

Supplementary Tables— **Observed ions in the HPLC - APCI-mass spectra of TAGs in positive and negative ion modes**

Table 1. Observed ions in the HPLC-APCI-mass spectra of major salmon TAGs in positive and negative ion modes

TAG	TCN	DBN	ECN	Ion observed in the mass spectra of TAG												
				Molecular ion						Fragmentation ions: [RCOO] ⁻						
				[M+H] ⁺	F1	m/z	F2	m/z	F3	m/z	R1	m/z	R2	m/z	R3	m/z
EEO	58	11	36	925.73	EE	643.48	EO	623.51	—	—	E	301.22	O	281.25	—	—
DDO	62	13	36	977.76	DD	695.51	DO	649.53	—	—	D	327.23	O	281.25	—	—
DPoPo	54	8	38	875.71	DPo	621.50	PoPo	547.48	—	—	D	327.23	Po	253.2173	—	—
EMM	48	5	38	797.67	EM	569.47	MM	495.45	—	—	E	301.22	M	227.20	—	—
DPoO	56	8	40	903.74	DPo	621.50	PoO	595.48	DO	649.53	D	327.23	Po	253.2173	O	281.25
DMO	54	7	40	877.73	DM	595.48	MO	549.50	DO	649.53	D	327.23	M	227.20	O	281.25
DMP	52	6	40	851.71	DM	595.48	MP	523.48	DP	623.51	D	327.23	M	227.20	P	255.23
DOO	58	8	42	931.77	DO	649.53	OO	603.55	—	—	D	327.23	O	281.25	—	—
EOP	54	6	42	879.74	EO	623.51	OP	577.53	EP	597.50	E	301.22	O	281.25	P	255.23
DPP	54	6	42	879.74	DP	623.51	PP	551.51	—	—	D	327.23	P	255.23	—	—
EOS	56	6	44	907.77	EO	623.51	OS	605.56	ES	625.53	E	301.22	O	281.25	S	283.26
DOS	58	7	44	933.79	DO	649.53	OS	605.56	DS	651.55	D	327.23	O	281.25	S	283.26
EPS	54	5	44	881.76	EP	597.50	PS	579.55	ES	625.53	E	301.22	P	255.23	S	283.26
DPS	56	6	44	907.77	DP	623.51	PS	579.55	DS	651.55	D	327.23	P	255.23	S	283.26
ESS	56	5	46	909.79	ES	625.53	SS	607.58	—	—	E	301.22	S	283.26	—	—
DSS	58	6	46	935.81	DS	651.55	SS	607.58	—	—	D	327.23	S	283.26	—	—
OOO	54	3	48	885.79	OO	603.55	—	—	—	—	O	281.25	—	—	—	—
OOP	52	2	48	859.77	OO	603.55	OP	577.53	—	—	O	281.25	P	255.23	—	—
OPP	50	1	48	833.76	OP	577.53	PP	551.51	—	—	O	281.25	P	255.23	—	—
OOS	54	2	50	887.81	OO	603.55	OS	605.56	—	—	O	281.25	S	283.26	—	—
PPS	50	0	50	835.77	PP	551.51	PS	579.55	—	—	P	255.23	S	283.26	—	—
OSS	54	1	52	889.82	OS	605.56	SS	607.58	—	—	O	281.25	S	283.26	—	—
PSS	52	0	52	863.81	PS	579.55	SS	607.58	—	—	P	255.23	S	283.26	—	—
SSS	54	0	54	891.84	SS	607.58	—	—	—	—	S	283.26	—	—	—	—

TCN: total carbon number; DB: number of double bonds; ECN: equivalent carbon number; ECN = TCN - (2 × DB);

F-1, F-2, and F-3: fragmentation ions of diacylglycerols; R¹, R², and R³: fragmentation ions of fatty acids.

Table 2. Observed ions in the HPLC–APCI-mass spectra of major anchovy TAGs in positive and negative ion modes

TAG	TCN	DB	ECN	Ion observed in the mass spectra of TAG																	
				Molecular						Fragmentation ions:[(M+H)RCOO]+						Fragmentation ions:[RCOO]-					
				[M+H] ⁺	F1	m/z	F2	m/z	F3	m/z	R1	m/z	R2	m/z	R3	m/z					
EEE	60	15	30	945.70	EE	643.48	—	—	—	—	E	301.22	—	—	—	—					
DDD	66	18	30	1023.74	DD	695.51	—	—	—	—	D	327.23	—	—	—	—					
EEO	58	11	36	925.73	EE	643.48	EO	623.51	—	—	E	301.22	O	281.25	—	—					
DDO	62	13	36	977.76	DD	695.51	DO	649.53	—	—	D	327.23	O	281.25	—	—					
DDP	60	12	36	951.74	DD	695.51	DP	623.51	—	—	D	327.23	P	255.23	—	—					
EPoPo	52	7	38	849.70	EPo	595.48	PoPo	547.48	—	—	E	301.22	Po	253.22	—	—					
EPoM	50	6	38	823.68	EPo	595.48	PoM	521.47	EM	569.47	E	301.22	Po	253.22	M	227.20					
EMM	48	5	38	797.67	EM	569.47	MM	495.45	—	—	E	301.22	M	227.20	—	—					
DMM	50	6	38	823.68	DM	595.48	MM	495.45	—	—	D	327.23	M	227.20	—	—					
DPoO	56	8	40	903.74	DPo	621.50	PoO	595.48	DO	649.53	D	327.23	Po	253.22	O	281.25					
DMO	54	7	40	877.73	DM	595.48	MO	549.50	DO	649.53	D	327.23	M	227.20	O	281.25					
DMP	52	6	40	851.71	DM	595.48	MP	523.48	DP	623.51	D	327.23	M	227.20	P	255.23					
EOP	54	6	42	879.74	EO	623.51	OP	577.53	EP	597.50	E	301.22	O	281.25	P	255.23					
DOP	56	7	42	905.76	DO	649.53	OP	577.53	DP	623.51	D	327.23	O	281.25	P	255.23					
DPP	54	6	42	879.74	DP	623.51	PP	551.51	—	—	D	327.23	P	255.23	—	—					
EPP	52	5	42	853.73	EP	597.50	PP	551.51	—	—	E	301.22	P	255.23	—	—					
EOS	56	6	44	907.77	EO	623.51	OS	605.56	ES	625.53	E	301.22	O	281.25	S	283.26					
EPS	54	5	44	881.76	EP	597.50	PS	579.55	ES	625.53	E	301.22	P	255.23	S	283.26					
DPS	56	6	44	907.77	DP	623.51	PS	579.55	DS	651.55	D	327.23	P	255.23	S	283.26					
ESS	56	5	46	909.79	ES	625.53	SS	607.58	—	—	E	301.22	S	283.26	—	—					
DSS	58	6	46	935.81	DS	651.55	SS	607.58	—	—	D	327.23	S	283.26	—	—					
OOO	54	3	48	885.79	OO	603.55	—	—	—	—	O	281.25	—	—	—	—					
OOP	52	2	48	859.77	OO	603.55	OP	577.53	—	—	O	281.25	P	255.23	—	—					
OPP	50	1	48	833.76	OP	577.53	PP	551.51	—	—	O	281.25	P	255.23	—	—					
PPS	50	0	50	835.77	PP	551.51	PS	579.55	—	—	P	255.23	S	283.26	—	—					
OSS	54	1	52	889.82	OS	605.56	SS	607.58	—	—	O	281.25	S	283.26	—	—					

TCN-total carbon number; DB-double bond number; ECN-equivalent carbon number, ECN = TCN - (2×DB);

F-1, F-2, and F-3: fragmentation ions of diacylglycerols; R¹, R², and R³: fragmentation ions of fatty acids.

Table 3. Observed ions in the HPLC–APCI-mass spectra of major tuna TAGs in positive and negative ion modes

TAG	TCN	DB	ECN	Ion observed in the mass spectra of TAG												
				Molecular ion Fragmentation ions:[(M+H)RCOO] ⁺							Fragmentation ions:[RCOO] ⁻					
				[M+H] ⁺	F1	m/z	F2	m/z	F3	m/z	R1	m/z	R2	m/z	R3	m/z
EEE	60	15	30	945.70	EE	643.48	—	—	—	—	E	301.22	—	—	—	—
DDD	66	18	30	1023.74	DD	695.51	—	—	—	—	D	327.23	—	—	—	—
DDO	62	13	36	977.76	DD	695.51	DO	649.53	—	—	D	327.23	O	281.25	—	—
DDP	60	12	36	951.74	DD	695.51	DP	623.51	—	—	D	327.23	P	255.23	—	—
DPoPo	54	8	38	875.71	DPo	621.50	PoPo	547.48	—	—	D	327.23	Po	253.2173	—	—
FMM	48	5	38	797.67	FM	569.47	MM	495.45	—	—	F	301.22	M	227.20	—	—
DPoO	56	8	40	903.74	DPo	621.50	PoO	595.48	DO	649.53	D	327.23	Po	253.2173	O	281.25
DMO	54	7	40	877.73	DM	595.48	MO	549.50	DO	649.53	D	327.23	M	227.20	O	281.25
DMP	52	6	40	851.71	DM	595.48	MP	523.48	DP	623.51	D	327.23	M	227.20	P	255.23
DOO	58	8	42	931.77	DO	649.53	OO	603.55	—	—	D	327.23	O	281.25	—	—
DOP	56	7	42	905.76	DO	649.53	OP	577.53	DP	623.51	D	327.23	O	281.25	P	255.23
EPP	52	5	42	853.73	EP	597.50	PP	551.51	—	—	E	301.22	P	255.23	—	—
EOS	56	6	44	907.77	EO	623.51	OS	605.56	ES	625.53	E	301.22	O	281.25	S	283.26
DOS	58	7	44	933.79	DO	649.53	OS	605.56	DS	651.55	D	327.23	O	281.25	S	283.26
EPS	54	5	44	881.76	EP	597.50	PS	579.55	ES	625.53	E	301.22	P	255.23	S	283.26
DPS	56	6	44	907.77	DP	623.51	PS	579.55	DS	651.55	D	327.23	P	255.23	S	283.26
ESS	56	5	46	909.79	ES	625.53	SS	607.58	—	—	E	301.22	S	283.26	—	—
DSS	58	6	46	935.81	DS	651.55	SS	607.58	—	—	D	327.23	S	283.26	—	—
OOO	54	3	48	885.79	OO	603.55	—	—	—	—	O	281.25	—	—	—	—
OOP	52	2	48	859.77	OO	603.55	OP	577.53	—	—	O	281.25	P	255.23	—	—
OPP	50	1	48	833.76	OP	577.53	PP	551.51	—	—	O	281.25	P	255.23	—	—
OOS	54	2	50	887.81	OO	603.55	OS	605.56	—	—	O	281.25	S	283.26	—	—
PPS	50	0	50	835.77	PP	551.51	PS	579.55	—	—	P	255.23	S	283.26	—	—
OSS	54	1	52	889.82	OS	605.56	SS	607.58	—	—	O	281.25	S	283.26	—	—
SSS	54	0	54	891.84	SS	607.58	—	—	—	—	S	283.26	—	—	—	—

TCN: total carbon number; DB: number of double bonds; ECN: equivalent carbon number; ECN = TCN - (2 × DB);

F-1, F-2, and F-3: fragmentation ions of diacylglycerols; R¹, R², and R³: fragmentation ions of fatty acids.