Supplements

Table 1S. Relative quantities[a] (%) of molecular species of TAGs identified in alga *S. bacillaris*, their retention times, equivalent carbon number, number of double bond(s), calculated *m/z* of $[DAG]^+$ and $[M+H]^+$.

						$[DAG]^+$			10 ºC			20 ºC			30 ºC	
RT	ECN	ACN	DB	TAG	$[M+H]^+$	1:2	1:3	2:3	906	493	NAP	906	493	NAP	493	NAP
20.2	30	60	15	EEE	955.77	643.48	643.48	643.48	0.2	0.2	0.3	0.1	0.1	0.1	0.0	0.0
21.6	30	56	13	PnEE	893.68	591.45	591.45	643.48	0.4	0.2	0.3	0.2	0.1	0.1	0.0	0.0
22.0	32	60	14	EEA	957.79	643.48	645.49	645.49	0.2	0.2	0.3	0.1	0.1	0.1	0.0	0.0
22.8	32	58	13	LnEE	921.71	619.48	619.48	643.48	1.2	0.4	0.3	0.9	0.3	0.1	0.1	0.0
23.3	32	56	12	PlEE	895.69	593.46	593.46	643.48	1.1	1.1	0.9	0.8	0.8	0.5	0.2	0.1
24.2	32	54	11	PnLnE	869.68	567.45	591.45	619.48	0.9	0.7	0.8	0.7	0.5	0.4	0.2	0.1
24.7	32	50	9	LnPnPn	817.65	567.45	567.45	539.42	0.2	0.3	0.3	0.1	0.1	0.1	0.0	0.0
28.0	32	48	8	PnPlPn	791.63	541.43	539.42	541.43	0.2	0.8	0.3	0.1	0.1	0.1	0.0	0.0
28.2	32	48	8	PlPnPn	791.63	541.43	541.43	539.42	0.2	0.7	0.4	0.1	0.1	0.1	0.0	0.0
32.8	34	60	13	AAE	949.72	647.50	645.49	645.49	0.2	0.1	0.3	0.1	0.1	0.1	0.0	0.0
33.1	34	58	12	AELn	923.72	645.49	621.49	619.48	1.3	0.8	0.3	1.2	0.4	0.1	0.1	0.0
34.2	34	58	12	EEL	923.72	643.48	621.49	621.49	0.6	0.4	0.3	0.5	0.2	0.1	0.1	0.0
35.6	34	56	11	LnELn	897.71	619.48	595.48	619.48	9.9	5.6	1.8	9.4	4.2	0.7	1.2	0.1
35.9	34	56	11	PoEE	897.71	595.48	595.48	643.48	0.5	0.5	0.5	0.5	0.4	0.3	0.1	0.0
36.2	34	54	10	PlLnE	871.69	569.46	593.46	619.48	0.3	0.2	0.1	0.2	0.1	0.1	0.0	0.0
37.4	34	52	9	PoPnE	845.68	543.45	595.48	591.45	0.4	0.2	0.3	0.3	0.2	0.1	0.0	0.0
38.6	34	52	9	PoEPn	845.68	595.48	543.45	591.45	0.3	0.2	0.3	0.2	0.1	0.1	0.0	0.0
40.8	34	48	7	PnPnPo	793.65	539.42	543.45	543.45	0.5	0.4	0.3	0.4	0.3	0.1	0.3	0.2
40.9	34	48	7	PlPnPl	793.64	543.44	541.43	543.44	0.5	0.7	0.4	0.3	0.2	0.2	0.3	0.2
41.0	34	48	7	PlPlPn	793.64	543.44	541.43	541.43	0.4	0.6	0.3	0.1	0.1	0.1	0.0	0.0
41.8	34	50	8	LPnPn	819.66	569.46	569.46	539.42	0.3	0.3	0.3	0.2	0.2	0.1	0.3	0.2
41.9	36	60	12	AAA	951.74	647.50	647.50	647.50	0.2	0.1	0.1	0.1	0.1	0.1	0.0	0.0
42.1	36	58	11	AEL	925.73	645.49	623.50	621.49	0.9	0.3	0.3	0.7	0.2	0.1	0.1	0.0
42.3	36	58	11	EEO	925.74	643.48	623.51	623.51	0.2	0.3	0.3	0.2	0.2	0.1	0.0	0.0

42.5	36	56	10	LnEL	899.72	619.48	597.49	621.49	6.4	3.2	0.8	6.0	2.6	0.4	0.9	0.1
43.0	36	56	10	PEE	899.72	597.49	597.49	643.48	0.3	0.4	0.3	0.2	0.2	0.1	0.0	0.0
43.5	36	54	9	LnEPo	873.71	619.48	571.48	595.48	0.6	0.4	0.4	0.5	0.3	0.2	0.1	0.0
44.6	36	52	8	PLnE	875.72	573.49	597.49	619.48	0.4	0.3	0.3	0.3	0.2	0.1	0.3	0.2
45.1	36	52	8	PoEPl	847.69	595.48	545.46	593.46	0.2	0.2	0.3	0.1	0.1	0.1	0.2	0.2
45.3	36	52	8	LLnPn	847.69	597.49	569.46	567.45	0.4	0.2	0.3	0.3	0.2	0.1	0.3	0.2
45.4	36	52	8	LnLnPl	847.69	595.48	569.46	569.46	10.1	11.4	5.9	9.2	8.7	3.5	8.6	3.5
45.8	36	50	7	PoPnLn	821.68	543.45	571.48	567.45	0.8	0.4	0.7	0.7	0.6	0.4	0.7	0.4
46.1	36	50	7	LnPlPl	821.67	569.46	569.46	543.44	0.6	0.3	0.3	0.5	0.3	0.1	0.4	0.2
46.8	36	48	6	PPnPn	795.66	545.46	545.46	539.42	0.6	0.4	0.4	0.5	0.3	0.1	0.4	0.2
47.3	38	58	10	AAL	927.74	647.50	623.50	623.50	1.0	0.5	0.3	0.9	0.3	0.1	0.1	0.0
47.5	38	58	10	EAO	927.75	645.49	623.51	625.52	0.9	0.6	0.3	0.8	0.5	0.1	0.2	0.0
47.8	38	56	9	LEL	901.73	621.49	599.50	621.49	4.0	2.0	0.4	3.5	1.6	0.2	0.4	0.1
47.9	38	56	9	LnEO	901.74	619.48	599.51	623.51	0.6	0.5	0.3	0.5	0.3	0.1	0.1	0.0
48.1	38	56	9	PAE	901.73	599.50	597.49	645.49	0.3	0.2	0.3	0.2	0.1	0.1	0.0	0.0
48.2	38	56	9	PoAA	901.73	597.49	597.49	647.50	0.3	0.2	0.3	0.2	0.1	0.1	0.0	0.0
48.3	38	54	8	LnAPo	875.72	621.49	571.48	597.49	0.1	0.6	0.3	0.7	0.4	0.1	0.4	0.2
50.0	38	54	8	LnEP	875.72	619.48	573.49	597.49	0.1	1.8	1.2	0.9	1.2	0.6	1.3	0.6
50.1	38	52	7	PPlE	849.70	547.47	597.49	593.46	0.4	0.9	0.3	0.3	0.1	0.1	0.2	0.2
50.2	38	52	7	PoPoE	849.71	547.48	595.48	595.48	0.4	0.4	0.3	0.3	0.3	0.1	0.4	0.2
50.3	38	52	7	LnPoLn	849.71	571.48	595.48	571.48	5.8	5.3	5.0	5.8	4.0	3.2	4.2	3.0
50.6	38	52	7	PlLLn	849.70	571.47	569.46	597.49	7.7	8.2	4.4	7.8	6.3	2.5	6.4	2.6
50.8	38	54	7	PoEL	875.72	595.48	573.49	621.49	0.4	0.3	0.3	0.3	0.2	0.1	0.3	0.2
51.1	38	52	7	LLnPl	849.70	597.49	571.47	569.46	0.3	0.3	0.3	0.2	0.2	0.1	0.3	0.2
54.2	38	50	6	LPlPl	823.68	571.47	571.47	543.44	0.3	0.2	0.3	0.2	0.2	0.1	0.3	0.2
54.3	38	50	6	MPoE	823.69	521.46	569.46	595.48	0.2	0.2	0.3	0.1	0.1	0.1	0.2	0.1
54.4	38	48	5	PlPlPo	797.67	543.44	545.46	545.46	0.3	0.1	0.1	0.3	0.2	0.2	0.3	0.2
54.5	38	48	5	PoPoPn	797.68	547.48	543.45	543.45	0.3	0.1	0.1	0.2	0.1	0.1	0.2	0.2
54.6	38	48	5	PPlPn	797.67	547.47	545.46	541.43	0.2	0.1	0.1	0.3	0.2	0.2	0.3	0.2
54.6	38	46	4	MPlPl	771.65	519.44	519.44	543.44	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2
54.7	40	58	9	ELnPo	929.75	619.48	595.48	851.71	0.2	0.2	0.3	0.1	0.1	0.1	0.0	0.0

54.7	40	56	8	ELPo	875.72	621.49	595.48	573.49	0.4	0.3	0.3	0.3	0.2	0.1	0.3	0.2
54.8	40	56	8	PAA	903.74	599.50	599.50	647.50	0.5	0.3	0.3	0.5	0.2	0.2	0.3	0.2
54.9	40	56	8	LnOA	903.75	599.51	621.49	625.52	0.5	0.4	0.4	0.4	0.3	0.3	0.3	0.2
55.0	42	56	8	ELO	903.75	621.49	623.51	601.52	0.4	0.7	0.4	0.3	0.5	0.2	0.6	0.2
55.1	40	54	7	PoAL	877.73	597.49	573.49	623.50	0.5	0.3	0.3	0.4	0.2	0.1	0.3	0.2
55.2	40	54	7	LnAP	877.73	621.49	573.49	599.50	1.5	1.8	0.8	1.2	1.4	0.5	1.6	0.5
55.6	40	54	7	PEL	877.73	597.49	575.50	621.49	0.5	1.0	0.5	0.5	0.8	0.3	0.9	0.3
57.4	40	52	6	LnPoL	851.72	571.48	597.49	573.49	3.7	3.2	3.0	3.4	2.5	1.8	2.8	1.9
58.1	40	52	6	LnPLn	851.72	573.49	595.48	573.49	8.3	10.6	12.6	8.1	9.6	8.5	10.2	8.0
58.3	42	56	7	EOO	905.77	623.51	623.51	603.54	0.2	0.2	0.4	0.1	0.1	0.2	0.2	0.2
58.6	42	54	6	PAL	879.74	599.50	575.50	623.50	0.7	0.7	0.3	0.7	0.9	0.3	0.1	0.3
58.7	42	54	6	PEO	879.75	597.49	577.52	623.51	0.1	0.1	0.3	0.1	0.2	0.3	0.2	0.3
58.9	42	52	5	PoOLn	853.74	575.51	571.48	599.51	0.3	0.2	0.1	0.2	0.1	0.1	0.2	0.2
59.0	40	52	6	PoEP	851.72	595.48	549.49	597.49	0.1	0.2	0.1	0.1	0.1	0.1	0.2	0.2
59.2	40	50	5	LnPoPo	825.71	571.48	571.48	547.48	0.2	0.3	0.7	0.3	0.3	0.6	0.4	0.6
59.5	40	48	4	PPoPn	799.69	549.49	545.46	543.45	0.3	0.2	0.1	0.4	0.3	0.1	0.4	0.2
59.7	40	48	4	PPlPl	799.68	547.47	547.47	543.44	0.1	0.1	0.7	0.1	0.2	0.5	0.2	0.4
60.0	42	52	5	LPoL	853.73	573.49	599.50	573.49	1.6	1.0	0.9	2.0	1.6	1.0	1.9	1.1
60.1	42	52	5	LnPL	853.73	573.49	597.49	575.50	4.8	5.5	7.0	5.5	9.4	7.6	10.1	7.3
60.2	40	48	4	LnMPo	799.69	545.46	571.48	521.46	1.7	1.0	1.2	2.0	1.6	1.0	1.7	1.2
60.2	42	52	5	LPoL	853.73	573.49	599.50	573.49	0.1	0.1	0.3	0.1	0.1	0.3	0.2	0.3
60.4	42	52	5	PoAP	853.73	597.49	549.49	599.50	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2
60.5	40	48	4	PoPlPo	799.69	545.46	547.48	545.46	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2
60.6	42	52	5	PEP	853.73	597.49	551.50	597.49	0.1	0.3	0.7	0.1	0.4	0.4	0.4	0.4
60.7	40	46	3	MPoPl	773.67	521.46	519.44	545.46	0.1	0.2	0.3	0.2	0.3	0.3	0.4	0.3
60.8	42	50	4	PLPl	827.71	575.50	547.47	571.47	0.9	1.3	1.2	0.9	1.8	1.6	1.8	1.6
60.9	40	46	3	MPPl	775.68	523.47	519.44	547.47	0.1	0.1	0.3	0.2	0.2	0.4	0.3	0.4
60.9	42	50	4	PoPoL	827.72	547.48	573.49	573.49	0.0	0.1	0.0	0.1	0.2	0.2	0.4	0.2
61.1	42	50	4	LnPoP	827.72	571.48	573.49	549.49	0.5	0.9	1.8	0.5	1.2	2.5	1.3	2.4
61.5	42	50	4	PoPlO	827.72	545.46	575.51	573.49	0.6	0.7	1.2	0.8	0.9	1.0	0.9	1.0
62.0	42	48	3	PPoPl	801.70	549.49	547.47	545.46	0.4	0.3	0.4	0.7	0.8	0.7	1.1	0.7

62.5	42	48	3	PPPn	801.70	551.50	545.46	545.46	0.3	0.2	0.3	0.6	0.5	0.4	0.7	0.5
62.8	42	48	3	PoML	801.70	521.46	573.49	547.47	0.0	0.0	0.0	0.1	0.1	0.2	0.2	0.4
64.2	42	48	3	LnMP	801.70	545.46	573.49	523.47	0.0	0.2	0.8	0.1	0.4	1.2	0.5	1.4
64.3	42	46	2	MPoPo	775.69	521.46	521.46	547.48	0.0	0.0	0.0	0.1	0.1	0.2	0.2	0.2
64.4	44	54	5	LLO	881.76	599.50	601.52	601.52	0.4	0.6	0.9	0.5	0.7	0.8	0.8	0.7
64.5	44	54	5	AOP	881.76	625.52	599.50	577.52	0.2	0.1	0.1	0.1	0.2	0.2	0.2	0.2
65.9	44	50	3	OPoPo	829.74	575.51	575.51	547.48	0.0	0.0	0.1	0.1	0.1	0.3	0.2	0.4
66.7	44	50	3	LPPo	829.73	575.50	573.49	549.49	0.2	0.3	1.2	0.3	0.7	1.4	0.9	1.8
68.1	44	50	3	LnPP	829.73	573.49	573.49	551.50	0.4	1.3	3.6	0.9	4.1	9.4	5.1	8.8
68.5	44	52	4	POLn	855.75	577.52	573.49	599.51	0.7	0.5	0.7	0.9	0.7	0.6	0.9	0.6
68.8	44	52	4	OPoL	855.75	575.51	601.52	573.49	0.1	0.2	0.9	0.2	0.4	0.8	0.5	0.7
68.9	44	52	4	LLP	855.74	599.50	575.50	575.50	2.3	4.6	3.4	3.3	6.5	4.2	6.8	4.2
69.2	44	52	4	PAP	855.74	599.50	551.50	599.50	0.0	0.3	0.4	0.1	0.4	0.4	0.5	0.4
69.5	44	50	3	PoPL	829.73	549.49	573.49	575.50	0.1	0.2	1.1	0.3	0.7	1.4	0.9	1.5
70.0	44	48	2	PPPl	803.71	551.50	547.47	547.47	0.0	0.2	0.1	0.3	0.4	0.3	0.6	0.4
70.3	44	48	2	PPoPo	803.72	549.49	549.49	547.48	0.0	0.0	0.3	0.1	0.1	0.5	0.2	0.6
70.9	44	48	2	LMP	803.71	547.47	575.50	523.47	0.0	0.0	0.3	0.1	0.2	0.7	0.3	0.7
71.5	44	46	1	PoMP	777.70	521.46	549.49	523.47	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.2
71.7	46	54	4	LOO	883.78	601.52	601.52	603.54	0.1	0.7	2.0	0.2	1.0	2.0	1.2	1.8
73.3	46	52	3	OPoO	857.77	575.51	603.54	575.51	0.0	0.0	0.4	0.1	0.1	0.7	0.2	0.7
74.1	46	52	3	OPL	857.76	577.52	601.52	575.50	0.1	0.8	1.5	0.3	1.7	3.4	2.0	3.5
74.3	46	50	2	OMO	831.75	549.49	603.54	549.49	0.0	0.0	0.0	0.1	0.1	0.3	0.2	0.4
74.5	46	50	2	OPPo	831.75	577.52	575.51	549.49	0.0	0.1	0.4	0.1	0.2	1.1	0.4	1.6
75.3	46	50	2	PPL	831.74	551.50	575.50	575.50	0.3	1.1	2.6	0.5	2.1	4.6	2.3	6.1
75.6	46	48	1	PPoP	805.73	549.49	551.50	549.49	0.0	0.2	1.1	0.1	0.3	1.9	0.5	2.0
75.8	46	48	1	PMO	805.73	523.47	577.52	549.49	0.0	0.0	0.3	0.1	0.1	0.6	0.2	0.7
76.2	46	46	0	PMP	779.71	523.47	551.50	523.47	0.0	0.0	0.4	0.1	0.1	0.9	0.2	1.0
78.8	48	52	2	OPO	859.78	577.52	603.54	577.52	0.0	0.2	1.5	0.1	0.5	2.7	0.7	3.0
80.1	48	50	1	OPP	833.76	577.52	577.52	551.50	0.0	0.3	2.1	0.1	0.8	5.6	0.9	5.5
81.3	48	48	0	PPP	807.74	551.50	551.50	551.50	0.0	0.3	1.8	0.1	0.7	4.1	0.7	4.3

[a] The values given in columns 906, 493, NAP, etc. are area ratios of TIC chromatograms and indicate approximate ratios of TAGs

Fig. 1S. Mass spectrum of picolinyl ester of 16:2n-6 acid. For explanation of values see the text.

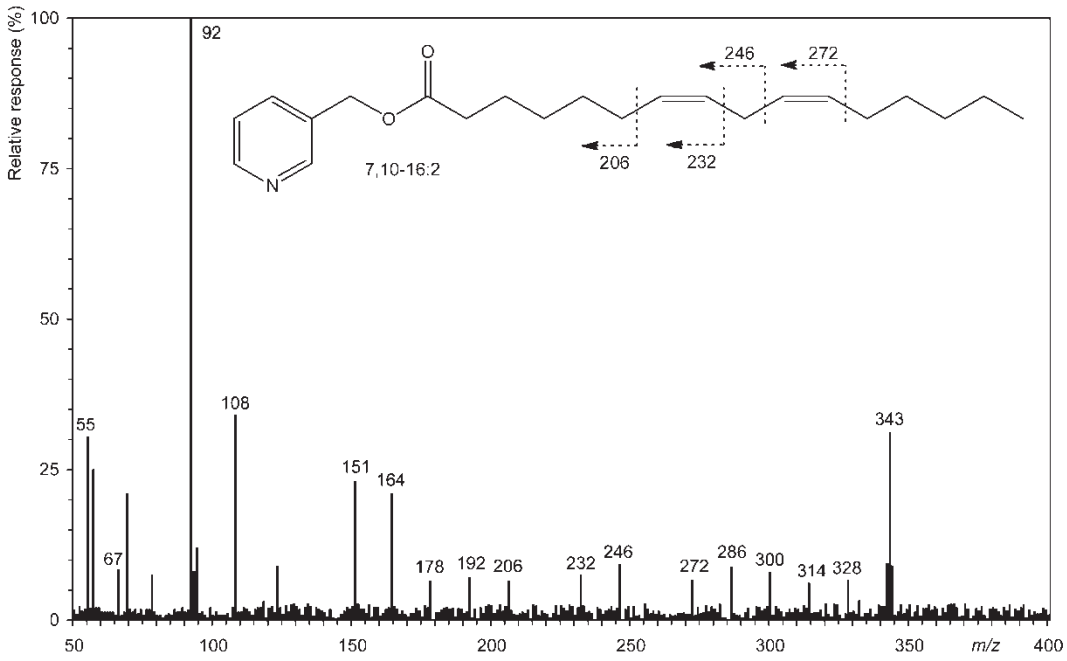


Fig. 2S. Mass spectrum of picolinyl ester of 16:3n-3 acid. For explanation of values see the text.

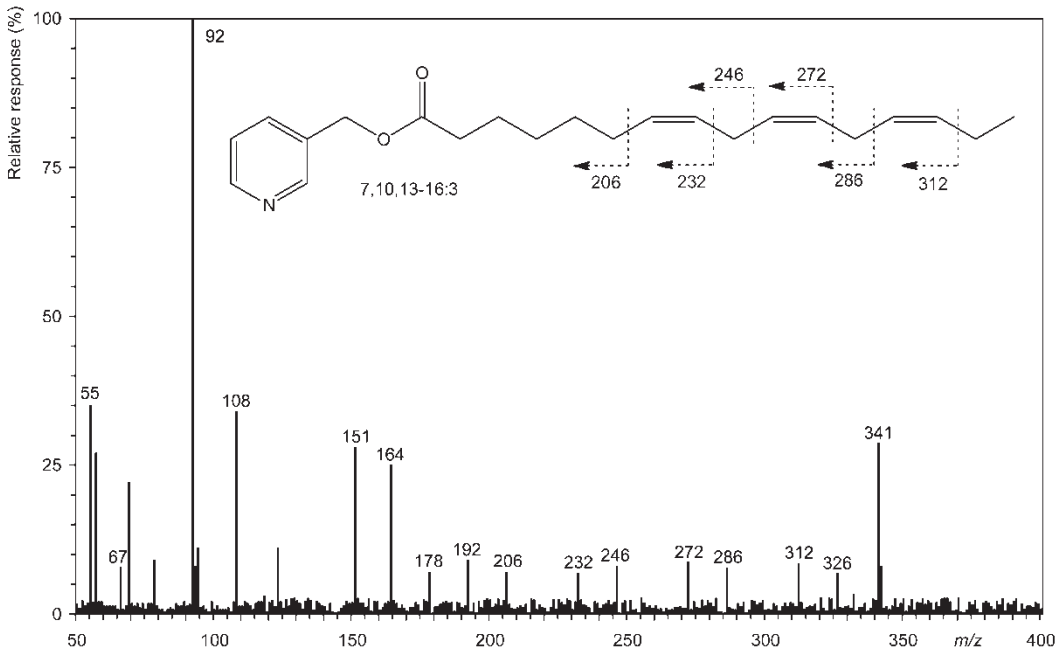
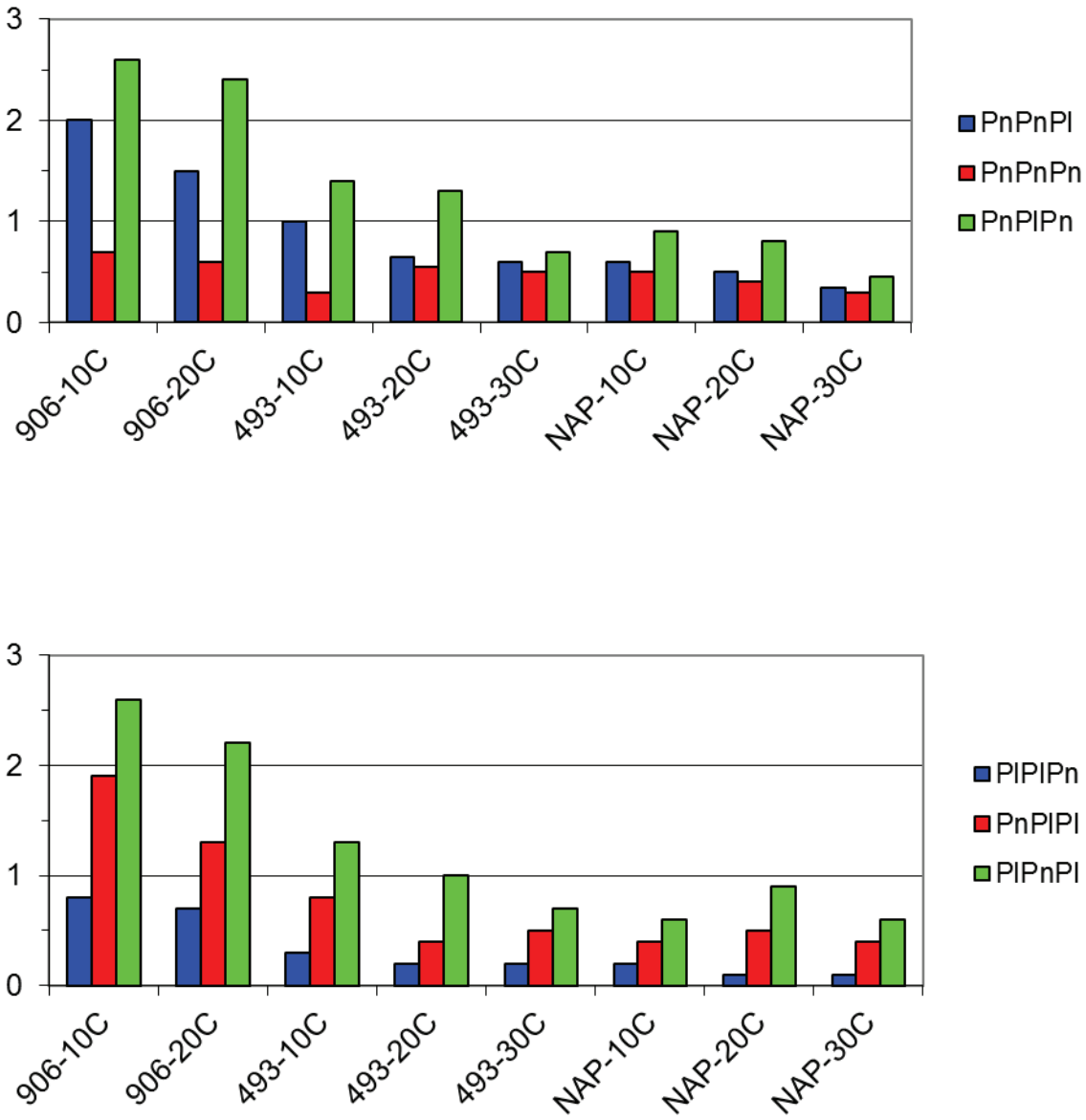
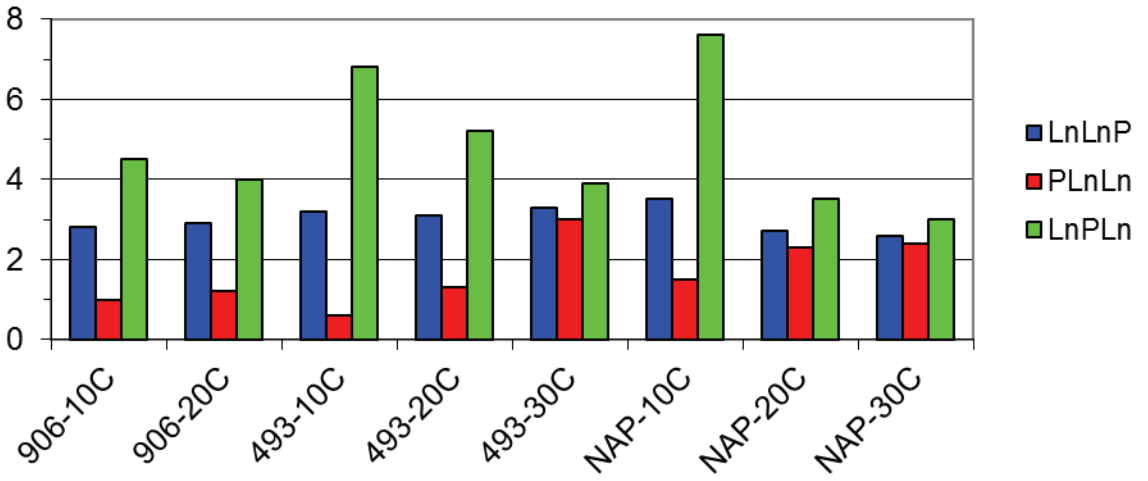


Fig. 3S. Ratio of different regioisomers and enantiomers of TAGs from *S. bacillaris*.




8
6
4
2
0
LnLnP
PLnLn
LnPLn
906-10C
906-20C
493-10C
493-20C
493-30C
NAP-10C
NAP-20C
NAP-30C

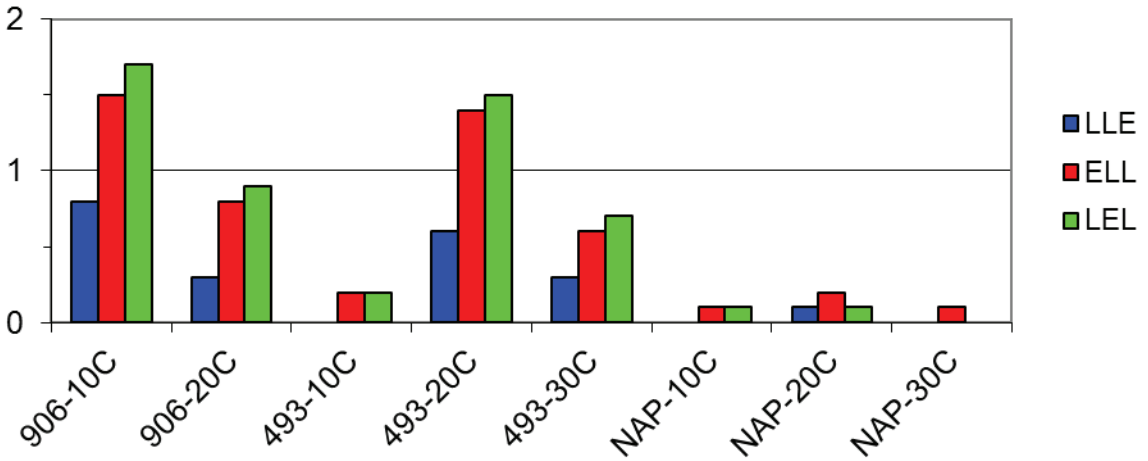

2
1
0
LLE
ELL
LEL
906-10C
906-20C
493-10C
493-20C
493-30C
NAP-10C
NAP-20C
NAP-30C

Fig. 4S. Principal component analysis (PCA) of the relative proportions of regioisomers and enantiomers of 30 most abundant TAGs in *S. bacillaris* strains cultivated at 10 °C, 20 °C and 30 °C. The first two canonical axes are plotted; they explained 80.0 % of the variability. For FA and TAGs abbreviations, see Tables 1 and 2.