC 20:2_20:4, PC 20:3_20:3, and further compounds

Linear model

```
PC aa C40:6 ~ b * ( PC 18:0_22:6
   + PC 18:1_22:5
   + PC 18:2_22:4 )
```

b = 0.91019

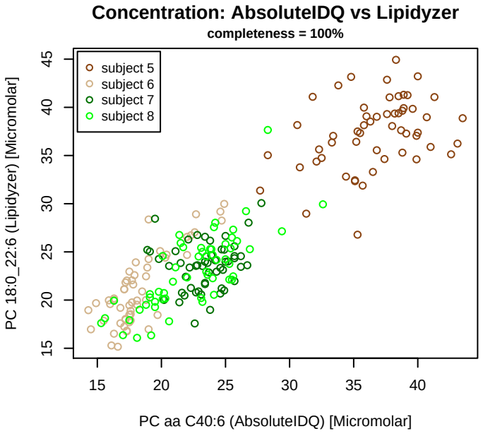
R^2 = 0.82665

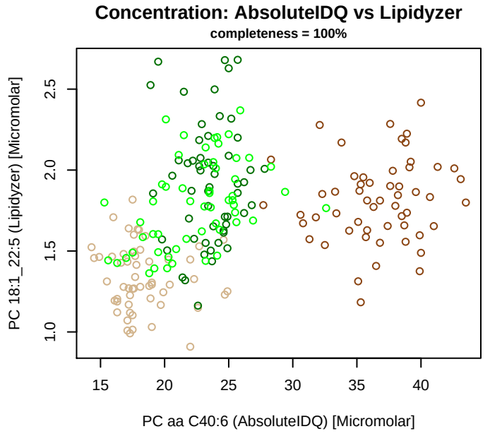
Ranges

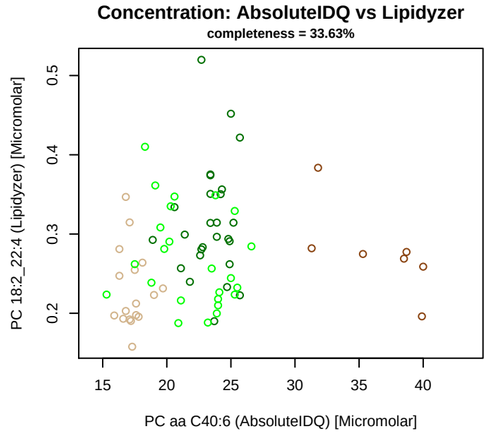
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	14.3	16.78	2.48
Max	43.5	43.62	0.12
Mean	25.21	24.91	0.3
Median	23.5	24.17	0.67
SD	7.46	5.35	2.11

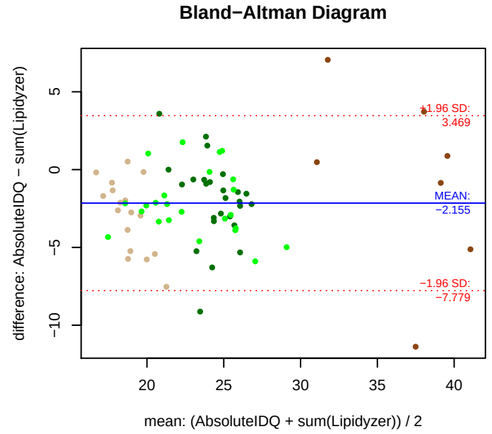
Composition: mean of proportions q

conc(PC aa C40:6) * 1.054 = conc(PC 18:0_22:6) [var(q)=1.054]
Percentiles: 5%−>0.8588, 25%−>0.9535, 75%−>1.1426, 95%−>1.2734
conc(PC aa C40:6) * 0.0718 = conc(PC 18:1_22:5) [var(q)=0.0718]
Percentiles: 5%−>0.0429, 25%−>0.0573, 75%−>0.0856, 95%−>0.1039
conc(PC aa C40:6) * 0.0126 = conc(PC 18:2_22:4) [var(q)=0.0126]
Percentiles: 5%−>0.0076, 25%−>0.0099, 75%−>0.0147, 95%−>0.0186









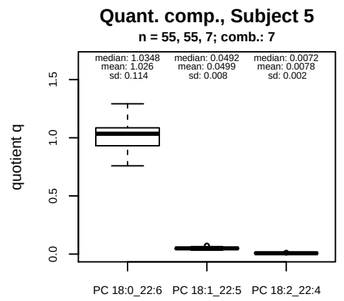
Stability of composition

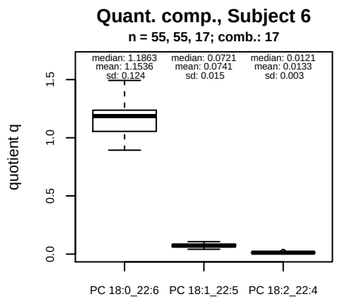
(PC 18:0_22:6 + PC 18:1_22:5 + PC 18:2_22:4) / PC aa C40:6
Shapiro−Wilk Test of log quotients, pv: 0.76064; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.82272; EQUAL
Wilcoxon: Challenge; sport: 1

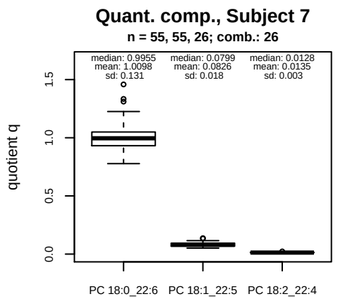
PC 18:0_22:6 / PC aa C40:6
Shapiro−Wilk Test of log quotients, pv: 0.25525; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.08; EQUAL
Wilcoxon: Challenge; fasting: 0.125; sport: 0.875; OLTT: 0.375

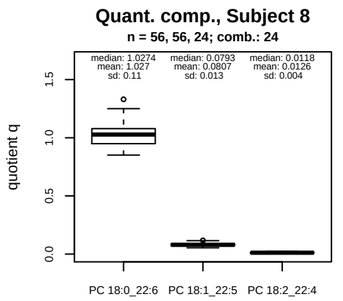
PC 18:1_22:5 / PC aa C40:6
Shapiro−Wilk Test of log quotients, pv: 0.04469; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.625; sport: 0.875; OLTT: 0.875

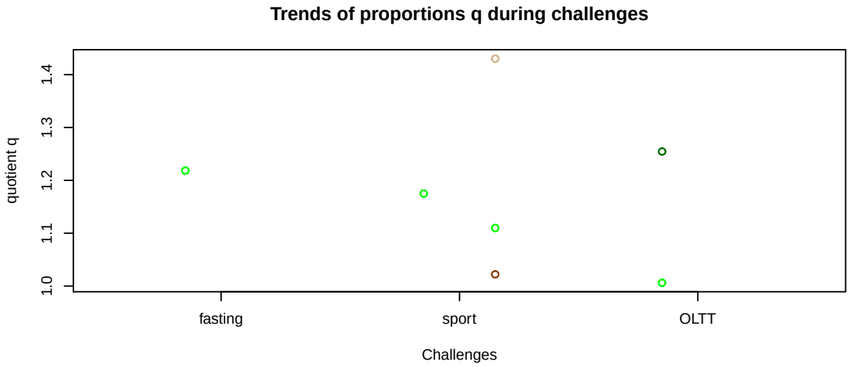
PC 18:2_22:4 / PC aa C40:6
Shapiro−Wilk Test of log quotients, pv: 0.65312; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.02697; EQUAL
Wilcoxon: Challenge; sport: 1

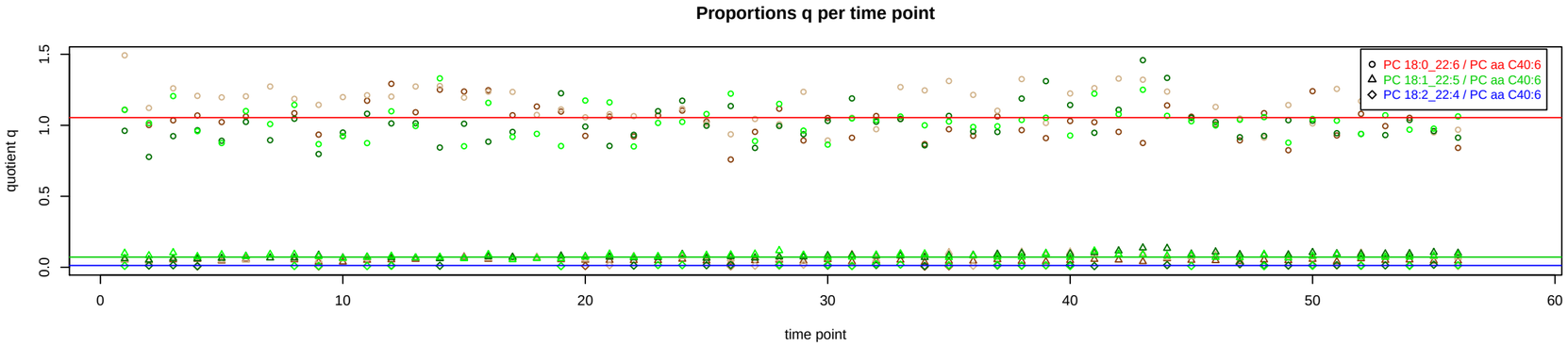












PC aa C42:0 = R

No independent Variable measured.

Qualitative composition

PC aa C42:0 consists of:
PC 16:0_26:0, PC 18:0_24:0, PC 20:0_22:0, PC 21:0_21:0, and further compounds

PC aa C42:1 = R

No independent Variable measured.

Qualitative composition

PC aa C42:1 consists of:
PC 18:0_24:1, PC 18:1_24:0, PC 20:0_22:1, PC 20:1_22:0, and further compounds

PC aa C42:2 = R

No independent Variable measured.

Qualitative composition

PC aa C42:2 consists of:
PC 16:0_26:2, PC 18:1_24:1, PC 18:2_24:0, PC 20:0_22:2, PC 20:2_22:0
and further compounds

PC aa C42:4 = R

No independent Variable measured.

Qualitative composition

PC aa C42:4 consists of:
PC 18:3_24:1, PC 18:4_24:0, PC 20:0_22:4, PC 20:2_22:2, PC 20:4_22:0
and further compounds

PC aa C42:5 = PC 20:0_22:5 + R

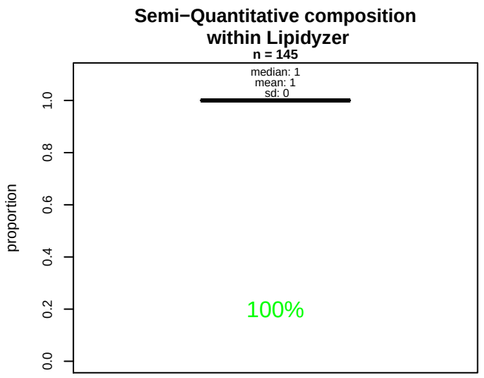
PC 20:0_22:5 excluded because of missingness > 75%

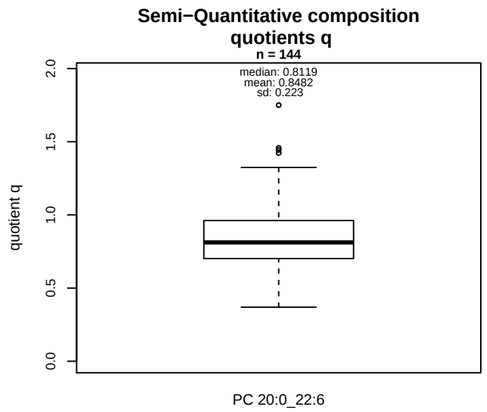
No independent Variable with coverage >0.25 out of PC 20:0_22:5

Qualitative composition

PC aa C42:5 consists of:
PC 20:0_22:5, PC 20:1_22:4, PC 20:3_22:2, PC 20:4_22:1, PC 20:5_22:0
and further compounds

PC aa C42:6 = PC 20:0_22:6 + R





Semi−Quantitative composition: Lipidyzer

PC aa C42:6 consists of:
PC 20:0_22:6 100%
and of (not quantified):
PC 20:5_22:1
and further compounds

Linear model

```
PC aa C42:6 ~ b * ( PC 20:0_22:6 )
```

b = 0.21904

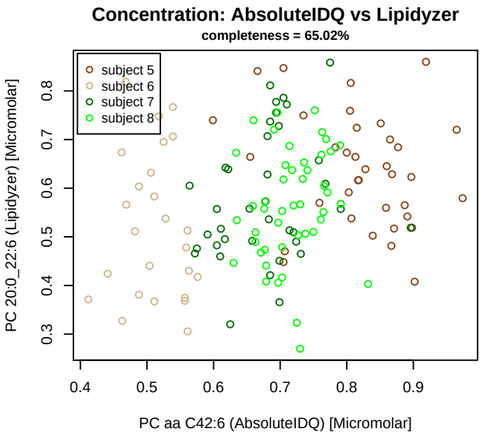
R^2 = 0.05859

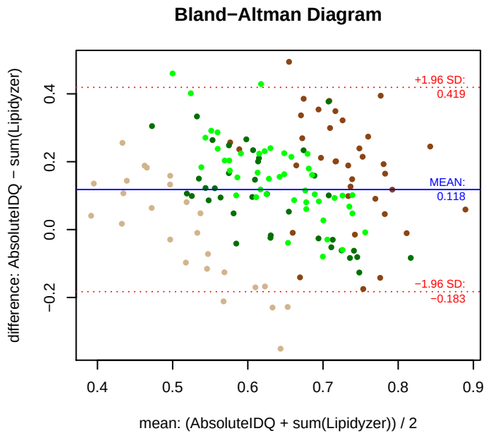
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	0.41	0.27	0.14
Max	0.97	0.86	0.11
Mean	0.69	0.58	0.11
Median	0.69	0.57	0.13
SD	0.13	0.13	0

Composition: mean of proportions q

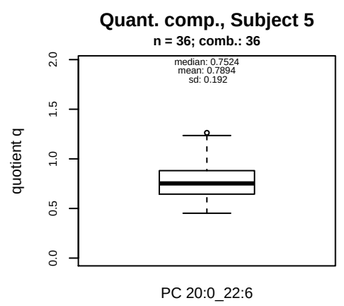
conc(PC aa C42:6) * 0.8482 = conc(PC 20:0_22:6) [var(q)=0.8482]
Percentiles: 5%−>0.5587, 25%−>0.703, 75%−>0.9614, 95%−>1.2468

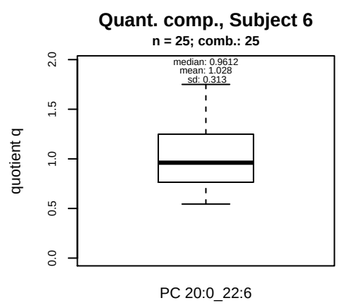


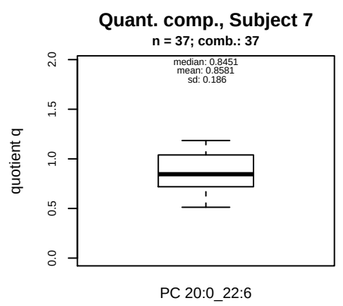


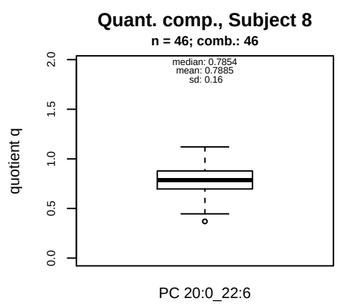
Stability of composition

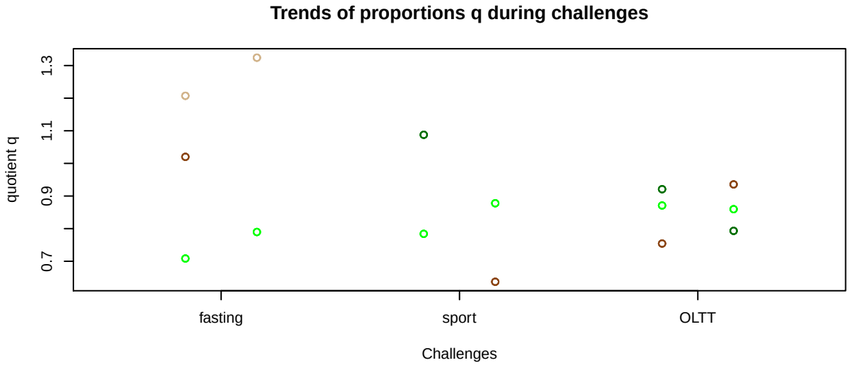
PC 20:0_22:6 / PC aa C42:6
Shapiro−Wilk Test of log quotients, pv: 0.79973; OK
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0.00367; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.5; sport: 1; OLTT: 1

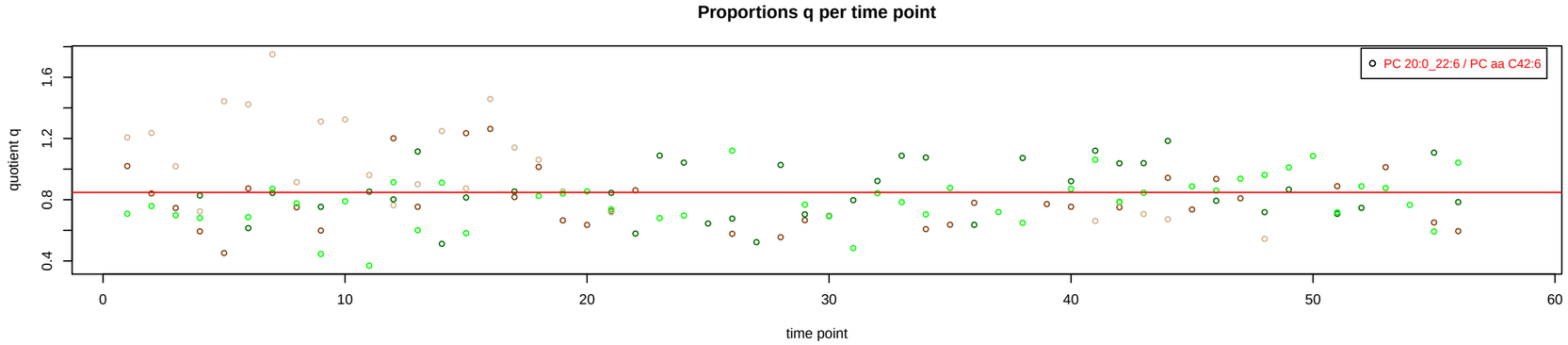












PC ae C30:0 = R

No independent Variable measured.

Qualitative composition

PC ae C30:0 consists of:
PC O−14:0_16:0, PC O−18:0_12:0, PC 10:0_19:0, PC 12:0_1
PC 13:0_16:0, PC 14:0_15:0, PC 20:0_9:0, PC 8:0_21:0,
[13C1]SM 33:0
and further compounds

PC ae C32:1 = PC 15:0_16:1 + PC 17:0_14:1 + R

PC 15:0_16:1, PC 17:0_14:1 excluded because of missingness > 75%

No independent Variable with coverage >0.25 out of PC 15:0_16:1, PC 17:0_14:1

Qualitative composition

PC ae C32:1 consists of:
PC 15:0_16:1, PC 17:0_14:1, PC O−14:0_18:1, PC O−16:0_1
PC O−18:0_14:1, PC O−20:1_12:0, PC 12:0_19:1, PC 13:0_1
PC 16:0_15:1
and further compounds

PC ae C32:2 = R

No independent Variable measured.

Qualitative composition

PC ae C32:2 consists of:
PC O−14:0_18:2, PC O−14:1_18:1, PC O−16:1_16:1, PC 13:
PC 15:1_16:1
and further compounds

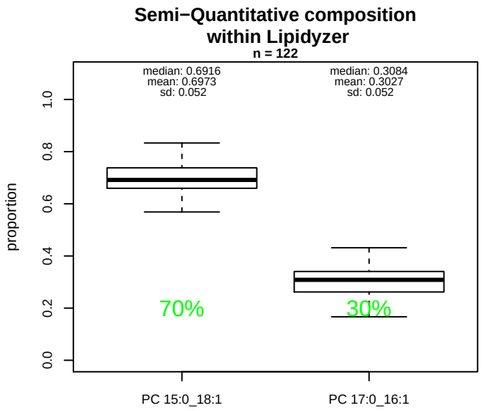
PC ae C34:0 = R

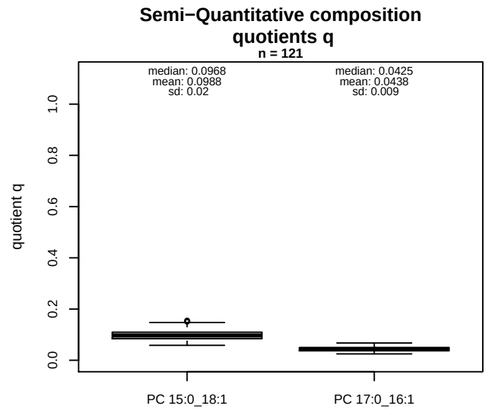
No independent Variable measured.

Qualitative composition

PC ae C34:0 consists of:
PC O−16:0_18:0, PC O−17:0_17:0, PC O−20:0_14:0, PC 10:
PC 11:0_22:0, PC 13:0_20:0, PC 15:0_18:0, PC 16:0_17:0,
PC 21:0_12:0
and further compounds

PC ae C34:1 = PC 15:0_18:1 + PC 17:0_16:1 + R





Semi−Quantitative composition: Lipidyzer

PC ae C34:1 consists of:
PC 15:0_18:1 69.7%
PC 17:0_16:1 30.3%
and of (not quantified):
PC O−16:0_18:1, PC O−18:0_16:1, PC O−20:0_14:1, PC O−
PC 13:0_20:1, PC 14:0_19:1, PC 14:1_19:0, PC 15:1_18:0,
[13C1]SM 37:1
and further compounds

Composition: mean of proportions q

conc(PC ae C34:1) * 0.0988 = conc(PC 15:0_18:1) [var(q)=0.0988]
Percentiles: 5%−>0.0705, 25%−>0.0843, 75%−>0.1097, 95%−>0.1373
conc(PC ae C34:1) * 0.0438 = conc(PC 17:0_16:1) [var(q)=0.0438]
Percentiles: 5%−>0.0307, 25%−>0.0371, 75%−>0.0499, 95%−>0.0601

Linear model

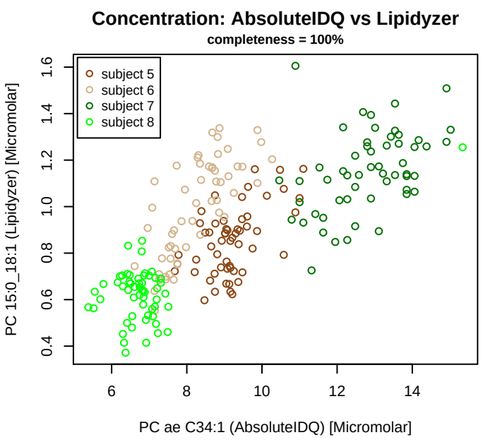
```
PC ae C34:1 ~ b * ( PC 15:0_18:1
   + PC 17:0_16:1 )
```

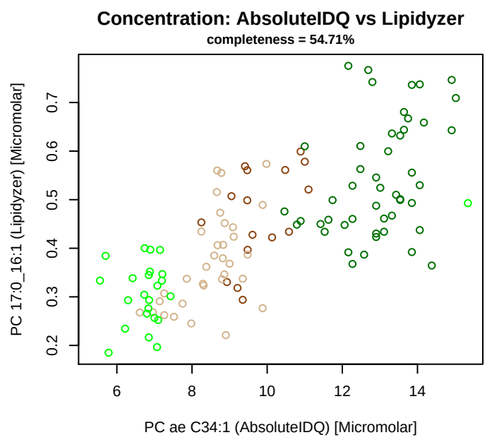
b = 4.14514

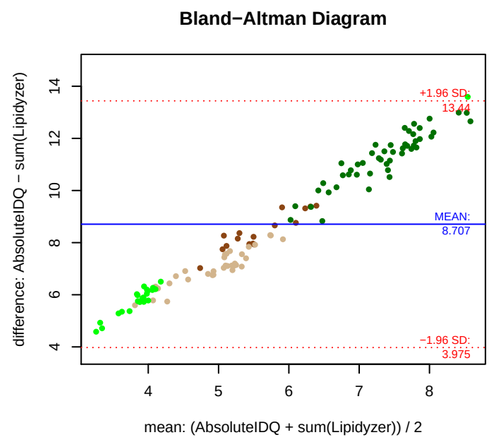
R^2 = 0.57752

Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	5.38	0.78	4.6
Max	15.34	2.26	13.08
Mean	9.27	1.45	7.82
Median	8.81	1.51	7.3
SD	2.43	0.35	2.08





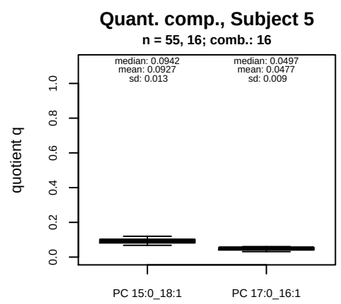


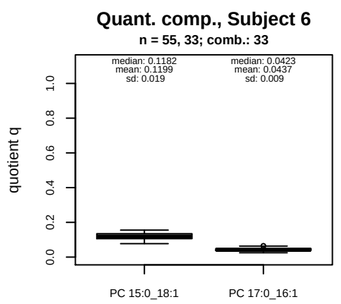
Stability of composition

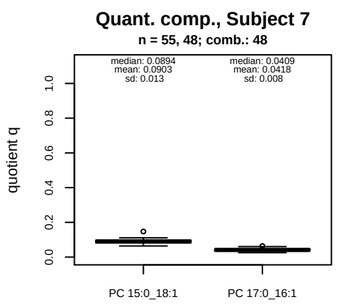
(PC 15:0_18:1 + PC 17:0_16:1) / PC ae C34:1
Shapiro−Wilk Test of log quotients, pv: 0.31322; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.0045; DIFFERENCE
Wilcoxon: Challenge; sport: 0.5; OLTT: 1

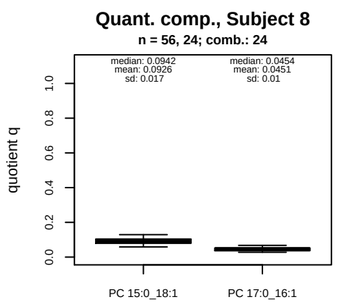
PC 17:0_16:1 / PC ae C34:1
Shapiro−Wilk Test of log quotients, pv: 0.65757; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.322; EQUAL
Wilcoxon: Challenge; sport: 0.75; OLTT: 1

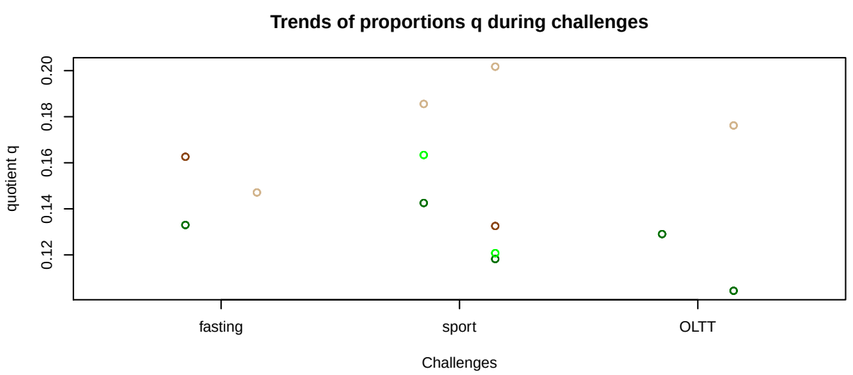
PC 15:0_18:1 / PC ae C34:1
Shapiro−Wilk Test of log quotients, pv: 0.37336; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.01068; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.625; OLTT: 0.875

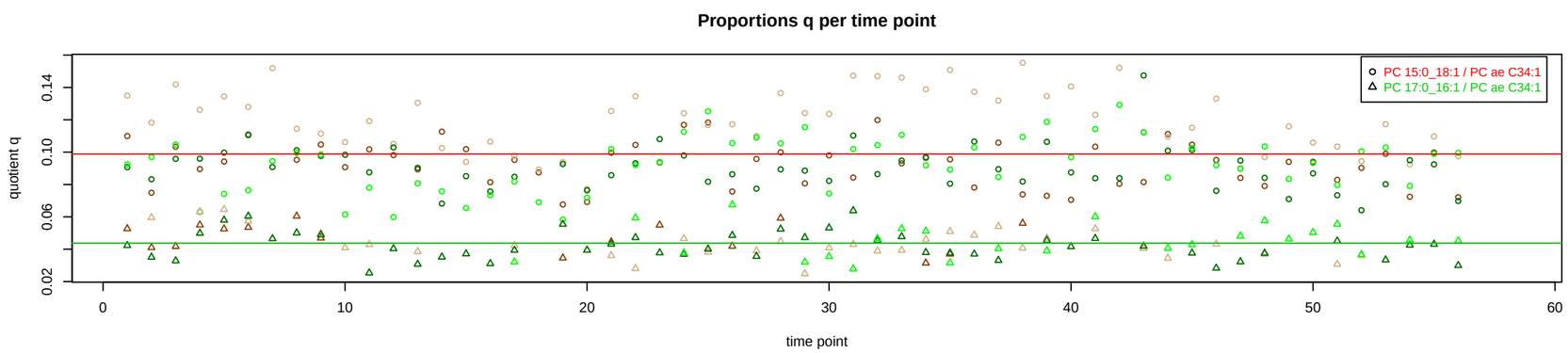




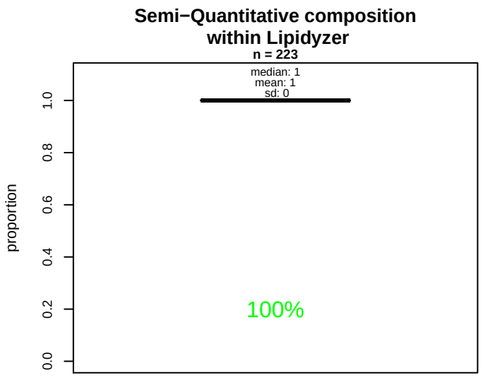


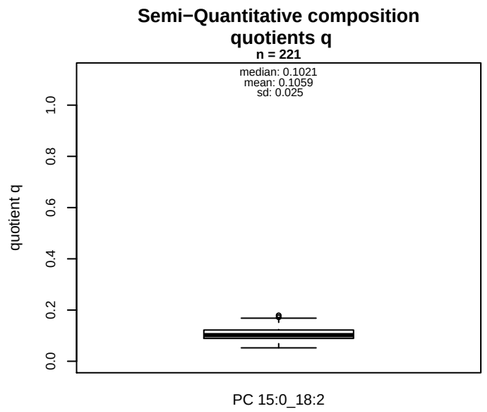






PC ae C34:2 = PC 15:0_18:2 + R





Semi−Quantitative composition: Lipidyzer

PC ae C34:2 consists of:
PC 15:0_18:2 100%
and of (not quantified):
PC O−16:0_18:2, PC O−16:1_18:1, PC O−20:1_14:1, PC 13:
PC 14:1_19:1, PC 15:1_18:1, PC 16:0_17:2, PC 16:1_17:1,
and further compounds

Composition: mean of proportions q

conc(PC ae C34:2) * 0.1059 = conc(PC 15:0_18:2) [var(q)=0.1059]
Percentiles: 5%−>0.0698, 25%−>0.0892, 75%−>0.1219, 95%−>0.1541

Linear model

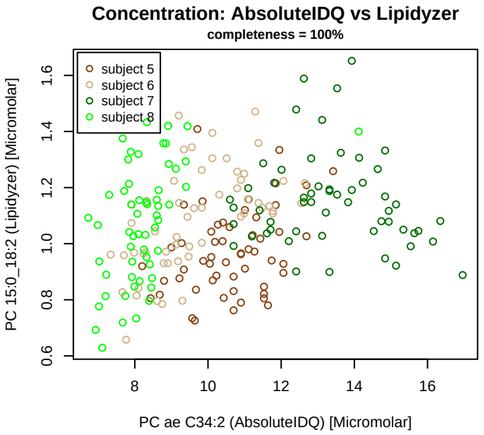
```
PC ae C34:2 ~ b * ( PC 15:0_18:2 )
```

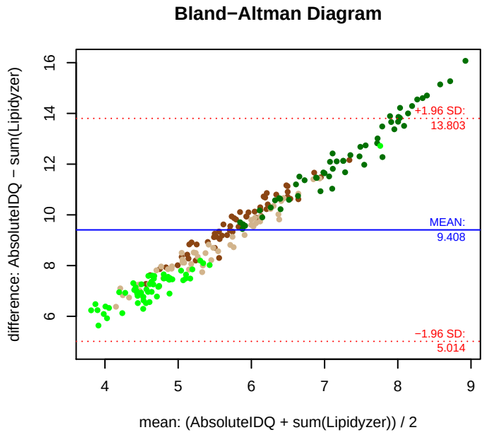
b = 3.24787

R^2 = 0.07136

Ranges

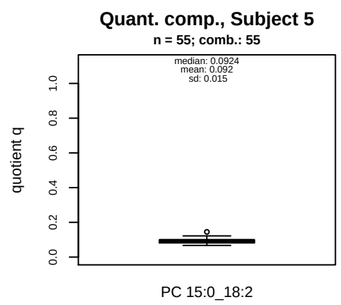
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	6.73	0.63	6.1
Max	16.96	1.65	15.31
Mean	10.48	1.07	9.41
Median	10.19	1.07	9.12
SD	2.28	0.19	2.1

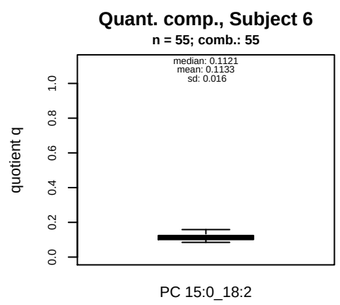


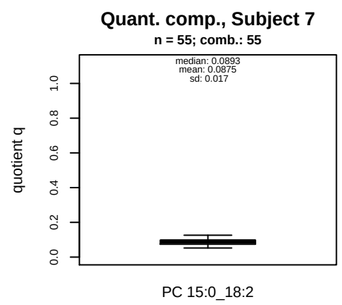


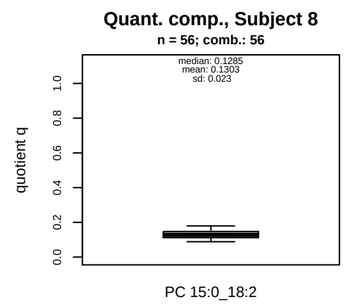
Stability of composition

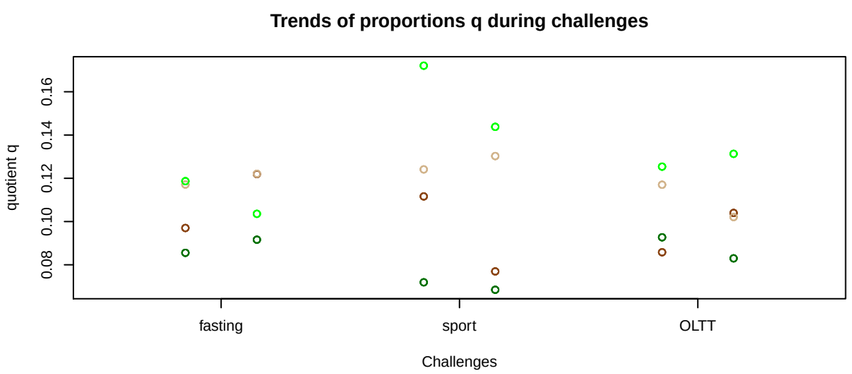
PC 15:0_18:2 / PC ae C34:2
Shapiro−Wilk Test of log quotients, pv: 0.62993; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.625; sport: 0.375; OLTT: 1

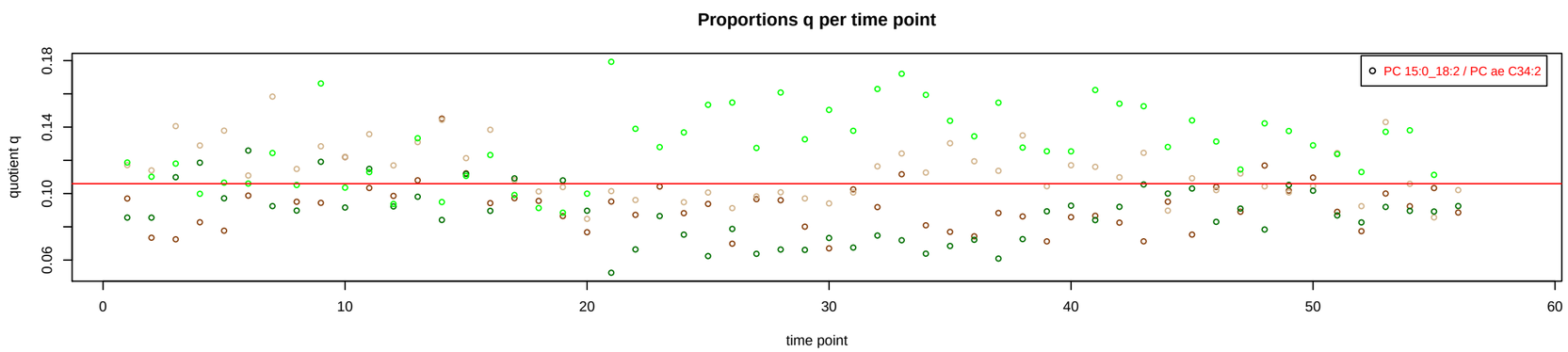












PC ae C34:3 = PC 15:0_18:3 + R

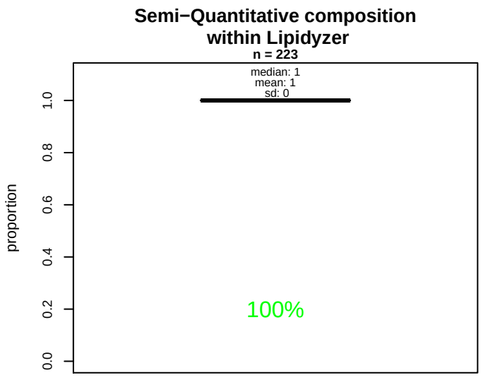
PC 15:0_18:3 excluded because of missingness > 75%

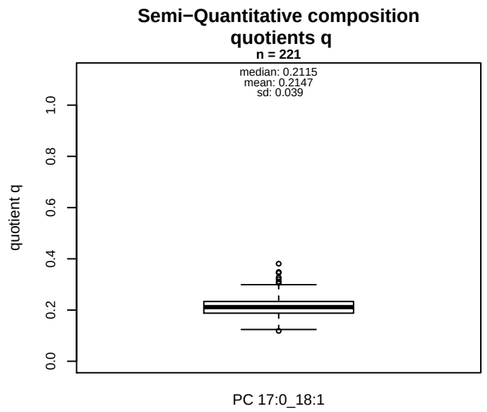
No independent Variable with coverage >0.25 out of PC 15:0_18:3

Qualitative composition

PC ae C34:3 consists of:
PC 15:0_18:3, PC O−16:0_18:3, PC O−16:1_18:2, PC 13:0_2
PC 16:1_17:2
and further compounds

PC ae C36:1 = PC 17:0_18:1 + R





Semi−Quantitative composition: Lipidyzer

PC ae C36:1 consists of:
PC 17:0_18:1 100%
and of (not quantified):
PC O−16:0_20:1, PC O−18:0_18:1, PC O−20:0_16:1, PC O−
PC 13:0_22:1, PC 14:1_21:0, PC 15:0_20:1, PC 15:1_20:0,
PC 16:0_19:1, PC 16:1_19:0, PC 17:1_18:0, PC 18:4_18:4,
[13C1]SM 39:1
and further compounds

Composition: mean of proportions q

conc(PC ae C36:1) * 0.2147 = conc(PC 17:0_18:1) [var(q)=0.2147]
Percentiles: 5%−>0.1601, 25%−>0.1877, 75%−>0.2335, 95%−>0.2878

Linear model

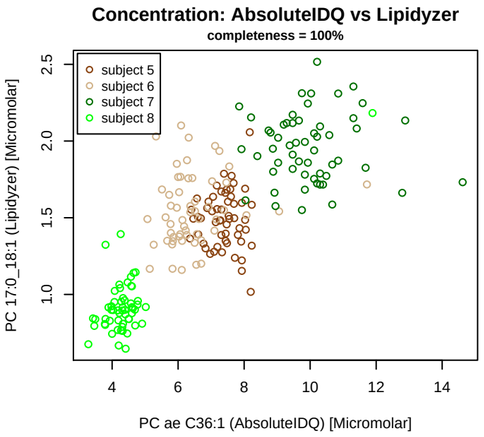
```
PC ae C36:1 ~ b * ( PC 17:0_18:1 )
```

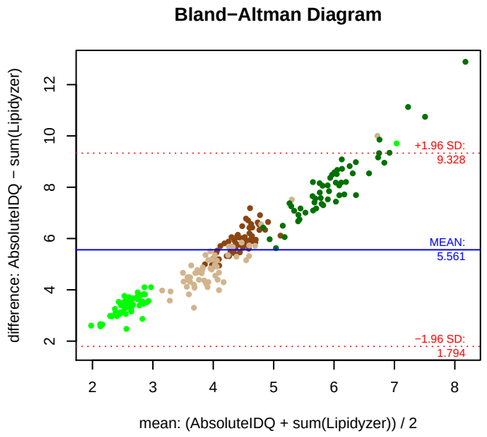
b = 4.23026

R^2 = 0.64372

Ranges

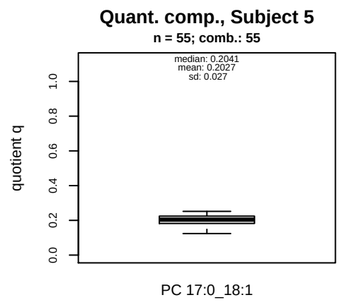
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	3.28	0.65	2.63
Max	14.62	2.52	12.1
Mean	7.04	1.48	5.56
Median	6.97	1.5	5.47
SD	2.25	0.42	1.82

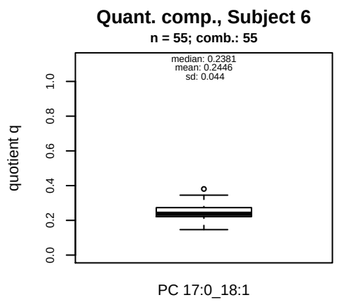


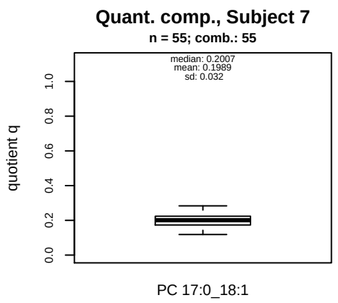


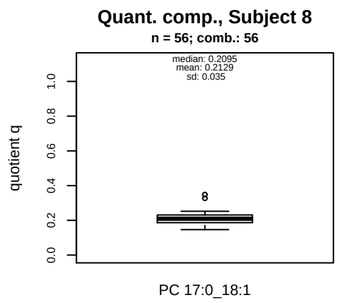
Stability of composition

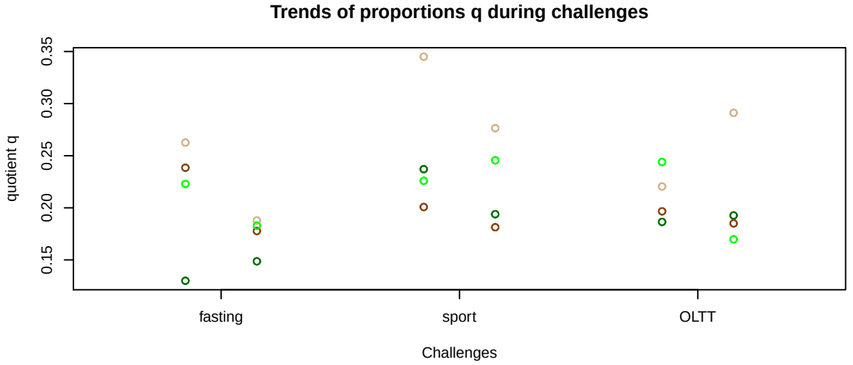
PC 17:0_18:1 / PC ae C36:1
Shapiro−Wilk Test of log quotients, pv: 0.04571; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.5455; EQUAL
Wilcoxon: Challenge; fasting: 0.25; sport: 0.375; OLTT: 0.875

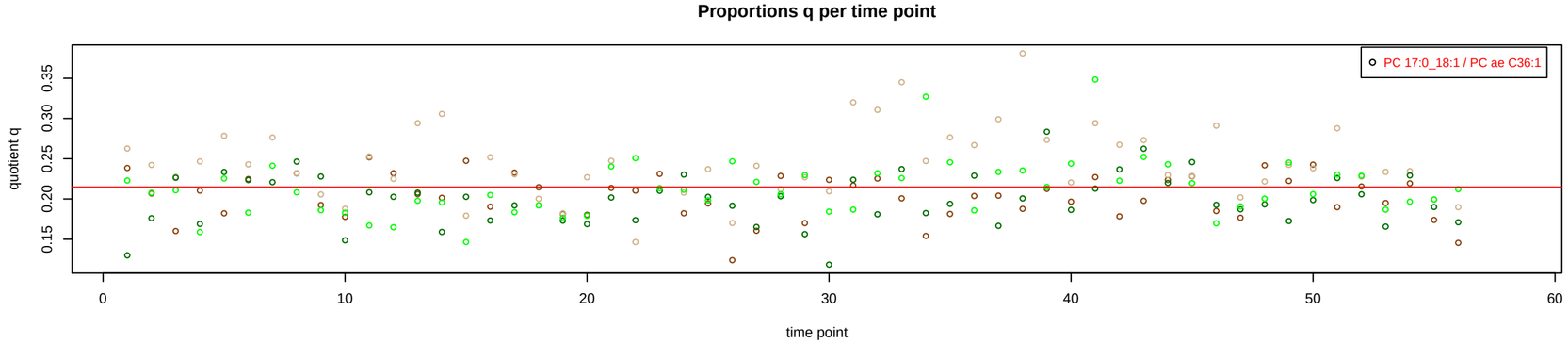




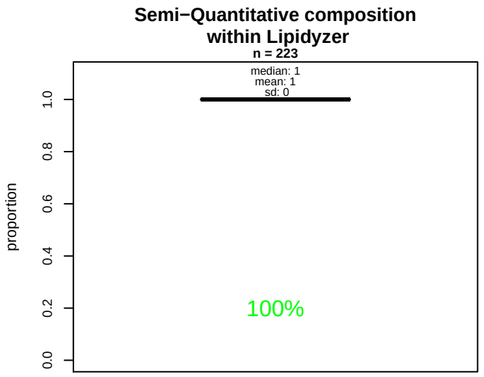


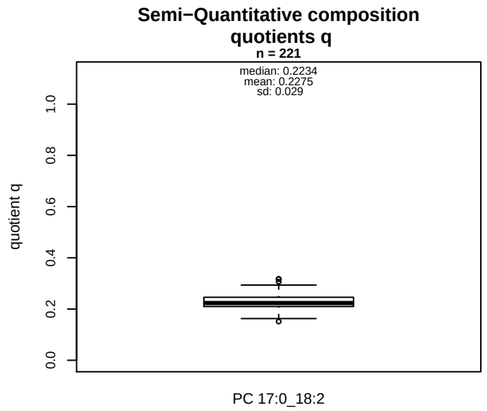






PC ae C36:2 = PC 17:0_18:2 + R





Semi−Quantitative composition: Lipidyzer

PC ae C36:2 consists of:
PC 17:0_18:2 100%
and of (not quantified):
PC O−16:0_20:2, PC O−18:0_18:2, PC O−18:1_18:1, PC O−PC 13:0_22:2, PC 15:0_20:2, PC 15:1_20:1, PC 16:1_19:1, [13C1]SM 39:2
and further compounds

Composition: mean of proportions q

conc(PC ae C36:2) * 0.2275 = conc(PC 17:0_18:2) [var(q)=0.2275]
Percentiles: 5%−>0.1837, 25%−>0.2098, 75%−>0.2459, 95%−>0.2799

Linear model

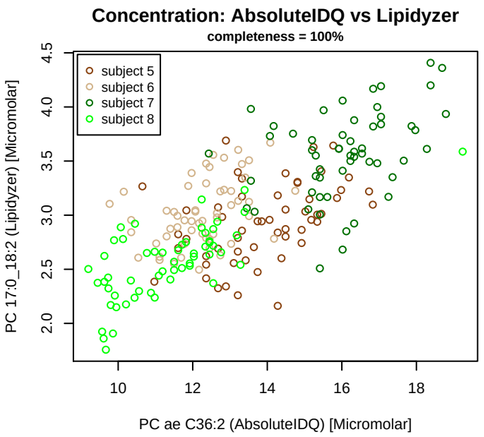
```
PC ae C36:2 ~ b * ( PC 17:0_18:2 )
```

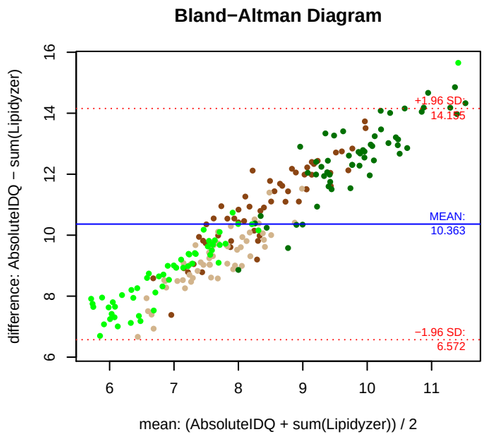
b = 3.27954

R^2 = 0.52816

Ranges

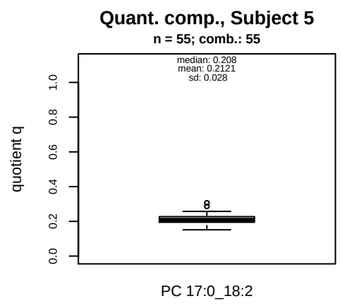
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	9.2	1.76	7.44
Max	19.24	4.41	14.83
Mean	13.38	3.02	10.36
Median	13.03	2.96	10.07
SD	2.27	0.51	1.76

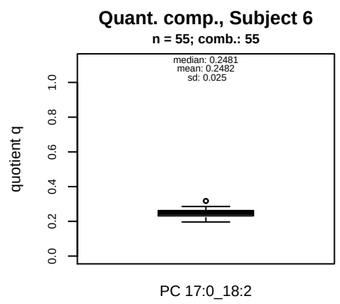


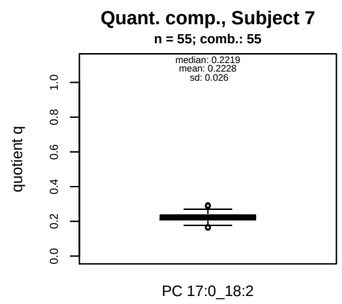


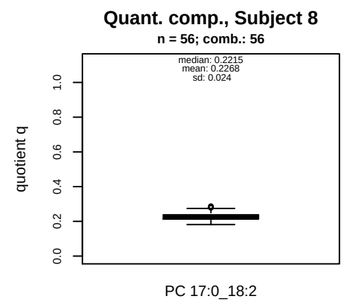
Stability of composition

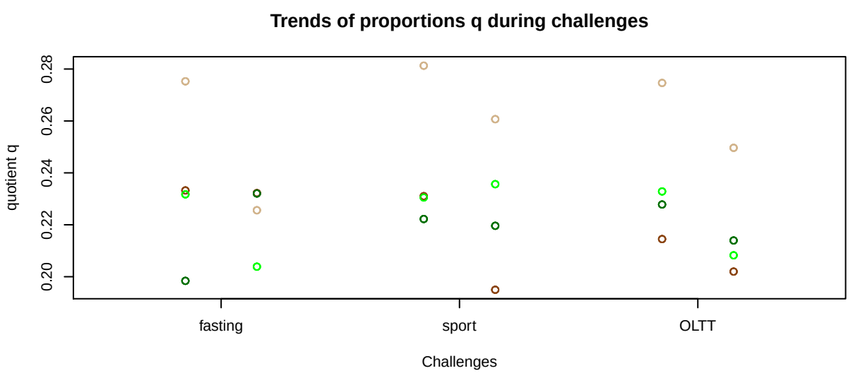
PC 17:0_18:2 / PC ae C36:2
Shapiro−Wilk Test of log quotients, pv: 0.867; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.19747; EQUAL
Wilcoxon: Challenge; fasting: 0.625; sport: 0.375; OLTT: 0.125

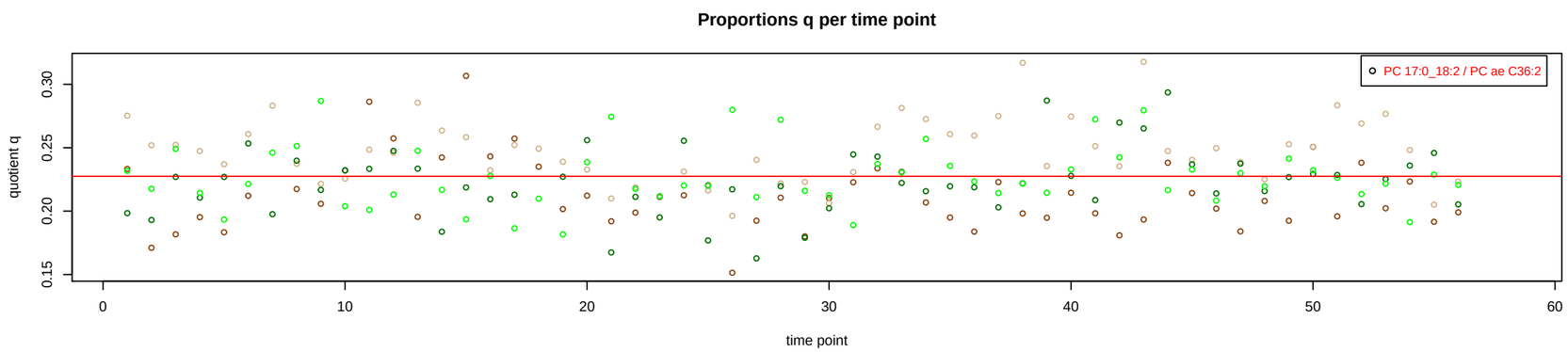








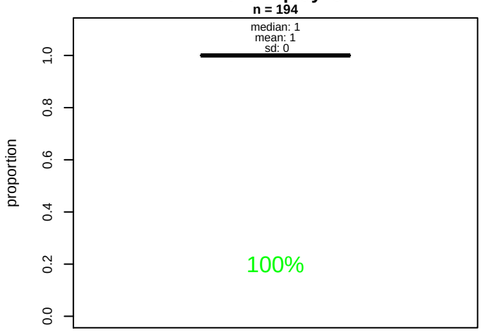




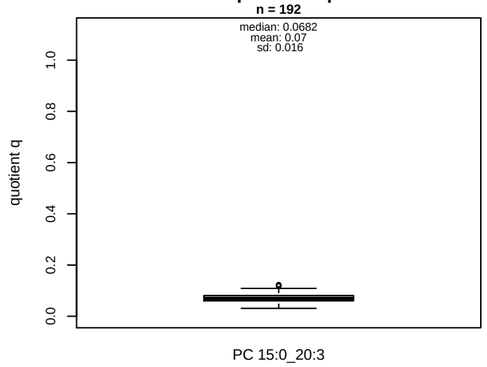
PC ae C36:3 = PC 15:0_20:3 + PC 17:0_18:3 + R

PC 17:0_18:3 excluded because of missingness > 75%

Semi−Quantitative composition within Lipidyzer



Semi−Quantitative composition quotients q



Semi−Quantitative composition: Lipidyzer

PC ae C36:3 consists of:
PC 15:0_20:3 100%
and of (not quantified):
PC 17:0_18:3, PC O−16:0_20:3, PC O−18:0_18:3, PC O−18:
PC O−16:1_20:2, PC 15:1_20:2, PC 17:1_18:2, PC 17:2_18:
and further compounds

Composition: mean of proportions q

conc(PC ae C36:3) * 0.07 = conc(PC 15:0_20:3) [var(q)=0.07]
Percentiles: 5%−>0.0458, 25%−>0.0603, 75%−>0.0809, 95%−>0.095

Linear model

```
PC ae C36:3 ~ b * ( PC 15:0_20:3 )
```

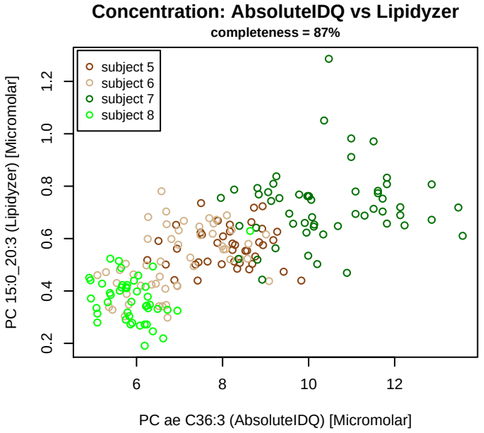
b = 8.36338

R^2 = 0.49946

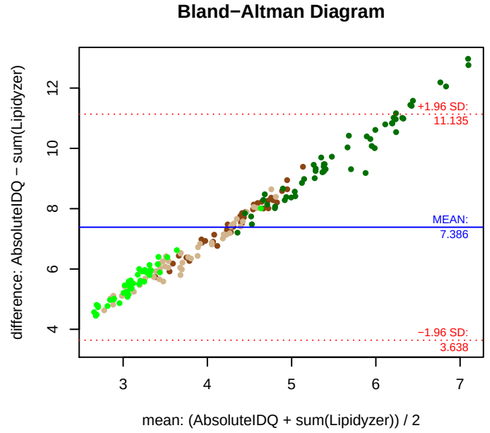
Ranges

Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	4.88	0.19	4.69
Max	13.58	1.29	12.29
Mean	7.83	0.55	7.28
Median	7.65	0.54	7.11
SD	1.97	0.17	1.8

Concentration: AbsoluteIDQ vs Lipidyzer



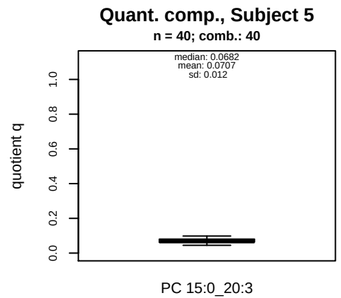
Bland−Altman Diagram



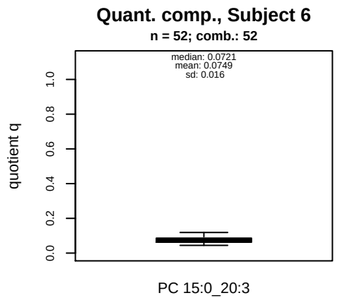
Stability of composition

PC 15:0_20:3 / PC ae C36:3
Shapiro−Wilk Test of log quotients, pv: 0.11199; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00182; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.25; sport: 0.75; OLTT: 0.625

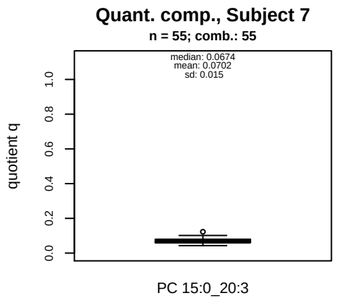
Quant. comp., Subject 5



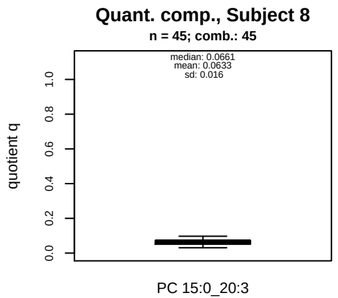
Quant. comp., Subject 6



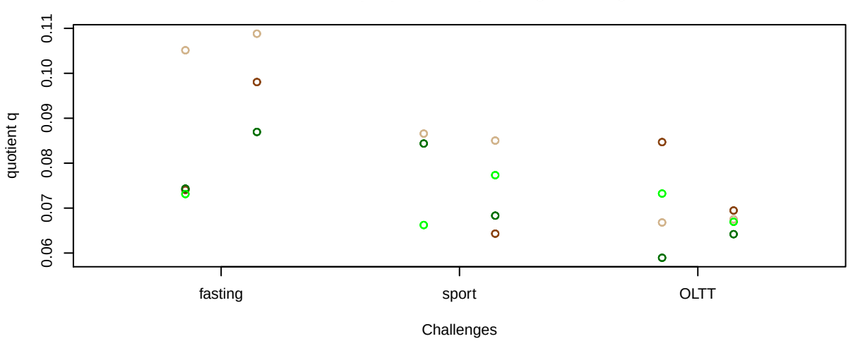
Quant. comp., Subject 7



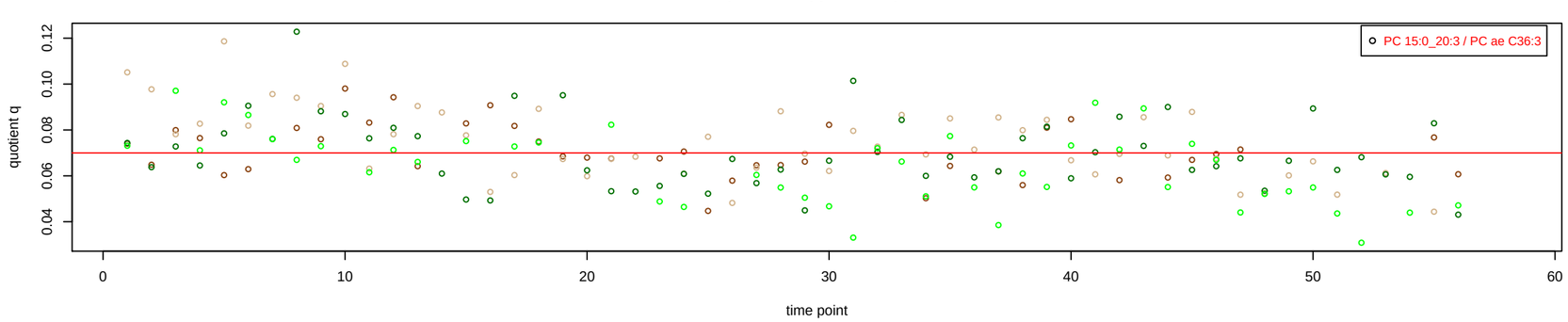
Quant. comp., Subject 8



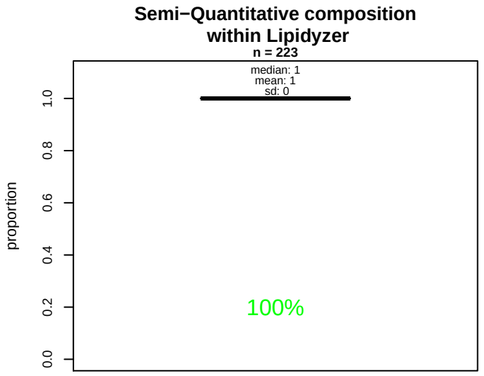
Trends of proportions q during challenges

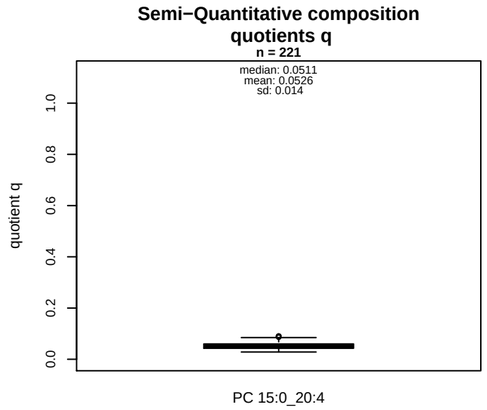


Proportions q per time point



PC ae C36:4 = PC 15:0_20:4 + R





Semi−Quantitative composition: Lipidyzer

PC ae C36:4 consists of:
PC 15:0_20:4 100%
and of (not quantified):
PC O−16:0_20:4, PC O−16:1_20:3, PC O−18:0_18:4, PC O−
PC O−18:2_18:2, PC 13:0_22:4, PC 15:1_20:3, PC 17:0_18:
PC 17:2_18:2
and further compounds

Composition: mean of proportions q

conc(PC ae C36:4) * 0.0526 = conc(PC 15:0_20:4) [var(q)=0.0526]
Percentiles: 5%−>0.0339, 25%−>0.0429, 75%−>0.0599, 95%−>0.0793

Linear model

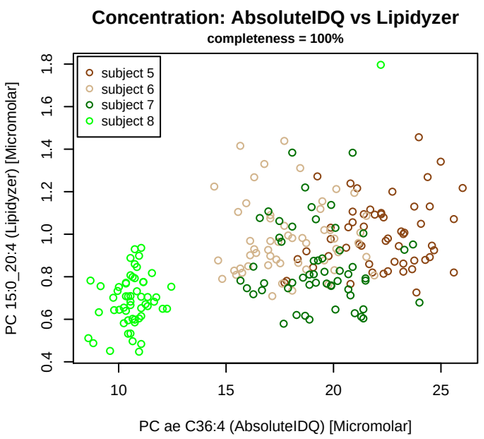
```
PC ae C36:4 ~ b * ( PC 15:0_20:4 )
```

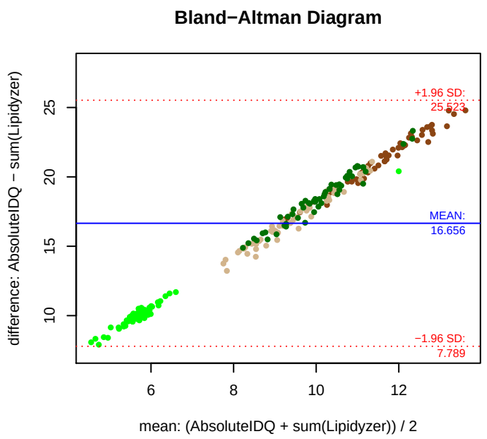
b = 11.15708

R^2 = 0.25993

Ranges

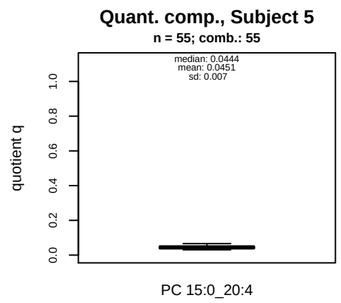
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	8.59	0.45	8.14
Max	26.01	1.8	24.21
Mean	17.54	0.88	16.66
Median	18.55	0.86	17.69
SD	4.63	0.21	4.42

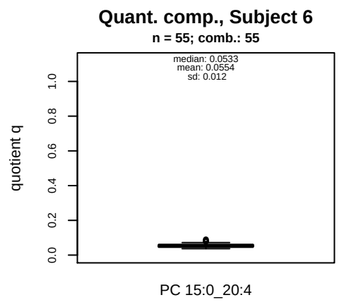


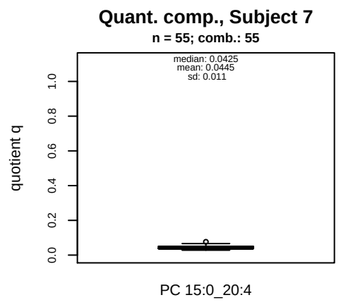


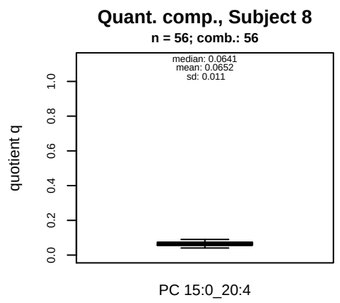
Stability of composition

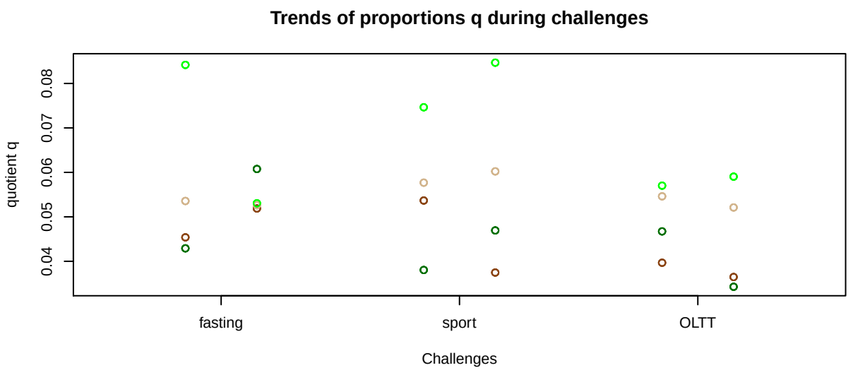
PC 15:0_20:4 / PC ae C36:4
Shapiro−Wilk Test of log quotients, pv: 0.32439: OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 1; sport: 0.875; OLTT: 0.25

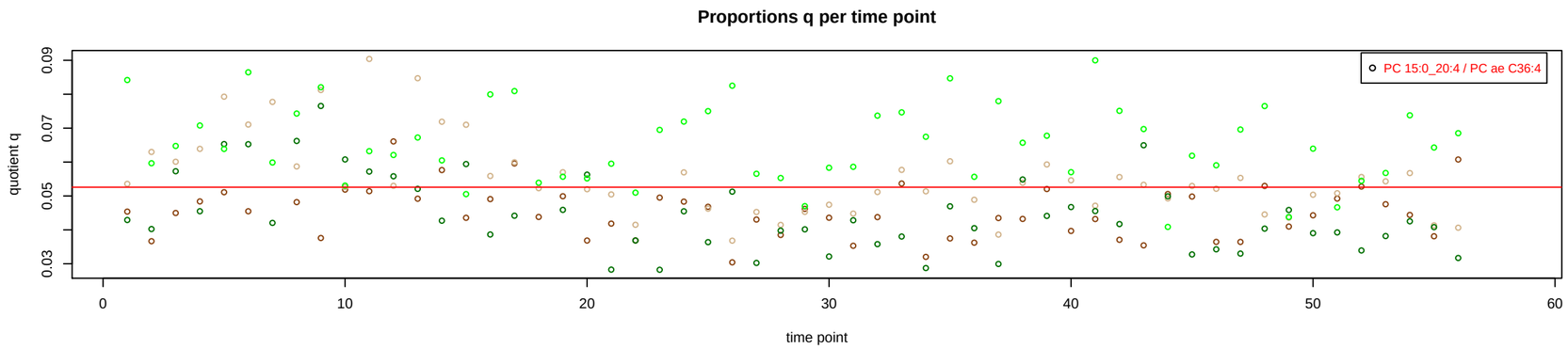












PC ae C36:5 = PC 15:0_20:5 + R

PC 15:0_20:5 excluded because of missingness > 75%

No independent Variable with coverage >0.25 out of PC 15:0_20:5

Qualitative composition

PC ae C36:5 consists of:
PC 15:0_20:5, PC O−16:0_20:5, PC O−16:1_20:4, PC O−18:
PC O−18:2_18:3, PC 15:1_20:4, PC 17:1_18:4, PC 17:2_18:
and further compounds

PC ae C38:0 = PC 18:2_20:5 + R

PC 18:2_20:5 excluded because of missingness > 75%

No independent Variable with coverage >0.25 out of PC 18:2_20:5

Qualitative composition

PC ae C38:0 consists of:
PC 18:2_20:5, PC O−16:0_22:0, PC O−18:0_20:0, PC 15:0_2
PC 16:0_21:0, PC 17:0_20:0, PC 18:0_19:0, PC 16:1_22:6,
PC 18:4_20:3
and further compounds

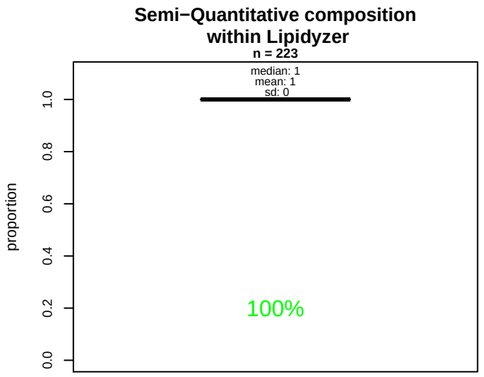
PC ae C38:2 = R

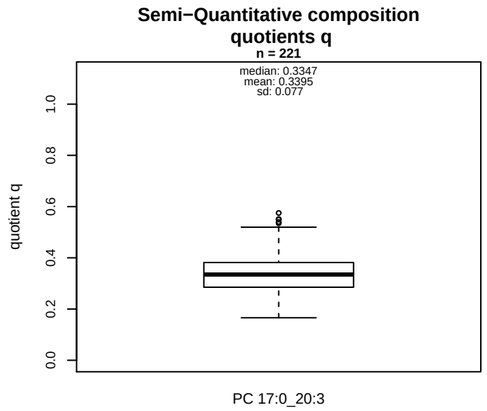
No independent Variable measured.

Qualitative composition

PC ae C38:2 consists of:
PC O−16:0_22:2, PC O−18:0_20:2, PC O−18:1_20:1, PC O−
PC O−16:1_22:1, PC 15:0_22:2, PC 15:1_22:1, PC 17:0_20:2
PC 17:1_20:1, PC 17:2_20:0, PC 18:1_19:1, PC 18:2_19:0,
PC 18:4_20:5
and further compounds

PC ae C38:3 = PC 17:0_20:3 + R





Semi−Quantitative composition: Lipidyzer

PC ae C38:3 consists of:
PC 17:0_20:3 100%
and of (not quantified):
PC O−18:0_20:3, PC O−16:1_22:2, PC O−18:1_20:2, PC O−
PC O−18:3_20:0, PC 15:1_22:2, PC 17:1_20:2, PC 17:2_20:
PC 18:3_19:0
and further compounds

Composition: mean of proportions q

conc(PC ae C38:3) * 0.3395 = conc(PC 17:0_20:3) [var(q)=0.3395]
Percentiles: 5%−>0.2248, 25%−>0.2852, 75%−>0.3816, 95%−>0.4767

Linear model

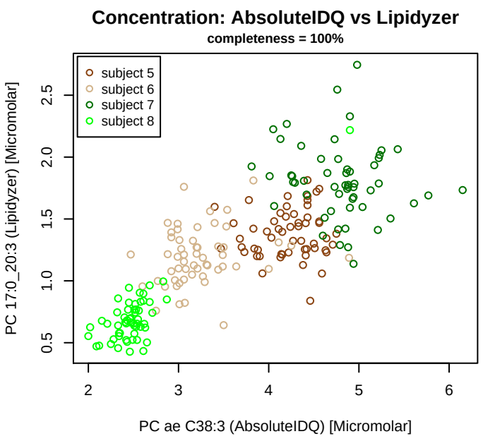
```
PC ae C38:3 ~ b * ( PC 17:0_20:3 )
```

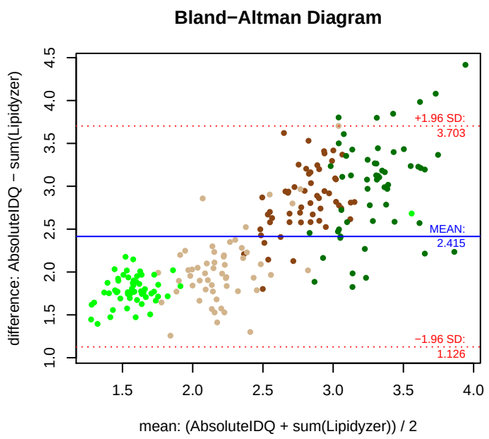
b = 1.66896

R^2 = 0.64485

Ranges

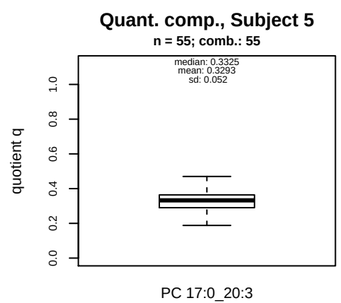
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	2	0.43	1.57
Max	6.15	2.75	3.4
Mean	3.68	1.27	2.41
Median	3.73	1.27	2.46
SD	0.97	0.47	0.5

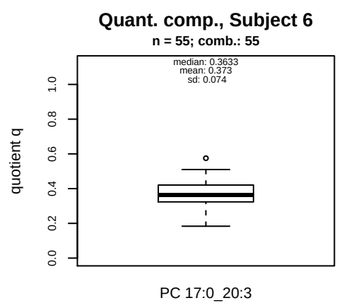


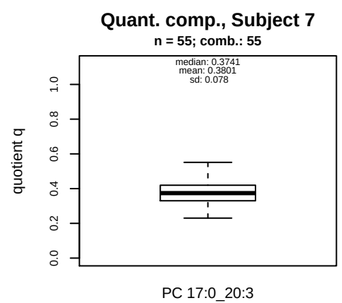


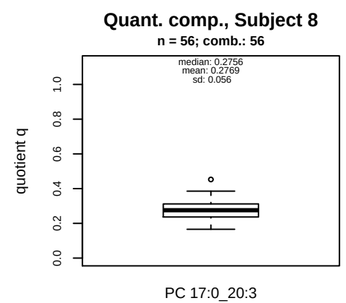
Stability of composition

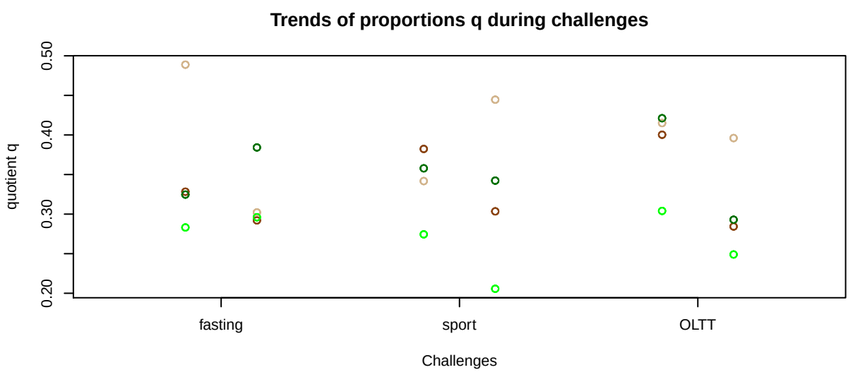
PC 17:0_20:3 / PC ae C38:3
Shapiro−Wilk Test of log quotients, pv: 0.30664; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.00011; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.875; sport: 0.875; OLTT: 0.125

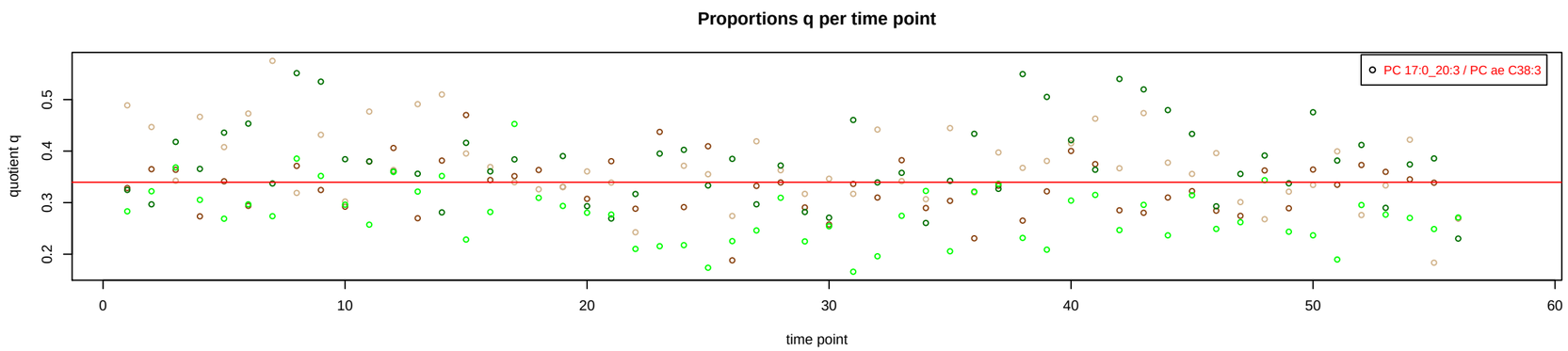




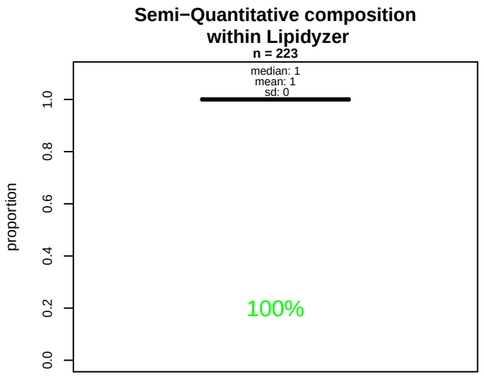


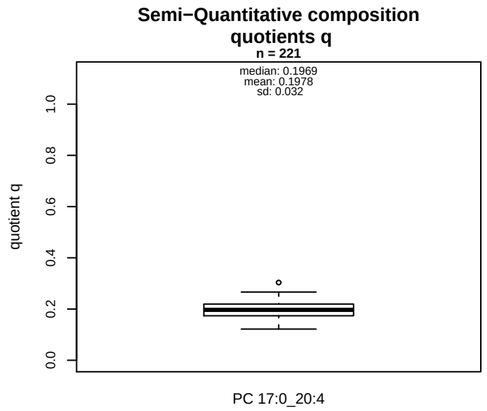






PC ae C38:4 = PC 17:0_20:4 + R





Semi−Quantitative composition: Lipidyzer

PC ae C38:4 consists of:
PC 17:0_20:4 100%
and of (not quantified):
PC O−16:0_22:4, PC O−18:0_20:4, PC O−20:0_18:4, PC O−
PC O−18:2_20:2, PC O−20:1_18:3, PC 15:0_22:4, PC 17:1_2
PC 18:4_19:0
and further compounds

Composition: mean of proportions q

conc(PC ae C38:4) * 0.1978 = conc(PC 17:0_20:4) [var(q)=0.1978]
Percentiles: 5%−>0.1495, 25%−>0.1737, 75%−>0.2195, 95%−>0.2547

Linear model

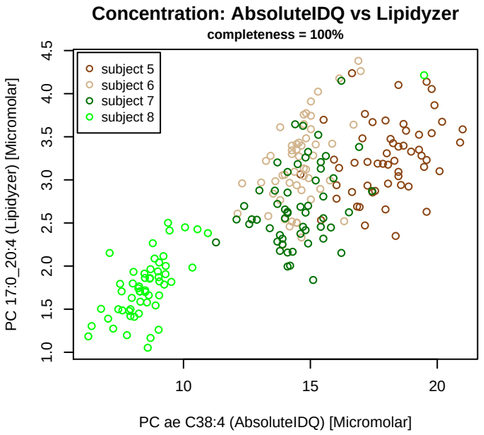
```
PC ae C38:4 ~ b * ( PC 17:0_20:4 )
```

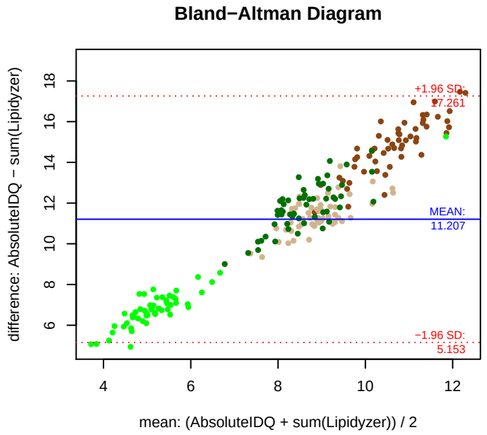
b = 3.91691

R^2 = 0.64147

Ranges

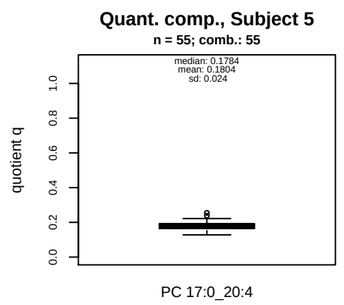
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	6.25	1.05	5.2
Max	21	4.38	16.62
Mean	13.93	2.73	11.2
Median	14.55	2.81	11.74
SD	3.65	0.75	2.91

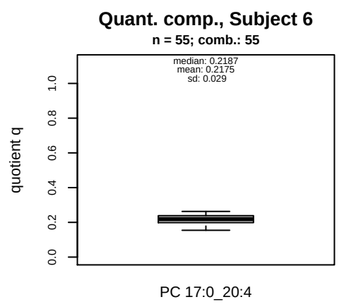


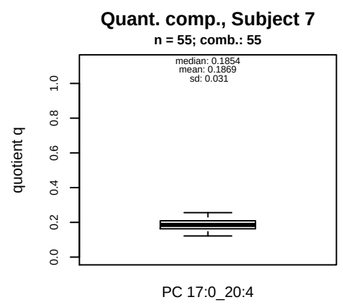


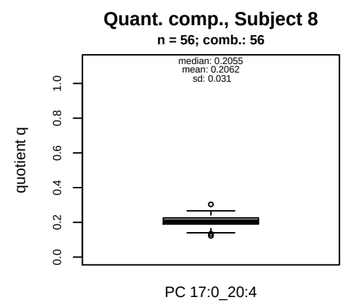
Stability of composition

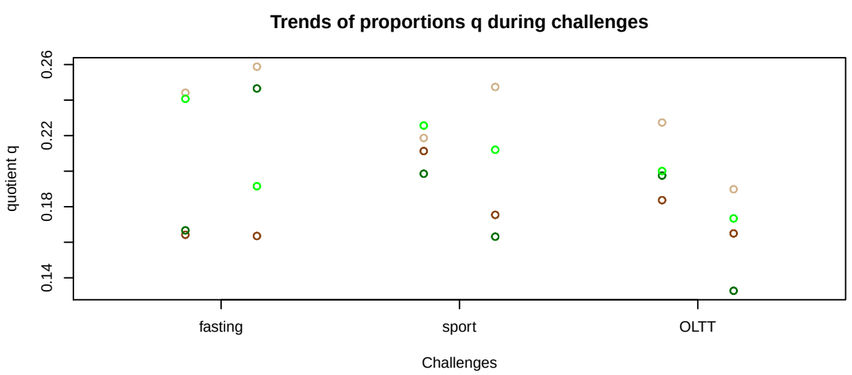
PC 17:0_20:4 / PC ae C38:4
Shapiro−Wilk Test of log quotients, pv: 0.19617; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.01837; EQUAL
Wilcoxon: Challenge; fasting: 0.875; sport: 0.375; OLTT: 0.125

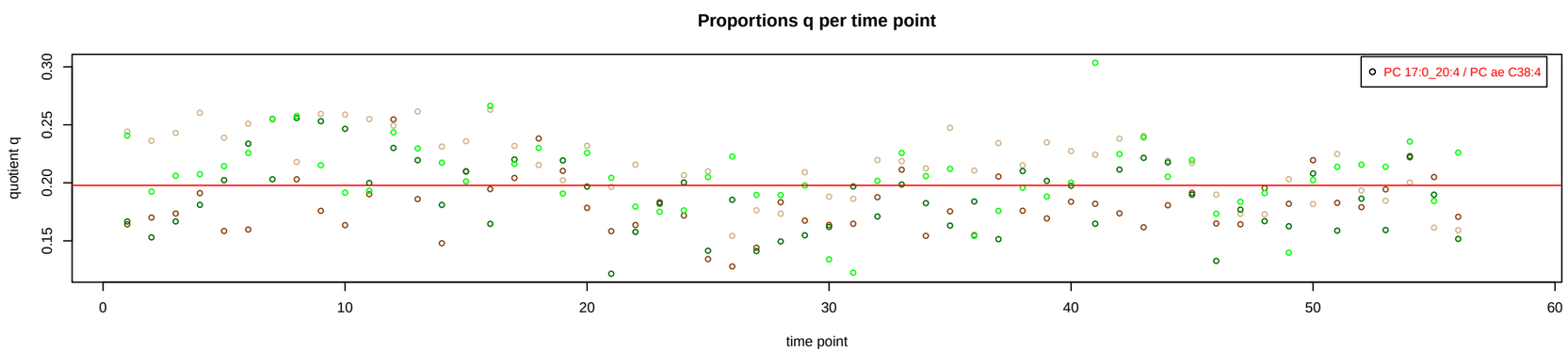






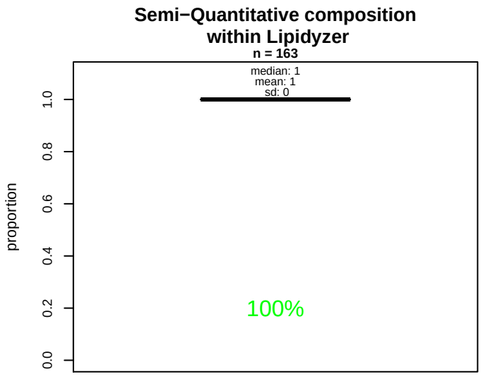


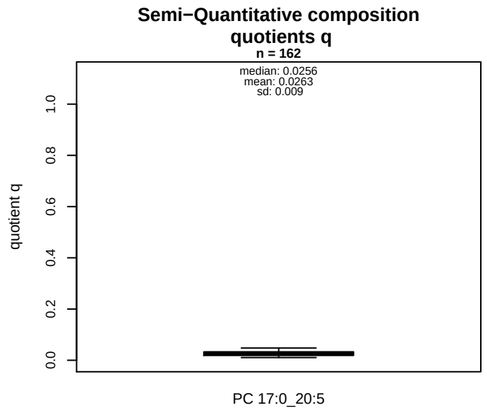




PC ae C38:5 = PC 15:0_22:5 + PC 17:0_20:5 + R

PC 15:0_22:5 excluded because of missingness > 75%





Semi−Quantitative composition: Lipidyzer

PC ae C38:5 consists of:
PC 17:0_20:5 100%
and of (not quantified):
PC 15:0_22:5, PC O−16:0_22:5, PC O−16:1_22:4, PC O−18:
PC O−18:1_20:4, PC O−18:2_20:3, PC O−18:4_20:1, PC 15:
PC 18:4_19:1
and further compounds

Composition: mean of proportions q

conc(PC ae C38:5) * 0.0263 = conc(PC 17:0_20:5) [var(q)=0.0263]
Percentiles: 5%−>0.0145, 25%−>0.0191, 75%−>0.0328, 95%−>0.0408

Linear model

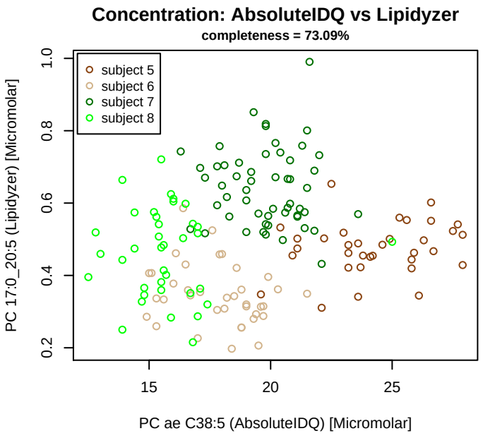
```
PC ae C38:5 ~ b * ( PC 17:0_20:5 )
```

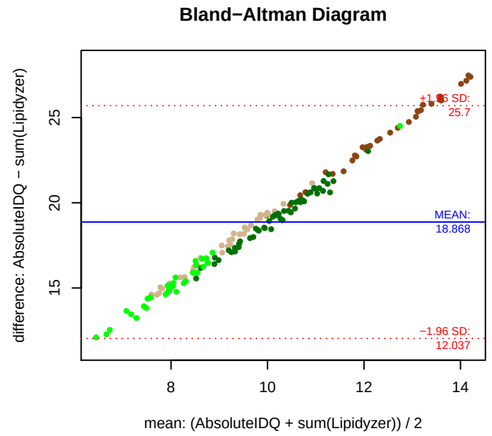
b = 3.44394

R^2 = 0.02174

Ranges

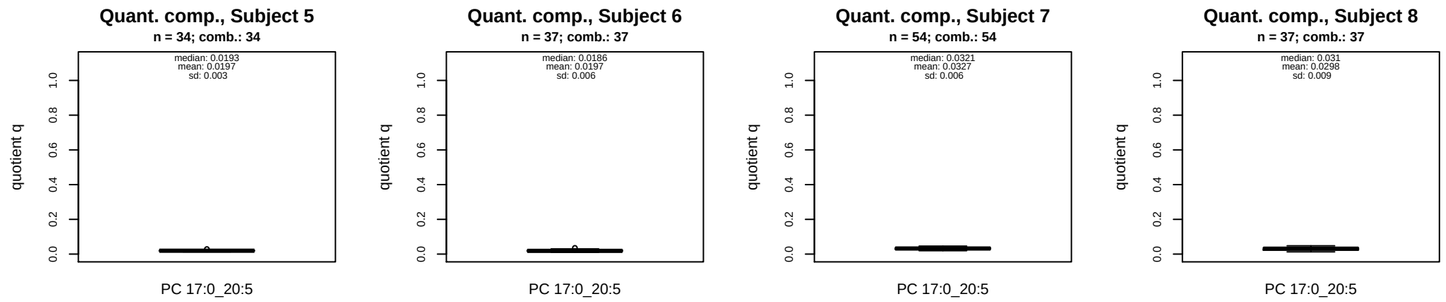
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	12.5	0.2	12.3
Max	27.9	0.99	26.91
Mean	19.34	0.5	18.84
Median	19	0.5	18.5
SD	3.67	0.15	3.52

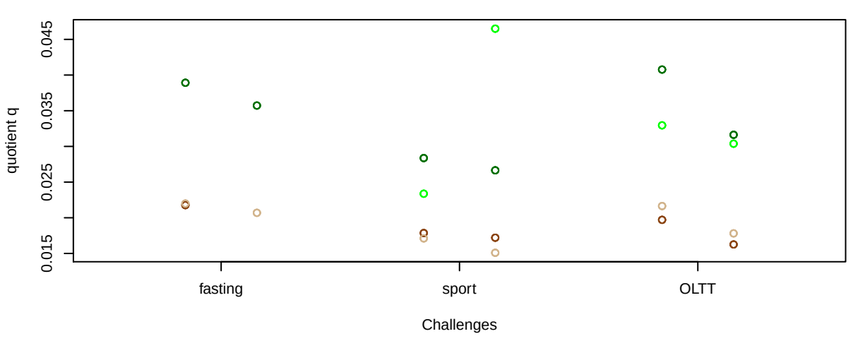


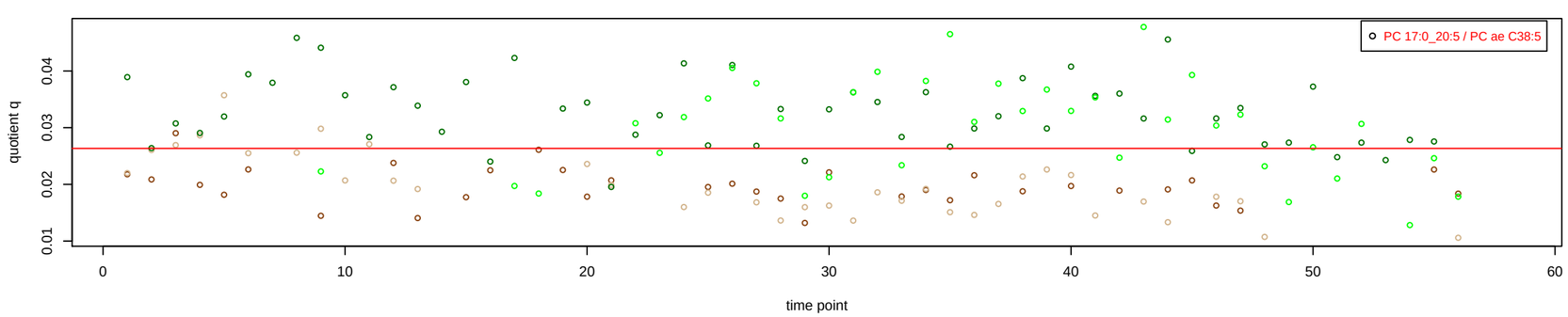


Stability of composition

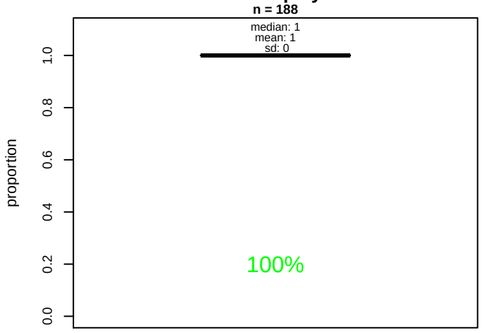
PC 17:0_20:5 / PC ae C38:5
Shapiro−Wilk Test of log quotients, pv: 0.02234; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.5; sport: 0.875; OLTT: 0.125

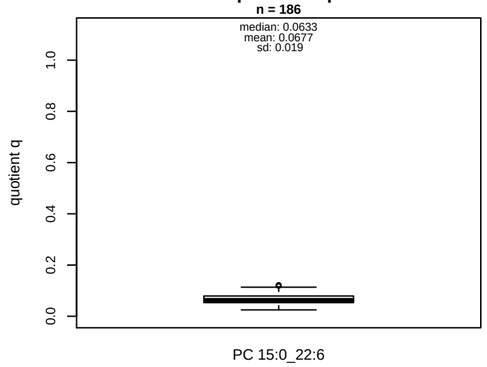






PC ae C38:6 = PC 15:0_22:6 + R





Semi−Quantitative composition: Lipidyzer

PC ae C38:6 consists of:
PC 15:0_22:6 100%
and of (not quantified):
PC O−16:0_22:6, PC O−18:1_20:5, PC O−18:2_20:5, PC 17:
PC 17:2_20:4
and further compounds

Composition: mean of proportions q

conc(PC ae C38:6) * 0.0677 = conc(PC 15:0_22:6) [var(q)=0.0677]
Percentiles: 5%−>0.0433, 25%−>0.0532, 75%−>0.0786, 95%−>0.1084

Linear model

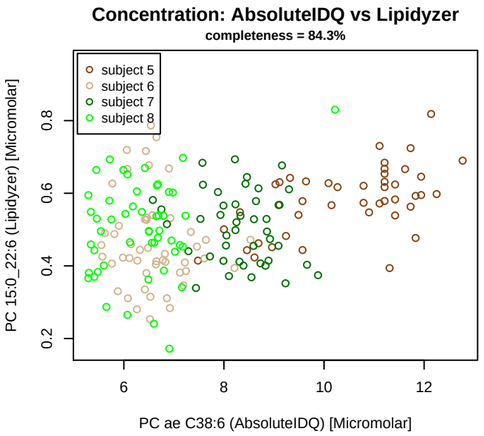
```
PC ae C38:6 ~ b * ( PC 15:0_22:6 )
```

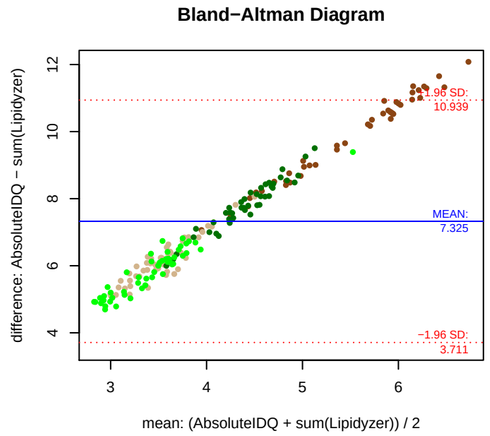
b = 5.55836

R^2 = 0.12603

Ranges

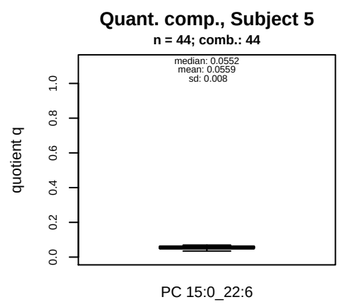
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	5.29	0.17	5.12
Max	12.77	0.96	11.81
Mean	7.85	0.51	7.34
Median	7.32	0.51	6.81
SD	1.87	0.12	1.75

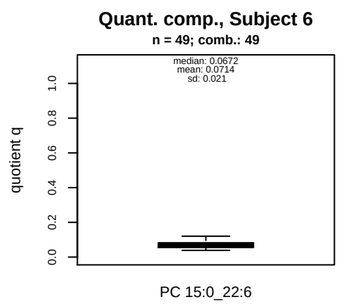


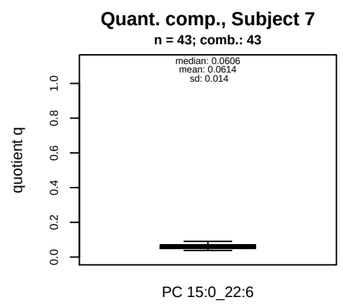


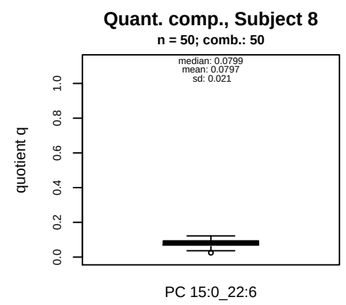
Stability of composition

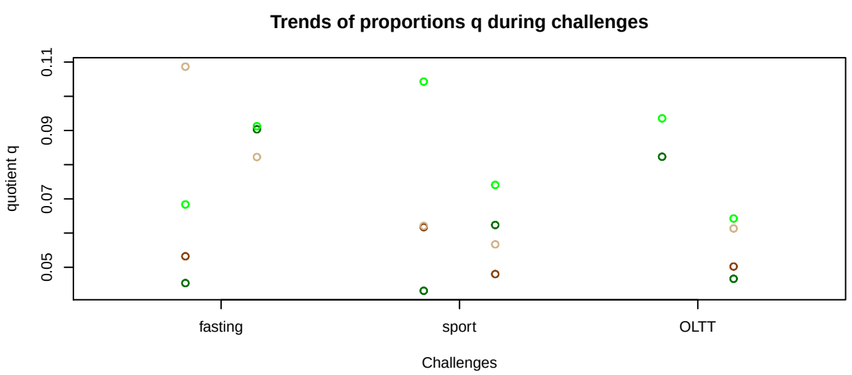
PC 15:0_22:6 / PC ae C38:6
Shapiro−Wilk Test of log quotients, pv: 0.22571; OK
SW: no; Kruskal: Comp. ~ Subject_ID −> pv = 0; DIFFERENCE
Wilcoxon: Challenge; fasting: 0.75; sport: 0.625; OLTT: 0.5

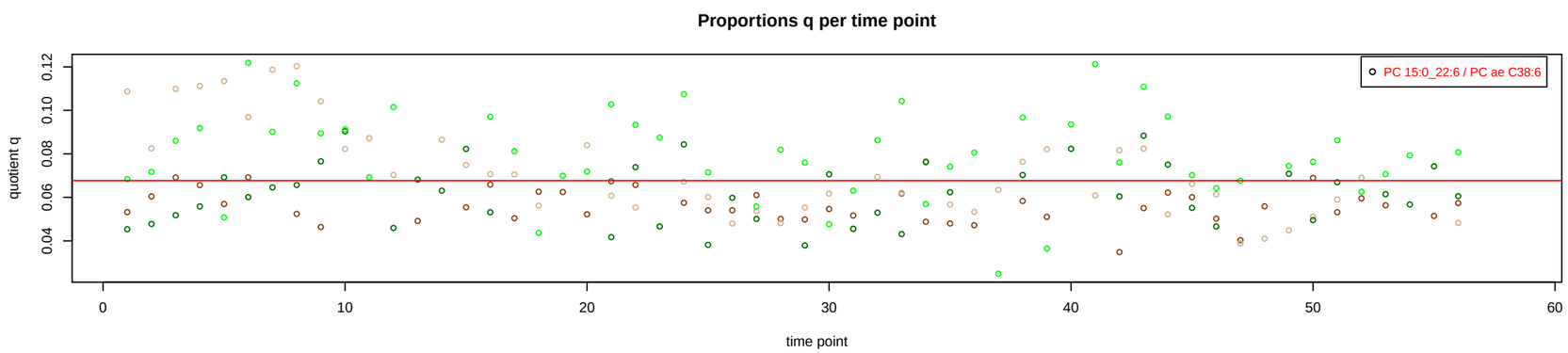




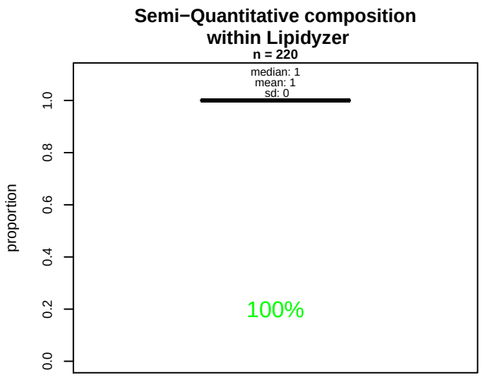


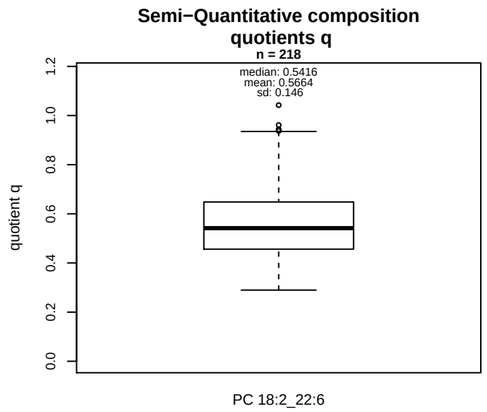






PC ae C40:1 = PC 18:2_22:6 + R





Semi−Quantitative composition: Lipidyzer

PC ae C40:1 consists of:
PC 18:2_22:6 100%
and of (not quantified):
PC O−18:0_22:1, PC O−18:1_22:0, PC O−20:0_20:1, PC 17:
PC 17:1_22:0, PC 18:1_21:0, PC 19:0_20:1, PC 19:1_20:0,
PC 20:4_20:4
and further compounds

Composition: mean of proportions q

conc(PC ae C40:1) * 0.5664 = conc(PC 18:2_22:6) [var(q)=0.5664]
Percentiles: 5%−>0.3782, 25%−>0.4566, 75%−>0.648, 95%−>0.8648

Linear model

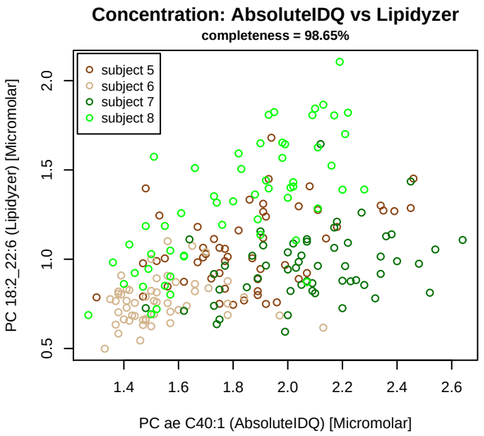
```
PC ae C40:1 ~ b * ( PC 18:2_22:6 )
```

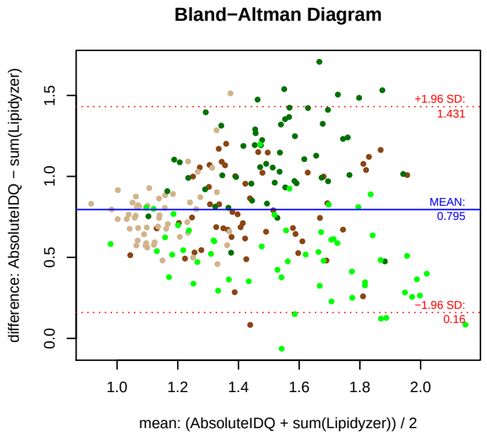
b = 0.44624

R^2 = 0.20278

Ranges

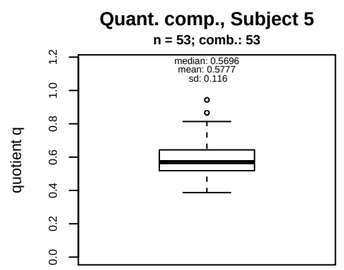
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	1.27	0.5	0.77
Max	2.64	2.11	0.53
Mean	1.82	1.03	0.79
Median	1.8	0.96	0.84
SD	0.31	0.31	0

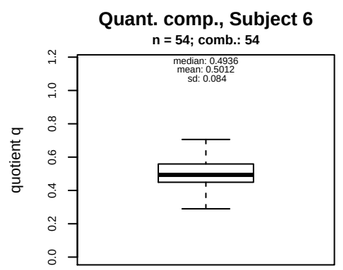


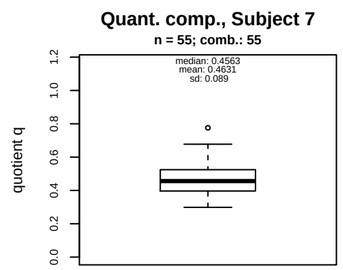


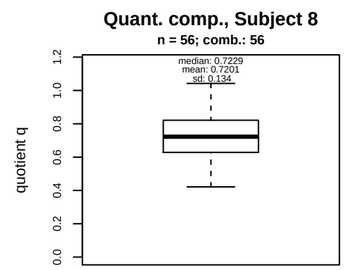
Stability of composition

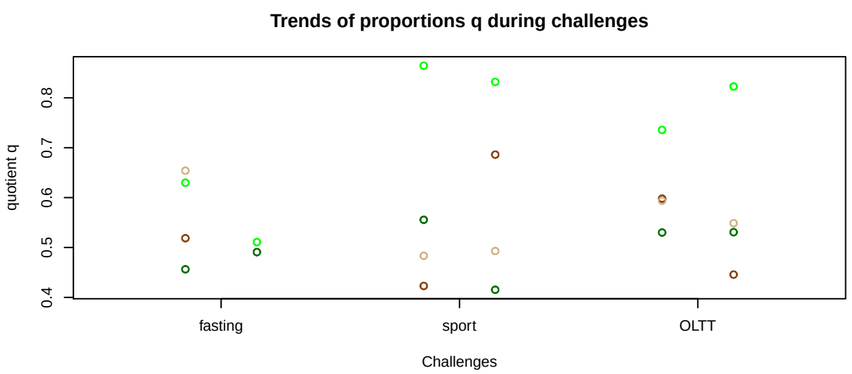
PC 18:2_22:6 / PC ae C40:1
Shapiro−Wilk Test of log quotients, pv: 0.32761; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 6e−05; DIFFERENCE
Wilcoxon: Challenge; fasting: 1; sport: 1; OLTT: 0.875

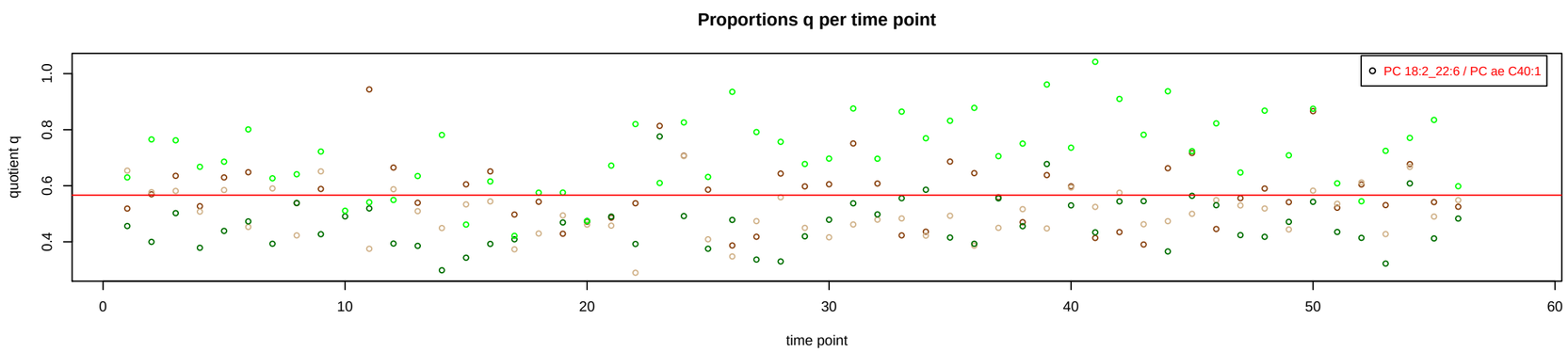












PC ae C40:2 = R

No independent Variable measured.

Qualitative composition

PC ae C40:2 consists of:
PC O−18:0_22:2, PC O−18:1_22:1, PC O−18:2_22:0, PC O−
PC O−20:1_20:1, PC 17:0_22:2, PC 17:1_22:1, PC 17:2_22:(
PC 18:2_21:0, PC 19:0_20:2, PC 19:1_20:1, PC 18:3_22:6,
[13C1]SM 43:2
and further compounds

PC ae C40:3 = R

No independent Variable measured.

Qualitative composition

PC ae C40:3 consists of:
PC O−18:1_22:2, PC O−18:2_22:1, PC O−20:0_20:3, PC O−
PC O−22:0_18:3, PC 17:1_22:2, PC 17:2_22:1, PC 18:3_21:(
PC 19:0_20:3, PC 19:1_20:2, PC 18:4_22:6, PC 20:5_20:5,
and further compounds

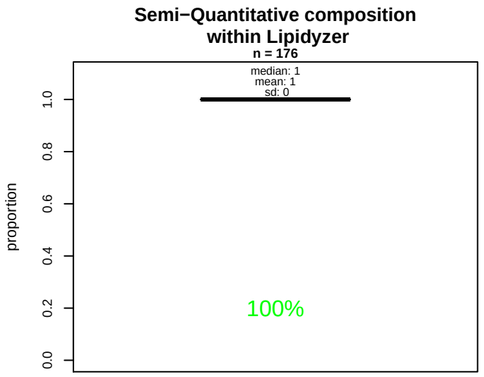
PC ae C40:4 = R

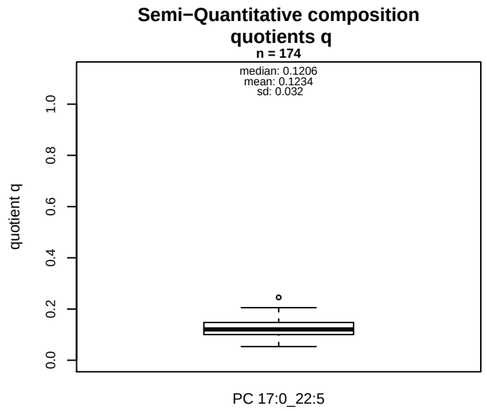
No independent Variable measured.

Qualitative composition

PC ae C40:4 consists of:
PC O−18:0_22:4, PC O−18:2_22:2, PC O−20:0_20:4, PC O−
PC 17:0_22:4, PC 17:2_22:2, PC 18:4_21:0, PC 19:0_20:4,
PC 19:1_20:3
and further compounds

PC ae C40:5 = PC 17:0_22:5 + R





Semi−Quantitative composition: Lipidyzer

PC ae C40:5 consists of:
PC 17:0_22:5 100%
and of (not quantified):
PC O−18:0_22:5, PC O−18:1_22:4, PC O−20:0_20:5, PC O−PC 16:0_23:5, PC 17:1_22:4, PC 19:0_20:5, PC 19:1_20:4, and further compounds

Composition: mean of proportions q

conc(PC ae C40:5) * 0.1234 = conc(PC 17:0_22:5) [var(q)=0.1234]
Percentiles: 5%−>0.0708, 25%−>0.1003, 75%−>0.1471, 95%−>0.1735

Linear model

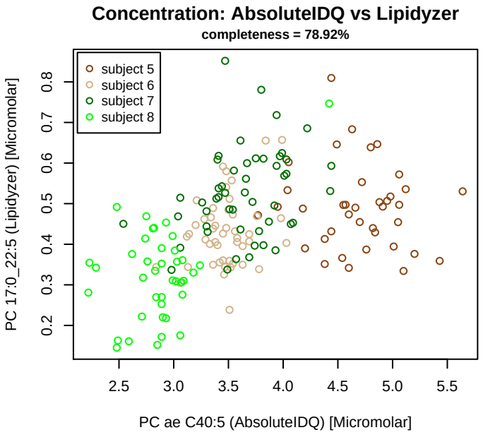
```
PC ae C40:5 ~ b * ( PC 17:0_22:5 )
```

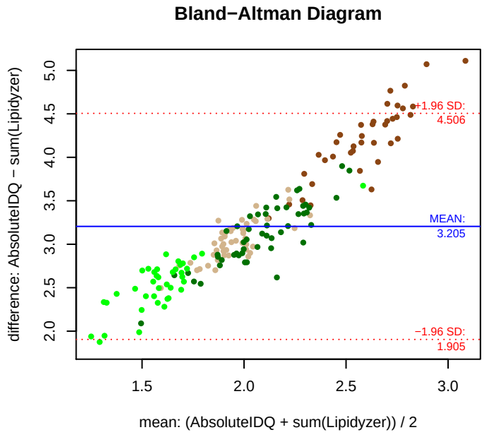
b = 2.47007

R^2 = 0.19655

Ranges

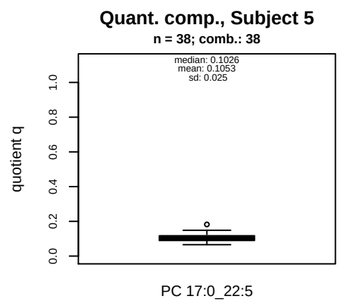
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	2.22	0.15	2.07
Max	5.64	0.85	4.79
Mean	3.66	0.45	3.22
Median	3.53	0.44	3.09
SD	0.73	0.13	0.6

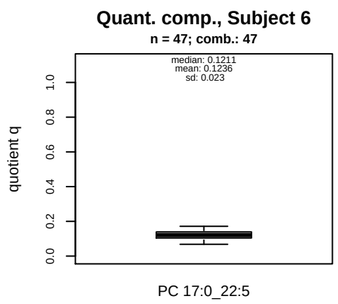


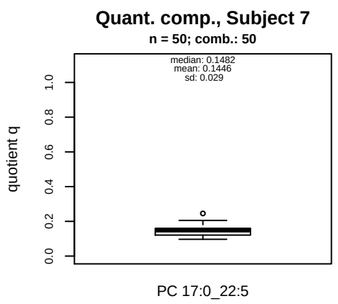


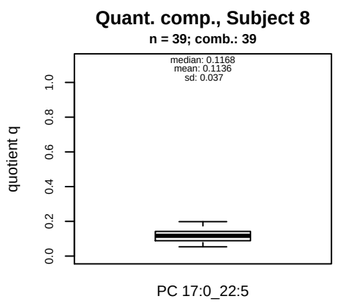
Stability of composition

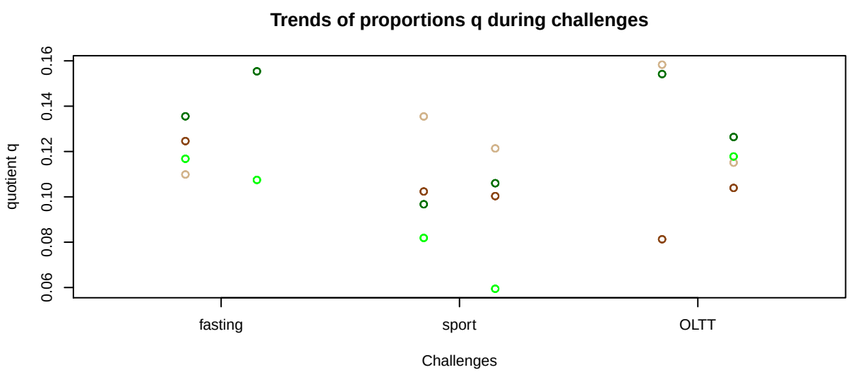
PC 17:0_22:5 / PC ae C40:5
Shapiro−Wilk Test of log quotients, pv: 0.00815; NO
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.09316; EQUAL
Wilcoxon: Challenge; fasting: 1; sport: 0.375; OLTT: 0.5

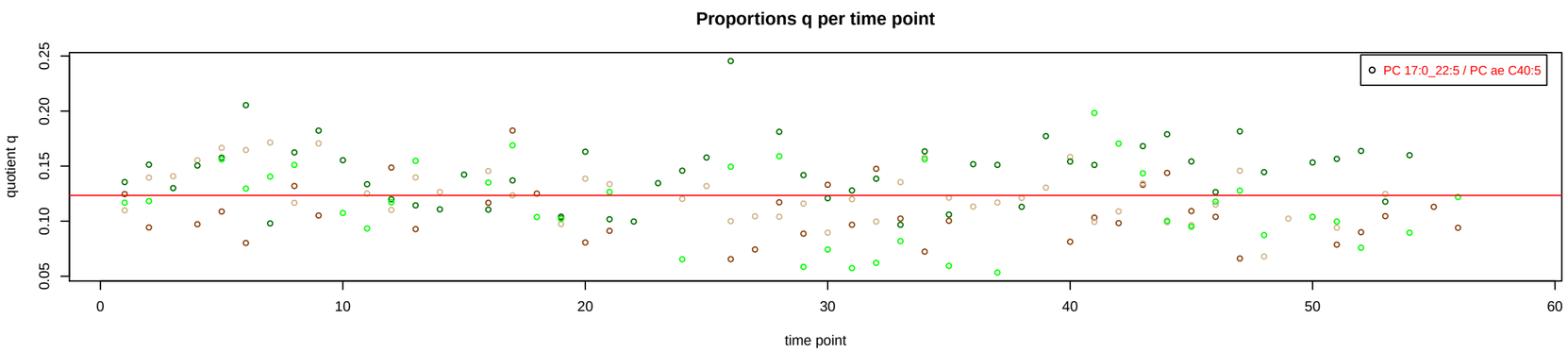




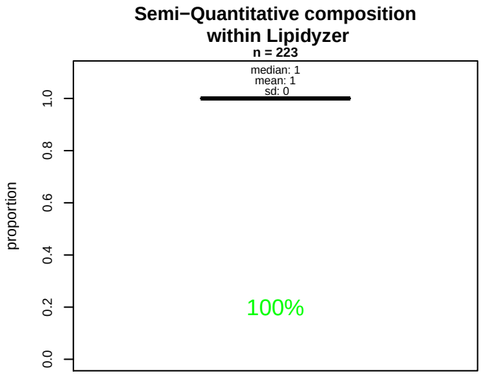


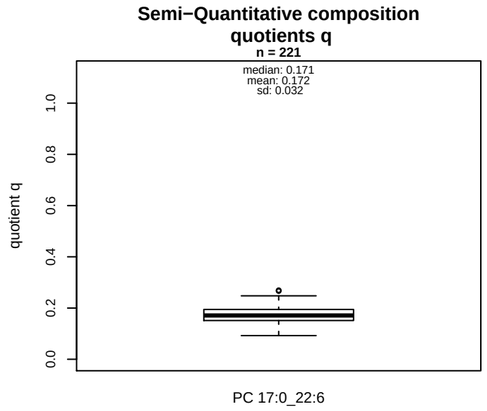






PC ae C40:6 = PC 17:0_22:6 + R





Semi−Quantitative composition: Lipidyzer

PC ae C40:6 consists of:
PC 17:0_22:6 100%
and of (not quantified):
PC O−18:0_22:6, PC O−18:2_22:4, PC O−20:1_20:5, PC 17:
PC 19:1_20:5
and further compounds

Composition: mean of proportions q

conc(PC ae C40:6) * 0.172 = conc(PC 17:0_22:6) [var(q)=0.172]
Percentiles: 5%−>0.1216, 25%−>0.1513, 75%−>0.1945, 95%−>0.2262

Linear model

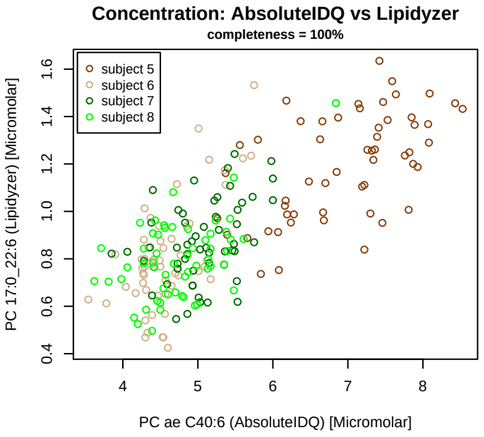
```
PC ae C40:6 ~ b * ( PC 17:0_22:6 )
```

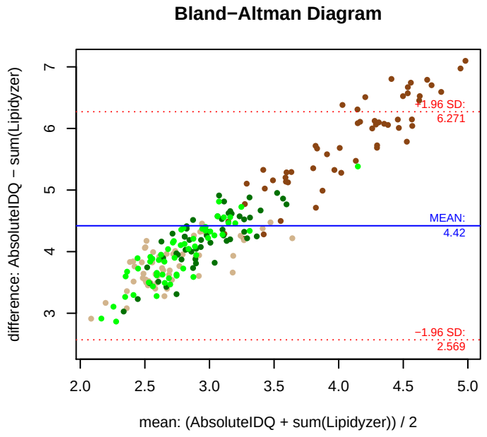
b = 3.28445

R^2 = 0.56301

Ranges

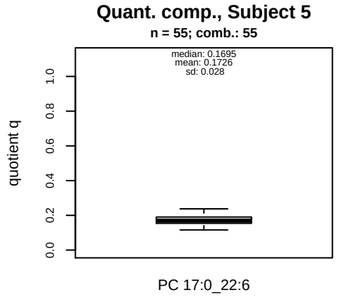
Measure	AbsoluteIDQ	sum(Lipidyzer)	delta
Min	3.54	0.43	3.11
Max	8.53	1.63	6.9
Mean	5.34	0.92	4.42
Median	5.01	0.87	4.14
SD	1.12	0.26	0.86

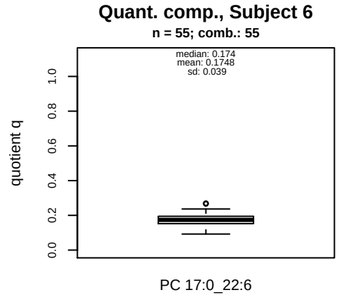


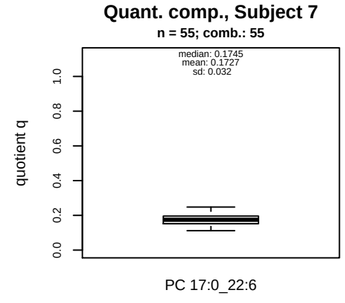


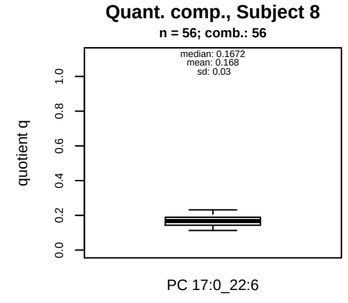
Stability of composition

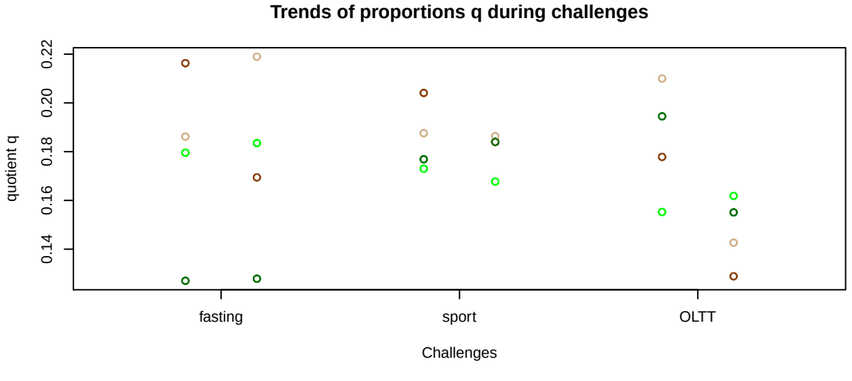
PC 17:0_22:6 / PC ae C40:6
Shapiro−Wilk Test of log quotients, pv: 0.15729; OK
SW: ok; ANOVA: Comp. ~ Subject_ID −> pv = 0.41419; EQUAL
Wilcoxon: Challenge; fasting: 0.875; sport: 0.625; OLTT: 0.25

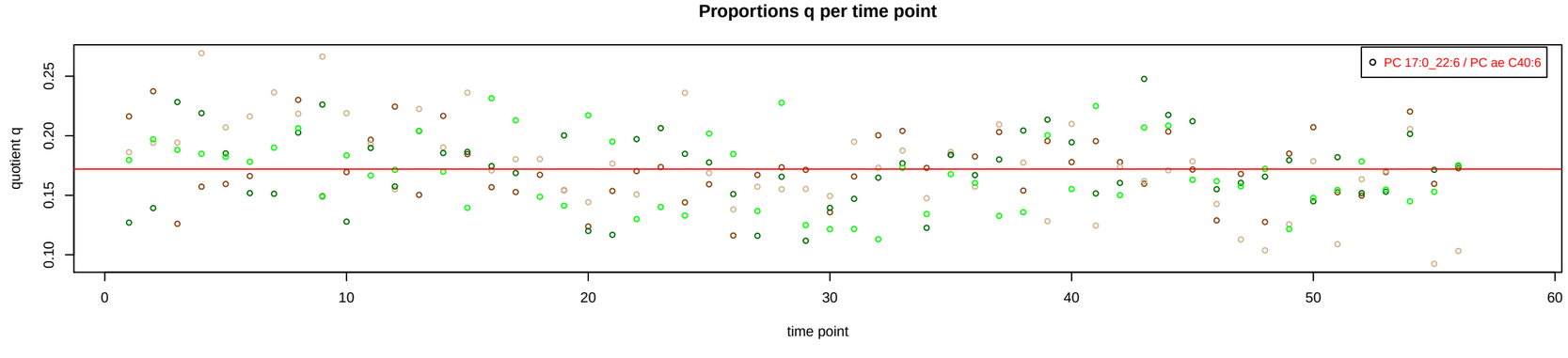












PC ae C42:0 = R

No independent Variable measured.

Qualitative composition

PC ae C42:0 consists of:
PC O−20:0_22:0, PC 19:0_22:0, PC 20:0_21:0, PC 23:0_18:(
PC 20:5_22:2
and further compounds

PC ae C42:1 = R

No independent Variable measured.

Qualitative composition

PC ae C42:1 consists of:
PC O−20:0_22:1, PC O−18:1_24:0, PC O−20:1_22:0, PC 19:
PC 19:1_22:0, PC 20:1_21:0, PC 20:2_22:6, PC 20:4_22:4,
and further compounds

PC ae C42:2 = R

No independent Variable measured.

Qualitative composition

PC ae C42:2 consists of:
PC O−20:0_22:2, PC O−18:2_24:0, PC O−20:1_22:1, PC O−
PC 19:0_22:2, PC 19:1_22:1, PC 20:2_21:0, PC 20:3_22:6,
PC 20:5_22:4
and further compounds

PC ae C42:3 = R

No independent Variable measured.

Qualitative composition

PC ae C42:3 consists of:
PC O−24:0_18:3, PC O−20:1_22:2, PC O−18:2_24:1, PC 21:
PC 19:1_22:2, PC 20:3_21:0, PC 20:5_22:5, PC 20:4_22:6,
and further compounds

PC ae C42:4 = R

No independent Variable measured.

Qualitative composition

PC ae C42:4 consists of:
PC O−20:0_22:4, PC 19:0_22:4, PC 20:4_21:0, PC 20:5_22:6
and further compounds

PC ae C42:5 = R

No independent Variable measured.

Qualitative composition

PC ae C42:5 consists of:
PC 20:5_21:0
and further compounds

PC ae C44:3 = R

No independent Variable measured.

Qualitative composition

PC ae C44:3 consists of:
PC 22:4_22:6
and further compounds

PC ae C44:4 = R

No independent Variable measured.

Qualitative composition

PC ae C44:4 consists of:
PC O−24:0_20:4, PC O−22:1_22:3, PC O−22:2_22:2, PC 21:
and further compounds

PC ae C44:5 = R

No independent Variable measured.

Qualitative composition

PC ae C44:5 consists of:
PC 22:6_22:6
and further compounds

PC ae C44:6 = R

No independent Variable measured.

Qualitative composition

PC ae C44:6 consists of:
PC 21:0_22:6
and further compounds