

Comprehensive LC–MS^E Lipidomic Analysis using a Shotgun Approach and Its Application to Biomarker Detection and Identification in Osteoarthritis Patients [*Journal of Proteome Research* 2010, 9, 2377–2389 DOI: 10.1021/pr901094j].

Jose M. Castro-Perez,* Jurre Kamphorst, Jeroen DeGroot, Floris Lafeber, Jeff Goshawk, Kate Yu, John P. Shockcor, Rob J. Vreeken, and Thomas Hankemeier

Page 2377: In the abstract, the total number of lipids identified and quantified was 275, not 284 as originally reported.

Page 2379: In section 2.5, ammonium acetate was mentioned twice. Both instances should be ammonium formate.

Page 2381: In section 3.5, the total number of fatty acids is listed twice should be 275, not 284 as originally reported.

There was an error in Table S1 in the Supporting Information. The corrected Table S1 is presented here.

Table S1. List of All Major Lipids Identified in the Human Extracted Plasma^a

class	formula	<i>m/z</i> found	ppm	time (min)	provisional assignment class		ionization mode	
ChoE	C ₄₇ H ₇₇ NO ₂	688.6016	−2.4	9.5	ChoE	20:5	[M + NH ₄] ⁺	
	C ₄₉ H ₇₉ NO ₂	714.6185	−0.6	9.61	ChoE	22:6	[M + NH ₄] ⁺	
	C ₄₅ H ₇₇ NO ₂	664.6057	3.6	9.67	ChoE	18:3	[M + NH ₄] ⁺	
	C ₄₇ H ₇₉ NO ₂	690.6189	0.1	9.72	ChoE	20:4	[M + NH ₄] ⁺	
	C ₄₅ H ₇₉ NO ₂	666.6193	0.6	9.84	ChoE	18:2	[M + NH ₄] ⁺	
	C ₄₅ H ₈₁ NO ₂	668.6337	−1.3	10.14	ChoE	18:1	[M + NH ₄] ⁺	
DG	C ₃₉ H ₇₁ NO ₅	634.5411	0	6.41	DG	36:4	[M + NH ₄] ⁺	
FA	C ₁₈ H ₃₀ O ₂	277.2150	−6.4	1.46	FA	18:3	[M − H] [−]	
	C ₂₂ H ₃₂ O ₂	327.2301	−7.1	1.52	FA	22:6	[M − H] [−]	
	C ₁₄ H ₂₈ O ₂	227.2023	5.1	1.55	FA	14:0	[M − H] [−]	
	C ₁₆ H ₃₀ O ₂	253.2170	0.9	1.65	FA	16:1	[M − H] [−]	
	C ₂₀ H ₃₂ O ₂	303.2309	−5	1.7	FA	20:4	[M − H] [−]	
	C ₁₈ H ₃₂ O ₂	279.2319	−1.9	1.8	FA	18:2	[M − H] [−]	
	C ₂₀ H ₃₄ O ₂	305.2476	−1.6	1.98	FA	20:3	[M − H] [−]	
	C ₁₆ H ₃₂ O ₂	255.2324	−0.1	2.12	FA	16:0	[M − H] [−]	
	C ₂₂ H ₃₆ O ₂	331.2635	−0.7	2.18	FA	22:4	[M − H] [−]	
	C ₁₈ H ₃₄ O ₂	281.2479	−0.6	2.24	FA	18:1	[M − H] [−]	
	C ₁₇ H ₃₄ O ₂	269.2484	1.2	2.47	FA	17:0	[M − H] [−]	
	C ₁₈ H ₃₆ O ₂	283.2638	0.2	2.86	FA	18:0	[M − H] [−]	
	C ₂₀ H ₃₈ O ₂	309.2786	−2.5	2.95	FA	20:1	[M − H] [−]	
	C ₂₀ H ₄₀ O ₂	311.2971	6.6	3.68	FA	20:0	[M − H] [−]	
	PC	C ₄₂ H ₇₆ NO ₈ P	754.5411	3.2	4.89	PC	34:4	[M + H] ⁺
		C ₄₀ H ₇₆ NO ₈ P	730.5409	3.1	4.4	PC	32:2	[M + H] ⁺
		C ₄₄ H ₇₈ NO ₈ P	780.5551	1	4.54	PC	36:5	[M + H] ⁺
C ₄₆ H ₇₆ NO ₈ P		802.5403	2	4.54	PC	38:8	[M + H] ⁺	
C ₄₆ H ₈₀ NO ₈ P		806.5709	1.2	4.55	PC	38:6	[M + H] ⁺	
C ₄₄ H ₇₆ NO ₈ P		778.5371	−2.1	4.59	PC	36:6	[M + H] ⁺	
C ₄₄ H ₈₀ NO ₈ P		782.5715	2	4.62	PC	36:4	[M + H] ⁺	
C ₄₂ H ₇₈ NO ₈ P		756.5535	−1.1	4.71	PC	34:3	[M + H] ⁺	
C ₄₂ H ₈₂ NO ₇ P		744.5935	3.8	4.71	PC-plasm	34:1	[M + H] ⁺	
C ₄₄ H ₈₀ NO ₈ P		782.5718	2.4	4.78	PC	36:4	[M + H] ⁺	
C ₄₆ H ₈₀ NO ₈ P		806.5729	3.7	4.78	PC	38:6	[M + H] ⁺	
C ₄₀ H ₇₈ NO ₈ P		732.5576	4.5	4.89	PC	32:1	[M + H] ⁺	

Table S1. Continued

class	formula	<i>m/z</i> found	ppm	time (min)	provisional assignment class		ionization mode
	C ₄₆ H ₇₈ NO ₈ P	804.5527	−2	4.93	PC	37:0	[M + H] ⁺
	C ₄₄ H ₈₀ NO ₈ P	782.5728	3.6	4.94	PC	36:4	[M + H] ⁺
	C ₃₅ H ₇₀ NO ₈ P	664.4935	2.7	4.96	PC	28:7	[M + H] ⁺
	C ₄₆ H ₈₂ NO ₈ P	808.5896	4.9	4.96	PC	38:5	[M + H] ⁺
	C ₄₂ H ₈₀ NO ₈ P	758.5718	2.4	5.02	PC	34:2	[M + H] ⁺
	C ₄₄ H ₇₈ NO ₈ P	780.5545	0.2	5.04	PC	36:5	[M + H] ⁺
	C ₄₄ H ₈₂ NO ₈ P	784.5876	2.5	5.09	PC	36:3	[M + H] ⁺
	C ₄₄ H ₈₀ NO ₇ P	766.5762	1.4	5.15	PC-plasm	36:4	[M + H] ⁺
	C ₄₄ H ₈₂ NO ₈ P	784.5876	2.5	5.15	PC	36:3	[M + H] ⁺
	C ₄₆ H ₈₂ NO ₈ P	808.5851	−0.6	5.15	PC	38:5	[M + H] ⁺
	C ₄₆ H ₈₀ NO ₈ P	806.5684	−1.9	5.18	PC	38:6	[M + H] ⁺
	C ₄₃ H ₈₂ NO ₈ P	772.5861	0.6	5.22	PC	35:2	[M + H] ⁺
	C ₄₆ H ₈₂ NO ₇ P	792.5931	3	5.23	PC-plasm	38:5	[M + H] ⁺
	C ₄₅ H ₈₂ NO ₈ P	796.5875	2.4	5.23	PC	37:4	[M + H] ⁺
	C ₄₆ H ₈₄ NO ₈ P	810.6044	3.9	5.23	PC	38:4	[M + H] ⁺
	C ₄₈ H ₈₂ NO ₈ P	832.5808	−5.8	5.23	PC	39:0	[M + H] ⁺
	C ₄₆ H ₈₀ NO ₇ P	790.5731	−2.5	5.3	PC-plasm	38:6	[M + H] ⁺
	C ₄₃ H ₈₂ NO ₈ P	772.5858	0.2	5.31	PC	35:2	[M + H] ⁺
	C ₄₄ H ₇₈ NO ₇ P	764.5595	0.1	5.32	PC-plasm	36:5	[M + H] ⁺
	C ₄₆ H ₈₄ NO ₈ P	810.6016	0.4	5.35	PC	38:4	[M + H] ⁺
	C ₄₈ H ₈₄ NO ₈ P	834.6031	2.2	5.36	PC	40:6	[M + H] ⁺
	C ₄₀ H ₈₀ NO ₈ P	734.5718	2.5	5.43	PC	32:0	[M + H] ⁺
	C ₄₄ H ₈₄ NO ₇ P	770.6059	−0.6	5.43	PC-plasm	36:2	[M + H] ⁺
	C ₄₆ H ₈₄ NO ₇ P	794.6064	0	5.43	PC-plasm	38:4	[M + H] ⁺
	C ₄₂ H ₈₂ NO ₈ P	760.5883	3.5	5.44	PC	34:1	[M + H] ⁺
	C ₄₈ H ₈₆ NO ₇ P	820.6230	1.2	5.44	PC-plasm	40:5	[M + H] ⁺
	C ₄₄ H ₈₀ NO ₈ P	782.5695	−0.6	5.45	PC	36:4	[M + H] ⁺
	C ₄₆ H ₈₄ NO ₈ P	810.6037	3	5.51	PC	38:4	[M + H] ⁺
	C ₄₈ H ₈₂ NO ₈ P	832.5830	−3.1	5.51	PC	40:7	[M + H] ⁺
	C ₄₈ H ₈₆ NO ₈ P	836.6119	−6	5.51	PC	40:5	[M + H] ⁺
	C ₄₆ H ₈₂ NO ₈ P	808.5830	−3.2	5.58	PC	38:5	[M + H] ⁺
	C ₄₄ H ₈₄ NO ₈ P	786.6025	1.6	5.59	PC	36:2	[M + H] ⁺
	C ₄₃ H ₇₈ NO ₈ P	768.5568	3.2	5.66	PC	35:4	[M + H] ⁺
	C ₄₃ H ₈₄ NO ₈ P	774.6008	−0.6	5.71	PC	35:1	[M + H] ⁺
	C ₄₂ H ₈₄ NO ₇ P	746.6033	−4.2	5.72	PC-plasm	34:0	[M + H] ⁺
	C ₄₆ H ₈₆ NO ₈ P	812.6152	−2.1	5.72	PC	38:3	[M + H] ⁺
	C ₄₈ H ₈₄ NO ₈ P	834.5981	−3.8	5.72	PC	40:6	[M + H] ⁺
	C ₄₂ H ₈₄ NO ₈ P	762.6032	2.6	5.91	PC	34:0	[M + H] ⁺
	C ₄₄ H ₈₂ NO ₈ P	784.5865	1.1	5.91	PC	36:3	[M + H] ⁺
	C ₄₄ H ₈₆ NO ₈ P	788.6165	−0.5	5.98	PC	36:1	[M + H] ⁺
	C ₄₆ H ₈₄ NO ₈ P	810.5992	−2.5	5.98	PC	38:4	[M + H] ⁺
	C ₄₆ H ₈₈ NO ₈ P	814.6338	1.5	6.03	PC	38:2	[M + H] ⁺
	C ₄₁ H ₇₆ NO ₈ P	742.5365	−2.9	6.06	PC	33:3	[M + H] ⁺
	C ₃₉ H ₇₈ NO ₈ P	720.5533	−1.4	6.06	PC	31:0	[M + H] ⁺
	C ₄₆ H ₉₂ NO ₈ P	818.6649	1.3	6.83	PC	38:0	[M + H] ⁺
	C ₅₂ H ₉₆ NO ₈ P	894.6934	−2	8.44	PC	44:4	[M + H] ⁺
	C ₅₀ H ₉₆ NO ₈ P	870.6982	3.5	8.57	PC	42:2	[M + H] ⁺
	C ₅₂ H ₉₈ NO ₈ P	896.7118	1.1	8.6	PC	44:3	[M + H] ⁺
	C ₅₂ H ₁₀₀ NO ₈ P	898.7225	−4.4	8.82	PC	44:2	[M + H] ⁺
	C ₅₄ H ₁₀₂ NO ₈ P	924.7462	4.4	8.83	PC	46:3	[M + H] ⁺
	C ₄₈ H ₉₄ NO ₈ P	844.6763	−3.8	8.9	PC	40:2	[M + H] ⁺
	C ₅₂ H ₁₀₂ NO ₈ P	900.7373	−5.3	9.02	PC	44:1	[M + H] ⁺
	C ₅₄ H ₁₀₆ NO ₈ P	928.7690	−4.8	9.21	PC	46:1	[M + H] ⁺
PE	C ₄₃ H ₇₆ NO ₈ P	764.5237	0.8	5.16	PE	38:5	[M − H] [−]

Table S1. Continued

class	formula	<i>m/z</i> found	ppm	time (min)	provisional assignment class		ionization mode
PG	C ₃₉ H ₇₄ NO ₈ P	714.5103	4	5.18	PE	34:2	[M – H] [–]
	C ₄₃ H ₇₈ NO ₈ P	766.5403	2.1	5.65	PE	38:4	[M – H] [–]
	C ₄₁ H ₇₈ NO ₈ P	742.5404	2.3	5.74	PE	36:2	[M – H] [–]
	C ₃₂ H ₆₃ O ₁₀ P	637.4073	–1.2	2.79	PG	26:0	[M – H] [–]
	C ₃₆ H ₇₁ O ₁₀ P	693.4739	4.6	4	PG	30:0	[M – H] [–]
PI	C ₅₂ H ₉₉ O ₁₀ P	913.6851	–5.1	6.26	PG	46:2	[M – H] [–]
	C ₄₅ H ₇₉ O ₁₃ P	857.5202	2.5	3.99	PI	36:4	[M – H] [–]
	C ₄₃ H ₇₉ O ₁₃ P	833.5187	0.8	4.07	PI	34:2	[M – H] [–]
	C ₄₉ H ₈₃ O ₁₃ P	909.5511	1.9	4.42	PI	40:6	[M – H] [–]
	C ₄₃ H ₈₁ O ₁₃ P	835.5377	4.8	4.5	PI	34:1	[M – H] [–]
PS	C ₄₇ H ₈₃ O ₁₃ P	885.5524	3.5	4.57	PI	38:4	[M – H] [–]
	C ₄₅ H ₈₃ O ₁₃ P	861.5481	–1.4	4.64	PI	36:2	[M – H] [–]
	C ₄₇ H ₈₅ O ₁₃ P	887.5643	–0.8	4.76	PI	38:3	[M – H] [–]
	C ₃₇ H ₇₂ NO ₁₀ P	720.4839	3.2	4.11	PS	31:0	[M – H] [–]
	C ₄₄ H ₈₀ NO ₁₀ P	812.5402	–4.9	4.32	PS	38:3	[M – H] [–]
	C ₄₂ H ₈₀ NO ₁₀ P	788.5465	2.9	4.42	PS	36:1	[M – H] [–]
	C ₄₆ H ₈₂ NO ₁₀ P	838.5621	2.7	4.42	PS	40:4	[M – H] [–]
	C ₄₄ H ₈₂ NO ₁₀ P	814.5624	3.1	4.53	PS	38:2	[M – H] [–]
	C ₄₆ H ₈₂ NO ₁₀ P	838.5647	5.8	4.56	PS	40:4	[M – H] [–]
	C ₄₈ H ₈₄ NO ₁₀ P	864.5773	2.1	4.56	PS	42:5	[M – H] [–]
	C ₄₆ H ₈₄ NO ₁₀ P	840.5766	1.3	4.66	PS	40:3	[M – H] [–]
	C ₄₃ H ₈₂ NO ₁₀ P	802.5607	1.1	4.73	PS	37:1	[M – H] [–]
	C ₄₈ H ₈₄ NO ₁₀ P	864.5776	2.4	4.79	PS	42:5	[M – H] [–]
	C ₃₉ H ₇₂ NO ₁₀ P	744.4801	–2	4.96	PS	33:2	[M – H] [–]
	C ₄₈ H ₈₆ NO ₁₀ P	866.5933	2.5	4.98	PS	42:4	[M – H] [–]
	C ₄₄ H ₈₄ NO ₁₀ P	816.5768	1.6	5.05	PS	38:1	[M – H] [–]
	C ₄₆ H ₈₆ NO ₁₀ P	842.5944	3.9	5.11	PS	40:2	[M – H] [–]
	C ₄₈ H ₈₆ NO ₁₀ P	866.5925	1.6	5.16	PS	42:4	[M – H] [–]
	C ₄₆ H ₈₆ NO ₁₀ P	842.5911	0	5.19	PS	40:2	[M – H] [–]
	C ₄₅ H ₈₆ NO ₁₀ P	830.5872	–4.7	5.26	PS	39:1	[M – H] [–]
	C ₄₅ H ₈₆ NO ₁₀ P	830.5933	2.6	5.31	PS	39:1	[M – H] [–]
	C ₄₆ H ₈₆ NO ₁₀ P	842.5946	4.1	5.37	PS	40:2	[M – H] [–]
	C ₅₀ H ₈₈ NO ₁₀ P	892.6071	0.4	5.37	PS	44:5	[M – H] [–]
	C ₄₄ H ₈₆ NO ₁₀ P	818.5949	4.6	5.46	PS	38:0	[M – H] [–]
	C ₄₈ H ₈₈ NO ₁₀ P	868.6103	4	5.53	PS	42:3	[M – H] [–]
	C ₅₀ H ₉₀ NO ₁₀ P	894.6236	1.3	5.54	PS	44:4	[M – H] [–]
	C ₄₅ H ₈₆ NO ₁₀ P	830.5903	–1	5.61	PS	39:1	[M – H] [–]
	C ₄₆ H ₈₈ NO ₁₀ P	844.6032	–4.2	5.61	PS	40:1	[M – H] [–]
	C ₅₀ H ₉₀ NO ₁₀ P	894.6234	1.1	5.72	PS	44:4	[M – H] [–]
	C ₄₈ H ₉₀ NO ₁₀ P	870.6227	0.3	5.74	PS	42:2	[M – H] [–]
	C ₄₅ H ₈₈ NO ₁₀ P	832.6057	–1.3	5.77	PS	39:0	[M – H] [–]
	C ₅₀ H ₉₂ NO ₁₀ P	896.6399	2	5.91	PS	44:3	[M – H] [–]
	C ₄₆ H ₉₀ NO ₁₀ P	846.6190	–4.1	6.01	PS	40:0	[M – H] [–]
	C ₄₃ H ₈₀ NO ₁₀ P	800.5396	–5.7	6.08	PS	37:2	[M – H] [–]
LPC	C ₂₄ H ₄₈ NO ₇ P	494.3251	0.8	1.15	LPC	16:1	[M + H] ⁺
	C ₂₈ H ₄₈ NO ₇ P	542.3225	–4.1	1.21	LPC	20:5	[M + H] ⁺
	C ₂₂ H ₄₇ NO ₇ P	468.3079	–2.3	1.21	LPC	14:0	[M + H] ⁺
	C ₂₆ H ₅₀ NO ₇ P	520.3397	–1.1	1.21	LPC	18:2	[M + H] ⁺
	C ₃₀ H ₅₀ NO ₇ P	568.3428	4.4	1.22	LPC	22:6	[M + H] ⁺
	C ₂₈ H ₅₀ NO ₇ P	544.3421	3.3	1.23	LPC	20:4	[M + H] ⁺
	C ₂₆ H ₅₀ NO ₇ P	520.3394	–1.7	1.26	LPC	18:2	[M + H] ⁺
	C ₂₃ H ₄₈ NO ₇ P	482.3244	–0.6	1.42	LPC	15:0	[M + H] ⁺
	C ₂₆ H ₄₈ NO ₇ P	518.3246	–0.1	1.43	LPC	18:3	[M + H] ⁺
	C ₂₄ H ₅₀ NO ₇ P	496.3399	–0.8	1.45	LPC	16:0	[M + H] ⁺

Table S1. Continued

class	formula	m/z found	ppm	time (min)	provisional assignment class		ionization mode
LPE	C ₂₆ H ₅₂ NO ₇ P	522.3538	−4.1	1.57	LPC	18:1	[M + H] ⁺
	C ₂₅ H ₅₂ NO ₇ P	510.3568	1.7	1.69	LPC	17:0	[M + H] ⁺
	C ₂₇ H ₅₀ NO ₇ P	532.3395	−1.5	1.69	LPC	19:3	[M + H] ⁺
	C ₂₆ H ₅₄ NO ₇ P	524.3726	1.9	1.84	LPC	18:0	[M + H] ⁺
	C ₂₄ H ₅₀ NO ₆ P	480.3436	−3.7	1.88	LPC	15:1	[M + H] ⁺
	C ₂₄ H ₅₂ NO ₆ P	482.3603	−1.7	1.93	LPC	15:0	[M + H] ⁺
	C ₂₆ H ₅₄ NO ₇ P	524.3726	1.9	1.97	LPC	18:0	[M + H] ⁺
	C ₂₈ H ₅₂ NO ₇ P	546.3549	−1.9	1.99	LPC	20:3	[M + H] ⁺
	C ₂₈ H ₅₂ NO ₇ P	546.3559	−0.1	2.02	LPC	20:3	[M + H] ⁺
	C ₂₆ H ₅₄ NO ₆ P	508.3758	−1.8	2.06	LPC	17:1	[M + H] ⁺
	C ₂₇ H ₅₆ NO ₇ P	538.3885	2.3	2.14	LPC	19:0	[M + H] ⁺
	C ₂₇ H ₅₆ NO ₇ P	538.3873	0.1	2.27	LPC	19:0	[M + H] ⁺
	C ₂₇ H ₄₄ NO ₇ P	524.2787	1.9	1.21	LPE	22:6	[M − H] [−]
	C ₂₅ H ₄₄ NO ₇ P	500.2798	4.2	1.25	LPE	20:4	[M − H] [−]
SM	C ₃₇ H ₇₅ N ₂ O ₆ P	675.5440	−0.1	4.7	SM	14:0	[M + H] ⁺
	C ₃₉ H ₇₇ N ₂ O ₆ P	701.5564	−4.7	4.23	SM	16:1	[M + H] ⁺
	C ₄₁ H ₇₅ N ₂ O ₆ P	723.5447	0.9	4.23	SM	18:4	[M + H] ⁺
	C ₃₈ H ₇₇ N ₂ O ₆ P	689.5617	2.9	4.45	SM	15:0	[M + H] ⁺
	C ₃₉ H ₇₉ N ₂ O ₆ P	703.5767	1.9	4.78	SM	16:0	[M + H] ⁺
	C ₄₁ H ₇₇ N ₂ O ₆ P	725.5600	0.4	4.78	SM	18:3	[M + H] ⁺
	C ₄₁ H ₈₁ N ₂ O ₆ P	729.5917	0.9	4.89	SM	18:1	[M + H] ⁺
	C ₄₃ H ₇₉ N ₂ O ₆ P	751.5771	2.3	4.89	SM	20:4	[M + H] ⁺
	C ₄₃ H ₈₁ N ₂ O ₆ P	753.5944	4.5	5.39	SM	20:3	[M + H] ⁺
	C ₄₀ H ₈₁ N ₂ O ₆ P	717.5898	−1.8	5.71	SM	17:0	[M + H] ⁺
	C ₄₇ H ₈₇ N ₂ O ₆ P	807.6346	−4.2	5.96	SM	24:4	[M + H] ⁺
	C ₄₃ H ₈₇ N ₂ O ₆ P	759.6407	3.6	5.98	SM	20:0	[M + H] ⁺
	C ₄₁ H ₈₃ N ₂ O ₆ P	731.6089	3	6	SM	18:0	[M + H] ⁺
	C ₄₇ H ₉₁ N ₂ O ₆ P	811.6653	−4.9	6.02	SM	24:2	[M + H] ⁺
	C ₄₉ H ₈₉ N ₂ O ₆ P	833.6518	−2.2	6.02	SM	26:5	[M + H] ⁺
	C ₄₇ H ₈₇ N ₂ O ₆ P	807.6377	−0.3	6.03	SM	24:4	[M + H] ⁺
	C ₄₅ H ₈₉ N ₂ O ₆ P	785.6536	0	6.06	SM	22:1	[M + H] ⁺
	C ₄₃ H ₈₅ N ₂ O ₆ P	757.6225	0.1	6.12	SM	20:1	[M + H] ⁺
	C ₃₇ H ₆₃ N ₂ O ₆ P	663.4521	2.9	6.18	SM	14:6	[M + H] ⁺
	C ₄₆ H ₉₁ N ₂ O ₆ P	799.6657	−4.5	6.2	SM	23:1	[M + H] ⁺
	C ₄₄ H ₈₉ N ₂ O ₆ P	773.6563	3.5	6.24	SM	21:0	[M + H] ⁺
	C ₄₆ H ₉₁ N ₂ O ₆ P	799.6701	1	6.3	SM	23:1	[M + H] ⁺
	C ₄₇ H ₉₃ N ₂ O ₆ P	813.6838	−1.4	6.43	SM	24:1	[M + H] ⁺
	C ₄₉ H ₉₁ N ₂ O ₆ P	835.6685	−0.9	6.43	SM	26:4	[M + H] ⁺
	C ₄₅ H ₉₁ N ₂ O ₆ P	787.6719	3.3	6.44	SM	22:0	[M + H] ⁺
	C ₄₇ H ₈₉ N ₂ O ₆ P	809.6506	−3.7	6.44	SM	24:3	[M + H] ⁺
	C ₄₇ H ₉₃ N ₂ O ₆ P	813.6871	2.7	6.54	SM	24:1	[M + H] ⁺
	C ₄₉ H ₉₁ N ₂ O ₆ P	835.6672	−2.5	6.54	SM	26:4	[M + H] ⁺
	C ₄₈ H ₉₅ N ₂ O ₆ P	827.7049	5.2	6.57	SM	25:1	[M + H] ⁺
	C ₄₆ H ₉₃ N ₂ O ₆ P	801.6882	4.1	6.68	SM	23:0	[M + H] ⁺
	C ₄₈ H ₉₁ N ₂ O ₆ P	823.6712	2.3	6.7	SM	25:3	[M + H] ⁺
	C ₄₇ H ₉₅ N ₂ O ₆ P	815.7028	2.7	6.91	SM	24:0	[M + H] ⁺
	C ₄₉ H ₉₃ N ₂ O ₆ P	837.6869	2.4	6.92	SM	26:3	[M + H] ⁺
	C ₄₅ H ₈₉ N ₂ O ₆ P	785.6570	4.3	8.38	SM	22:1	[M + H] ⁺
	C ₄₉ H ₉₅ N ₂ O ₆ P	839.7038	3.8	8.72	SM	26:2	[M + H] ⁺
	C ₄₆ H ₉₃ N ₂ O ₆ P	801.6851	0.2	8.78	SM	23:0	[M + H] ⁺
	C ₄₉ H ₉₇ N ₂ O ₆ P	841.7189	3.2	8.9	SM	26:1	[M + H] ⁺
	C ₅₃ H ₁₀₁ N ₂ O ₆ P	893.7510	3.9	8.92	SM	30:3	[M + H] ⁺
	C ₄₈ H ₉₇ N ₂ O ₆ P	829.7124	−4.6	8.97	SM	25:0	[M + H] ⁺
	C ₄₀ H ₇₅ N ₂ O ₆ P	711.5465	3.4	9.11	SM	17:3	[M + H] ⁺

Table S1. Continued

class	formula	<i>m/z</i> found	ppm	time (min)	provisional assignment class		ionization mode
TG	C ₅₀ H ₉₉ N ₂ O ₆ P	855.7324	0.6	9.21	SM	27:1	[M + H] ⁺
	C ₅₂ H ₁₀₅ N ₂ O ₆ P	885.7817	3.2	9.44	SM	29:0	[M + H] ⁺
	C ₅₅ H ₁₀₉ N ₂ O ₆ P	925.8089	−1.3	9.48	SM	32:1	[M + H] ⁺
	C ₄₇ H ₈₉ NO ₆	764.6807	5.1	8.03	TG	44:2	[M + NH ₄] ⁺
	C ₄₉ H ₉₁ NO ₆	790.6967	5.3	8.11	TG	46:3	[M + NH ₄] ⁺
	C ₅₃ H ₉₅ NO ₆	842.7266	3.3	8.23	TG	50:5	[M + NH ₄] ⁺
	C ₅₇ H ₉₉ NO ₆	894.7515	−4	8.23	TG	54:7	[M + NH ₄] ⁺
	C ₄₅ H ₈₉ NO ₆	740.6752	−2.1	8.24	TG	42:0	[M + NH ₄] ⁺
	C ₅₇ H ₉₉ NO ₆	894.7515	−4	8.25	TG	54:7	[M + NH ₄] ⁺
	C ₅₀ H ₉₃ NO ₆	804.7063	−2.2	8.25	TG	47:3	[M + NH ₄] ⁺
	C ₅₅ H ₉₇ NO ₆	868.7400	0.7	8.3	TG	52:6	[M + NH ₄] ⁺
	C ₄₇ H ₉₁ NO ₆	766.6937	1.6	8.3	TG	44:1	[M + NH ₄] ⁺
	C ₄₉ H ₉₃ NO ₆	792.7114	4.2	8.3	TG	46:2	[M + NH ₄] ⁺
	C ₆₁ H ₁₀₁ NO ₆	944.7735	3	8.31	TG	58:10	[M + NH ₄] ⁺
	C ₅₁ H ₉₅ NO ₆	818.7251	1.7	8.33	TG	48:3	[M + NH ₄] ⁺
	C ₅₁ H ₉₅ NO ₆	818.7239	0.1	8.34	TG	48:3	[M + NH ₄] ⁺
	C ₅₉ H ₁₀₁ NO ₆	920.7708	0.1	8.34	TG	56:8	[M + NH ₄] ⁺
	C ₄₆ H ₉₁ NO ₆	754.6968	5.8	8.36	TG	43:0	[M + NH ₄] ⁺
	C ₅₃ H ₉₇ NO ₆	844.7397	0.4	8.36	TG	50:4	[M + NH ₄] ⁺
	C ₅₃ H ₉₇ NO ₆	844.7397	0.4	8.39	TG	50:4	[M + NH ₄] ⁺
	C ₅₇ H ₁₀₁ NO ₆	896.7740	3.7	8.41	TG	54:6	[M + NH ₄] ⁺
	C ₅₅ H ₉₉ NO ₆	870.7558	0.8	8.42	TG	52:5	[M + NH ₄] ⁺
	C ₆₁ H ₁₀₃ NO ₆	946.7879	1.6	8.43	TG	58:9	[M + NH ₄] ⁺
	C ₅₀ H ₉₅ NO ₆	806.7217	−2.5	8.47	TG	47:2	[M + NH ₄] ⁺
	C ₅₂ H ₉₇ NO ₆	832.7440	5.5	8.49	TG	49:3	[M + NH ₄] ⁺
	C ₅₉ H ₁₀₃ NO ₆	922.7908	4.8	8.54	TG	56:7	[M + NH ₄] ⁺
	C ₅₇ H ₁₀₁ NO ₆	896.7720	1.5	8.55	TG	54:6	[M + NH ₄] ⁺
	C ₄₉ H ₉₅ NO ₆	794.7220	−2.2	8.57	TG	46:1	[M + NH ₄] ⁺
	C ₅₃ H ₉₉ NO ₆	846.7567	2	8.58	TG	50:3	[M + NH ₄] ⁺
	C ₅₁ H ₉₇ NO ₆	820.7375	−2.3	8.58	TG	48:2	[M + NH ₄] ⁺
	C ₅₅ H ₁₀₁ NO ₆	872.7720	1.5	8.62	TG	52:4	[M + NH ₄] ⁺
	C ₅₃ H ₉₉ NO ₆	846.7554	0.4	8.63	TG	50:3	[M + NH ₄] ⁺
	C ₅₇ H ₁₀₃ NO ₆	898.7861	−0.3	8.64	TG	54:5	[M + NH ₄] ⁺
	C ₄₈ H ₉₅ NO ₆	782.7242	0.6	8.65	TG	45:0	[M + NH ₄] ⁺
	C ₅₂ H ₉₉ NO ₆	834.7592	5	8.67	TG	49:2	[M + NH ₄] ⁺
	C ₅₄ H ₁₀₁ NO ₆	860.7722	1.8	8.7	TG	51:3	[M + NH ₄] ⁺
	C ₅₀ H ₉₇ NO ₆	808.7390	−0.5	8.7	TG	47:1	[M + NH ₄] ⁺
	C ₅₉ H ₁₀₅ NO ₆	924.8026	0.7	8.75	TG	56:6	[M + NH ₄] ⁺
	C ₄₉ H ₉₇ NO ₆	796.7368	−3.3	8.78	TG	46:0	[M + NH ₄] ⁺
	C ₅₁ H ₉₉ NO ₆	822.7565	1.8	8.79	TG	48:1	[M + NH ₄] ⁺
	C ₅₃ H ₁₀₁ NO ₆	848.7715	1	8.8	TG	50:2	[M + NH ₄] ⁺
	C ₅₅ H ₁₀₃ NO ₆	874.7885	2.5	8.82	TG	52:3	[M + NH ₄] ⁺
	C ₅₈ H ₁₀₈ NO ₆	916.8366	3.6	8.82	TG	55:3	[M + NH ₄] ⁺
	C ₆₁ H ₁₁₅ NO ₆	958.8865	6.5	8.82	TG	58:3	[M + NH ₄] ⁺
	C ₅₇ H ₁₀₅ NO ₆	900.8053	3.7	8.83	TG	54:4	[M + NH ₄] ⁺
	C ₅₄ H ₁₀₃ NO ₆	862.7913	5.8	8.92	TG	51:2	[M + NH ₄] ⁺
	C ₆₁ H ₁₀₉ NO ₆	952.8344	1.2	8.99	TG	58:6	[M + NH ₄] ⁺
	C ₅₁ H ₁₀₁ NO ₆	824.7726	2.3	8.99	TG	48:0	[M + NH ₄] ⁺
	C ₅₉ H ₁₀₇ NO ₆	926.8182	0.5	9	TG	56:5	[M + NH ₄] ⁺
	C ₅₃ H ₁₀₃ NO ₆	850.7871	0.9	9	TG	50:1	[M + NH ₄] ⁺
	C ₅₅ H ₁₀₅ NO ₆	876.8063	4.9	9	TG	52:2	[M + NH ₄] ⁺
	C ₆₀ H ₁₁₅ NO ₆	946.8836	3.6	9	TG	57:2	[M + NH ₄] ⁺
	C ₅₈ H ₁₁₁ NO ₆	918.8494	0.4	9.01	TG	55:2	[M + NH ₄] ⁺
	C ₆₁ H ₁₁₇ NO ₆	960.8916	−4.5	9.01	TG	58:2	[M + NH ₄] ⁺

Table S1. Continued

class	formula	<i>m/z</i> found	ppm	time (min)	provisional assignment class		ionization mode
	C ₅₉ H ₁₀₉ NO ₆	928.8317	−1.7	9.02	TG	56:4	[M + NH ₄] ⁺
	C ₅₇ H ₁₀₇ NO ₆	902.8207	3.4	9.04	TG	54:3	[M + NH ₄] ⁺
	C ₅₁ H ₁₀₁ NO ₆	824.7700	−0.8	9.06	TG	48:0	[M + NH ₄] ⁺
	C ₅₄ H ₁₀₅ NO ₆	864.8056	4.2	9.07	TG	51:1	[M + NH ₄] ⁺
	C ₅₆ H ₁₀₇ NO ₆	890.8201	2.7	9.08	TG	53:2	[M + NH ₄] ⁺
	C ₅₄ H ₁₀₅ NO ₆	864.8061	4.8	9.12	TG	51:1	[M + NH ₄] ⁺
	C ₅₉ H ₁₁₁ NO ₆	930.8494	0.4	9.21	TG	56:3	[M + NH ₄] ⁺
	C ₅₅ H ₁₀₉ NO ₆	880.8375	4.8	9.21	TG	52:0	[M + NH ₄] ⁺
	C ₅₅ H ₁₀₇ NO ₆	878.8224	5.4	9.21	TG	52:1	[M + NH ₄] ⁺
	C ₅₄ H ₉₉ NO ₆	858.7546	−0.6	9.22	TG	51:4	[M + NH ₄] ⁺
	C ₅₇ H ₁₀₉ NO ₆	904.8358	2.8	9.22	TG	54:2	[M + NH ₄] ⁺
	C ₅₄ H ₁₀₇ NO ₆	866.8201	2.8	9.31	TG	51:0	[M + NH ₄] ⁺
	C ₅₉ H ₁₁₃ NO ₆	932.8600	1.4	9.45	TG	56:2	[M + NH ₄] ⁺
	C ₅₇ H ₁₁₁ NO ₆	906.8511	2.4	9.46	TG	54:1	[M + NH ₄] ⁺
	C ₅₈ H ₁₁₃ NO ₆	920.8690	4.8	9.52	TG	55:1	[M + NH ₄] ⁺
	C ₅₉ H ₁₁₅ NO ₆	934.8801	−0.2	9.59	TG	56:1	[M + NH ₄] ⁺
	C ₅₇ H ₁₁₃ NO ₆	908.8682	4	9.59	TG	54:0	[M + NH ₄] ⁺
	C ₆₀ H ₁₁₇ NO ₆	948.9012	5.6	9.7	TG	57:1	[M + NH ₄] ⁺
	C ₆₁ H ₁₁₃ NO ₆	956.8646	2.2	9.8	TG	58:4	[M + NH ₄] ⁺
	C ₅₆ H ₁₀₉ NO ₆	892.8337	0.4	9.9	TG	53:1	[M + NH ₄] ⁺
	C ₆₃ H ₁₂₁ NO ₆	988.9258	−1.4	9.93	TG	60:2	[M + NH ₄] ⁺
	C ₆₅ H ₁₂₃ NO ₆	1014.9415	−1.4	9.93	TG	62:3	[M + NH ₄] ⁺
	C ₆₂ H ₁₂₁ NO ₆	976.9298	2.7	9.95	TG	59:1	[M + NH ₄] ⁺
	C ₆₂ H ₁₂₃ NO ₆	978.9465	3.7	10.09	TG	59:0	[M + NH ₄] ⁺
	C ₆₅ H ₁₂₅ NO ₆	1016.9623	3.7	10.12	TG	62:2	[M + NH ₄] ⁺
	C ₆₃ H ₁₂₃ NO ₆	990.9436	0.7	10.12	TG	60:1	[M + NH ₄] ⁺

^a The *m/z* of the most abundant ion, the mass error, retention time, provisional lipid assignment and the ionization mode (positive/negative) are given.

DOI: 10.1021/pr200420k

Published on Web 05/31/2011