

Supporting material for

**Quantification of Branched Chain Fatty Acids in Polar and Neutral Lipids of Cheese
and Fish Samples**

SIMONE HAUFF AND WALTER VETTER*

University of Hohenheim, Institute of Food Chemistry,

Garbenstrasse 28, D-70599 Stuttgart, Germany

*Corresponding author

Walter Vetter

University of Hohenheim

Institute of Food Chemistry (170b)

Garbenstr. 28

D-70599 Stuttgart, Germany

Phone +49 711 459 24016

Email: w-vetter@uni-hohenheim.de

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Table S1: Concentrations [mg/100 g], and the sum [mg/100 g] of individual fatty acids in the phospholipids of cheese samples. The DPPC_{eq} reflects the phospholipid content [%] of each sample, calculated by means of the factor 0.696 with the sum of all fatty acids (16)

FAME	gouda	emmental	butter cheese	organic camembert	organic brie	org. alpine cheese	org. curd cheese	cow mozzarella	mozzarella	feta (cow)	feta	goat cream	goat cheese	Bavaria blue	limburger	romadur	roquefort
8:0	<0.4	<0.4	<0.4	3.0	<0.4	<0.4	4.0	<0.4	2.7	<0.4	2.2	2	5.9	21.7	<0.4	1.3	9.8
10:0	<0.4	1.5	<0.4	7.3	<0.4	<0.4	4.2	<0.4	6.4	<0.4	14.9	12.7	6.7	26.2	0.5	8.7	22.7
11:0	<0.4	<0.4	<0.4	0.3	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	0.6	<0.4	0.7	0.5	0.3	<0.4	0.7
12:0	3.8	3.1	<0.4	10.4	0.2	<0.4	5.3	4.7	11.5	3.2	17.6	13.7	24	29.6	3.9	17.6	16.4
13:0	<0.4	<0.4	<0.4	0.4	0.2	<0.4	0.7	0.6	0.9	0.3	1.2	1.1	3.2	1.6	0.4	1.1	0.7
14:0/14:1	42.5	17.4	<0.4	46.9	25.3	10.5	33.0	24.9	66.8	35.7	90.7	53.2	95.9	110.9	21.3	100.6	51.3
15:0/15:1	12.1	4.4	5.0	7.5	7.3	4.3	6.9	7	12.5	6.4	16.8	8.4	17.1	12.4	5.1	18.1	6.7
16:0	175.2	69.8	189.8	129.8	145	79.5	111	111	236.5	235.8	388.7	175.4	572.8	265.8	113.3	361.9	159.9
17:0	3.8	1.7	<0.4	3	2.5	1.4	1.6	2.2	3.4	2.0	6.1	3.1	7.1	7.7	2.8	5.2	0.5
18:0	113.6	59.2	118.1	80.3	70.0	41.9	51.3	82.6	129	119.9	206.6	136.7	337.0	117.0	95.6	206.8	81.9
20:0	<0.4	0.8	2.1	1.2	0.8	0.4	0.7	1.3	2.0	1.4	3.3	1.7	5.2	1.4	1.5	3.2	1.7
21:0	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
22:0	<0.4	<0.4	<0.4	0.7	0.3	<0.4	<0.4	0.8	0.9	<0.4	1.4	0.6	1.4	0.8	0.7	1.7	1.1
24:0	<0.4	<0.4	<0.4	<0.4	0.3	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	0.9	<0.4	<0.4	<0.4	<0.4	<0.4
16:1	22.6	2.1	<0.4	6.7	8.3	2.2	4.9	3.8	13.8	4.5	17.7	2.4	12.1	8.5	5.4	22.7	3.8
17:1	<0.4	<0.4	<0.4	2.1	1.5	<0.4	<0.4	<0.4	1.8	1.1	3.4	<0.4	<0.4	3.3	<0.4	3.6	2.4
18:1	110.5	58.0	70.9	106.2	111.2	47.6	85.8	89.7	132.0	96.6	178.6	109.5	169.1	116	82.0	178.2	65.0
18:1tr	12.8	6.5	8.9	21.6	25.3	5.3	15.5	12.0	20.6	9.7	27.5	12.3	19.5	16	15.0	25.6	12.3
20:1	<0.4	<0.4	<0.4	1	3.5	<0.4	2.1	<0.4	4.1	0.8	6.4	<0.4	1.8	0.5	2.3	6.1	<0.4
22:1	<0.4	<0.4	<0.4	0.2	0.6	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
24:1	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
18:2 isomers	20.8	11.2	<0.4	41.1	54.2	6.5	17.9	18.9	22.3	13.8	20.9	24.8	30.4	25.0	20.7	26.7	16.6
20:2	<0.4	<0.4	<0.4	0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
22:2	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
18:3 isomers	<0.4	2.1	<0.4	20.2	13.6	0.9	2.3	2	2.5	1.1	2.6	1.8	4.7	<0.4	2.8	2.7	5.3
20:3 isomers	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
20:4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
20:5	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
22:6	<0.4	<0.4	<0.4	0.2	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
i14:0	0.4	0.2	<0.4	0.4	0.2	<0.4	0.1	<0.4	0.5	0.2	0.7	0.3	0.8	1.1	0.2	0.8	0.5
i15:0	1.3	0.5	<0.4	0.9	0.7	0.4	0.9	0.6	2.2	0.8	2.6	0.8	3.1	1.8	1.4	3.6	1.1
a15:0	2.0	1.6	<0.4	1.9	1.3	0.7	1.6	1.1	2.9	1.5	4.3	1.5	3.8	3.2	1.2	4.2	1.7
i16:0	1.0	0.5	<0.4	0.8	0.6	0.3	0.7	0.7	1.1	0.5	1.7	1.0	2.0	1.7	0.7	1.5	0.8
i17:0	1.9	0.6	<0.4	1.0	0.7	0.5	0.7	1.1	1.2	0.5	2.4	1.1	2.1	1.4	0.9	1.7	0.9
a17:0	2.8	1.3	<0.4	2.0	1.4	0.8	1.6	1.8	2.3	1.4	4.4	2.1	3.8	2.8	1.6	3.1	2.0
i18:0	0.3	0.2	<0.4	0.2	0.2	<0.4	<0.4	0.3	0.2	<0.4	<0.4	0.3	0.6	<0.4	0.3	0.4	<0.4
Σall FAs	527	243	395	495	475	203	349	367	677	537	1021	566	1325	777	380	1006	456
DPPC _{eq}	0.76	0.35	0.57	0.71	0.68	0.29	0.50	0.53	0.97	0.77	1.47	0.81	1.90	1.12	0.55	14.5	0.66

^{a)} <0.4: Limit of quantification typically 0.4 mg/100 g total lipid

Table S2: Concentrations [mg/100 g], and the sum [mg/100 g] of several fatty acids in the phospholipids of fish samples. The DPPC_{eq} reflects the phospholipid content [%] of each sample, calculated by means of the factor 0.696 with the sum of all fatty acids (16)

FAME	tuna	salmon	pollack	rainbow trout	gilthead seabream	sea bass	brown trout
8:0	6.5	5.2	9.7	1.9	<0.4	2.2	2.6
10:0	13.9	6.0	5.1	3.9	11.0	3.5	9.9
11:0	<0.4	0.9	0.8	0.3	4.2	0.6	1.2
12:0	71.1	10.3	5.8	3.9	13.5	7.5	59.6
13:0	2.7	1.5	0.7	0.6	4.7	3.5	3.0
14:0/14:1	177.1	76.9	118.9	95.2	941.1	682.0	297.4
15:0/15:1	65.7	17.6	21.4	38.3	107.9	84.5	95.2
16:0	1909.6	840.8	1421.3	1566.4	2873.8	3116.1	3876.4
17:0	48.7	11.6	5.9	23.4	34.4	43.9	71.6
18:0	966.3	442.4	303.5	426.2	702.4	858.6	1318.2
20:0	<0.4	6.0	5.7	6.2	25.0	2.4	28.0
21:0	<0.4	0.2	<0.4	<0.4	<0.4	1.4	<0.4
22:0	13.3	2.5	2.1	2.5	<0.4	9.8	23.0
24:0	6.2	0.9	1.3	<0.4	3.5	3.8	<0.4
16:1	71.7	40.1	99.0	100.6	452.5	505.5	630.4
17:1	<0.4	1.5	60.5	9.5	34.3	39.8	3.9
18:1	691.4	243.0	387.7	578.4	1619.7	2308.8	1317.8
18:1tr	73.1	84.7	183.5	143.8	212.7	315.2	<0.4
20:1	<0.4	54.9	197.1	5.2	34.3	278.2	188.8
22:1	<0.4	19.4	<0.4	31.3	66.7	40.8	<0.4
24:1	<0.4	1.3	<0.4	<0.4	<0.4	17.8	<0.4
18:2 isomers	62.1	180.9	101.3	199.2	96.0	165.8	446.3
20:2	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	4.1
22:2	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
18:3 isomers	21.2	30.7	12.2	41.4	<0.4	4.3	114.7
20:3 isomers	<0.4	1.3	<0.4	14.3	4.3	4.5	<0.4
20:4	<0.4	20.3	<0.4	51.1	<0.4	<0.4	<0.4
20:5	<0.4	286.9	705.64	249.4	27.8	<0.4	992.3
22:6	<0.4	1799.7	2092.5	3567.2	<0.4	<0.4	3508.5
i14:0	1.5	0.4	0.2	0.3	2.9	2.0	2.9
i15:0	4.4	1.8	1.9	1.7	25.0	16.0	30.3
a15:0	5.4	2.1	1.8	1.2	8.5	5.1	9.6
i16:0	3.0	0.8	0.8	1.5	7.5	6.9	5.8
i17:0	5.3	2.0	2.9	5.0	15.8	19.4	19.5
a17:0	5.6	1.7	1.8	2.8	12.4	12.2	11.9
i18:0	1.4	0.4	<0.4	0.8	1.9	2.9	1.6
Σall FAs	4261	4192	5741	7172	7344	8563	13072
DPPC _{eq}	6.12	6.02	8.25	10.3	10.6	12.3	18.8

^{a)} <0.4: Limit of quantification typically 0.4 mg/100 g total lipid

Table S3: Proportions [%] of 15:0, 17:0 and some branched chain fatty acids found in the polar lipids of selected fish and cheese samples

	PLs						total BCFA
	15:0 [%]	17:0 [%]	i15:0 [%]	a15:0 [%]	i17:0 [%]	a17:0 [%]	[%]
tuna	23.8	18.9	81.4	84.3	84.2	84.9	96.4
salmon	7.9	10.8	4.1	11.3	5.2	7.6	5.7
pollack	23.0	29.7	65.1	64.5	74.2	63.9	90.2
rainbow							
trout	7.7	12.8	1.9	3.0	8.4	6.1	4.5
gilthead							
seabream	28.2	42.6	29.4	29.4	34.2	32.4	31.1
sea bass	28.9	30.9	24.6	26.9	33.7	34.6	27.8
brown trout	24.4	28.5	14.2	27.7	27.3	30.3	23.8
Mean	20.1	23.1	16.1	22.5	24.8	25.5	21.2
mozzarella							
cow	0.5	0.8	0.5	0.4	0.7	0.4	0.5
emmental	0.3	0.4	0.3	0.4	0.3	0.2	0.3
limburg	0.4	0.6	0.8	0.3	0.4	0.4	0.4
alpine cheese	0.3	0.3	0.2	0.2	0.2	0.2	0.2
feta cow	0.5	0.7	0.5	0.4	0.3	0.5	0.4
Mean	0.4	0.5	0.4	0.3	0.3	0.3	0.4

Figure S1: Bar graphs of the branched chain fatty acid distribution in the neutral lipids (top) and the polar lipids (bottom) of cheeses (left panels) and fish (right panels) and the polar lipid content (right-handed scales) shown as blue line in the lower graphs.

