

Supporting Information

Title: Accurate Lamb Origin Identification and Molecular Differentiation Analysis Using Rapid Evaporative Ionization Mass Spectrometry

Haiyan Gao^{1,2#}, Yueguang Lv^{1#}, Wenjing Zhao², Songying Wang², Jiayu Zhao¹, Yisheng Xu³, Yuhan Shang¹, Renyu Zhang^{4*}, Qiang Ma^{1*}

¹Chinese Academy of Inspection and Quarantine, Beijing 100176, China

²Inner Mongolia Autonomous Region Administration of Market Supervision Evaluation and Inspection Center, Hohhot 010070, China

³Waters Technology Co., Ltd., Beijing 100176, China

⁴Food Technology & Processing, Smart Foods & Bioproducts, AgResearch Ltd., Te Ohu Rangahau Kai, Palmerston North 4474, New Zealand

Email: maqiang@caiq.org.cn; renyu.zhang@agresearch.co.nz

[#]These authors contributed equally to this work

Figure S1 Optimization of REIMS parameters.

Figure S2 Clustering analysis results of lamb from the four regions.

Table S1 The identified compounds in lamb samples.

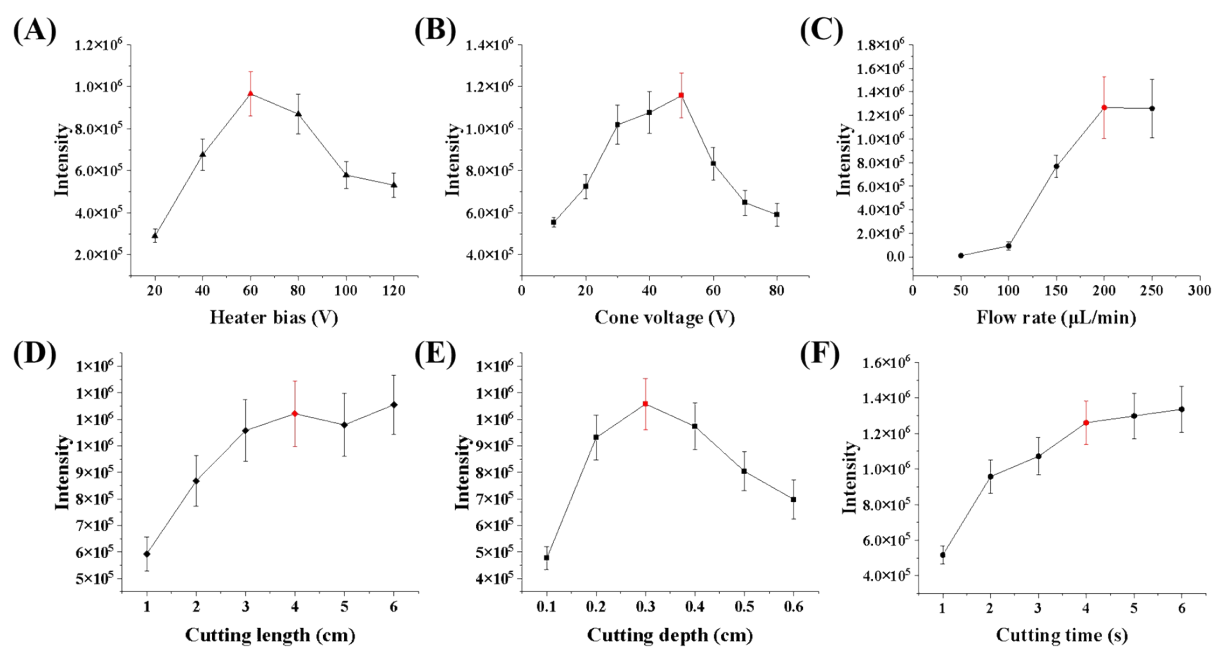


Figure S1. Optimization of REIMS parameters.

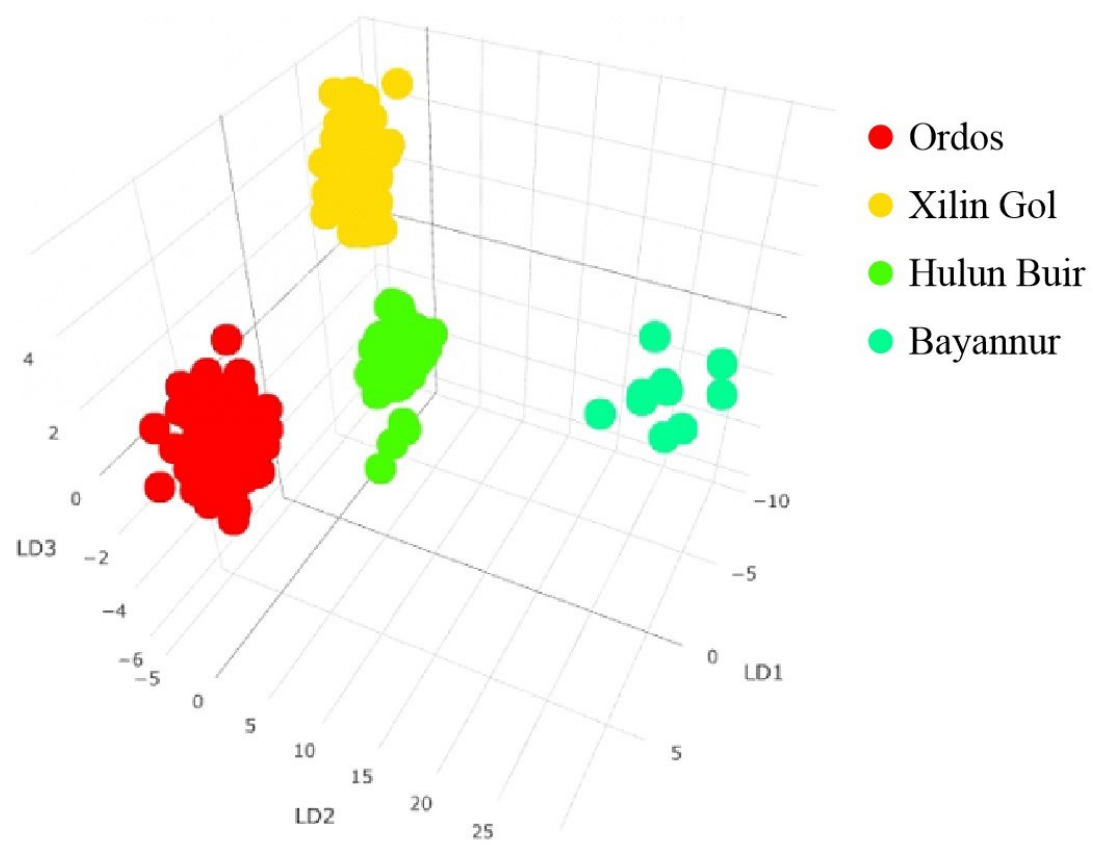


Figure S2. Clustering analysis results of lamb from the four regions.

Table S1 The identified compounds in lamb samples.

ID	Measured <i>m/z</i>	Compounds	Category	Formulas	Theoretical <i>m/z</i>	Relative error (ppm)
1	128.0351	Pyroglutamic acid	Amino acids	C ₅ H ₇ NO ₃	128.0353	−1.7
2	128.0351	Pyrrolidonecarboxylic acid	Amino acids	C ₅ H ₇ NO ₃	128.0353	−1.7
3	134.0467	Adenine	Small-molecule metabolites	C ₅ H ₅ N ₅	134.0472	−3.9
4	135.0308	Hypoxanthine	Small-molecule metabolites	C ₅ H ₄ N ₄ O	135.0312	−3.2
5	225.0986	Carnosine	Small-molecule metabolites	C ₉ H ₁₄ N ₄ O ₃	225.0993	−3.2
6	239.1150	Homocarnosine	Organic acids	C ₁₀ H ₁₆ N ₄ O ₃	239.1150	0.2
7	239.1150	Anserine	Organic acids	C ₁₀ H ₁₆ N ₄ O ₃	239.1150	0.2
8	255.2344	Palmitic acid	Fatty acids	C ₁₆ H ₃₂ O ₂	255.2330	5.7
9	255.2344	Isopalmitic acid	Fatty acids	C ₁₆ H ₃₂ O ₂	255.2330	5.7
10	269.2504	Heptadecanoic acid	Fatty acids	C ₁₇ H ₃₄ O ₂	269.2486	6.7
11	277.2196	Alpha-Linolenic acid	Fatty acids	C ₁₈ H ₃₀ O ₂	277.2173	8.3
12	279.2344	Linoleic acid	Fatty acids	C ₁₈ H ₃₂ O ₂	279.2330	5.2
13	279.2344	Linoelaidic acid	Fatty acids	C ₁₈ H ₃₂ O ₂	279.2330	5.2
14	279.2344	Octadecadienoic acid	Fatty acids	C ₁₈ H ₃₂ O ₂	279.2330	5.2
15	279.2344	Bovinic acid	Fatty acids	C ₁₈ H ₃₂ O ₂	279.2330	5.2
16	281.2496	Oleic acid	Fatty acids	C ₁₈ H ₃₄ O ₂	281.2486	3.6
17	281.2496	Petroselinic acid	Fatty acids	C ₁₈ H ₃₄ O ₂	281.2486	3.6
18	283.2655	Ethyl hexadecanoate	Fatty acids	C ₁₈ H ₃₆ O ₂	283.2643	4.4
19	283.2655	16-Methylheptadecanoic acid	Fatty acids	C ₁₈ H ₃₆ O ₂	283.2643	4.4
20	301.2205	Eicosapentaenoic acid	Fatty acids	C ₂₀ H ₃₀ O ₂	301.2173	10.6
21	303.2361	Arachidonic acid	Fatty acids	C ₂₀ H ₃₂ O ₂	303.2330	10.4
22	307.2763	Eicosadienoic acid	Fatty acids	C ₂₀ H ₃₆ O ₂	307.2643	39.2

23	307.2763	Sclareol	Small-molecule metabolites	C ₂₀ H ₃₆ O ₂	307.2643	39.2
24	327.2356	Docosahexaenoic acid	Fatty acids	C ₂₂ H ₃₂ O ₂	327.2330	8.1
25	329.2520	Docosapentaenoic acid (22n-3)	Fatty acids	C ₂₂ H ₃₄ O ₂	329.2486	10.3
26	478.2844	LysoPE(18:1(9Z)/0:0)	Lipids	C ₂₃ H ₄₆ NO ₇ P	478.2939	-19.9
27	514.2650	Taurocholic acid	Bile acids	C ₂₆ H ₄₅ NO ₇ S	514.2844	-37.7
28	655.4788	CerPE 34:3;O2	Lipids	C ₃₆ H ₆₉ N ₂ O ₆ P	655.4821	-5.0
29	655.4788	PA O-34:3	Lipids	C ₃₇ H ₆₉ O ₇ P	655.4708	12.2
30	657.4992	CerPE 34:2;O2	Lipids	C ₃₆ H ₇₁ N ₂ O ₆ P	657.4977	2.3
31	657.4992	PA O-34:2	Lipids	C ₃₇ H ₇₁ O ₇ P	657.4865	19.3
32	669.4905	PA 36:2	Lipids	C ₃₉ H ₇₃ O ₈ P	699.497	-9.3
33	669.4905	CerPE 36:3;O3	Lipids	C ₃₈ H ₇₃ N ₂ O ₇ P	699.5083	-25.4
34	671.5057	PA O-35:2	Lipids	C ₃₈ H ₇₃ O ₇ P	671.5021	5.4
35	671.5057	CerPE 35:2;O2	Lipids	C ₃₇ H ₇₃ N ₂ O ₆ P	671.5134	-11.5
36	671.5057	CerPE 34:3;O3	Lipids	C ₃₆ H ₆₉ N ₂ O ₇ P	671.477	42.7
37	673.4922	CerPE 34:2;O3	Lipids	C ₃₆ H ₇₁ N ₂ O ₇ P	673.4926	-0.6
38	673.4922	PA 34:1	Lipids	C ₃₇ H ₇₁ O ₈ P	673.4814	16.0
39	673.4922	PA O-35:1	Lipids	C ₃₈ H ₇₅ O ₇ P	673.5178	-38.0
40	679.4797	PA O-36:5	Lipids	C ₃₉ H ₆₉ O ₇ P	679.4708	13.1
41	679.4797	PG O-30:0	Lipids	C ₃₆ H ₇₃ O ₉ P	679.492	-18.1
42	679.4797	PG 29:0	Lipids	C ₃₅ H ₆₉ O ₁₀ P	679.4556	35.5
43	681.4939	PA O-36:4	Lipids	C ₃₉ H ₇₁ O ₇ P	681.4865	10.9
44	683.5057	PA O-36:3	Lipids	C ₃₉ H ₇₃ O ₇ P	683.5021	5.3
45	683.5057	CerPE 36:3;O2	Lipids	C ₃₈ H ₇₃ N ₂ O ₆ P	683.5134	-11.3
46	685.5098	PA O-36:2	Lipids	C ₃₉ H ₇₅ O ₇ P	685.5178	-11.7
47	685.5098	CerPE 36:2;O2	Lipids	C ₃₈ H ₇₅ N ₂ O ₆ P	685.529	-28.0
48	685.5098	DG 42:11	Lipids	C ₄₅ H ₆₆ O ₅	685.4838	37.9
49	685.5098	PA 35:2	Lipids	C ₃₈ H ₇₁ O ₈ P	685.4814	41.4
50	687.5114	CerPE 35:2;O3	Lipids	C ₃₇ H ₇₃ N ₂ O ₇ P	687.5083	4.5
51	687.5114	DG 42:10	Lipids	C ₄₅ H ₆₈ O ₅	687.4994	17.5
52	687.5114	PA 35:1	Lipids	C ₃₈ H ₇₃ O ₈ P	687.497	20.9
53	687.5114	PA O-36:1	Lipids	C ₃₉ H ₇₇ O ₇ P	687.5334	-32.0
54	687.5114	CerPE 36:1;O2	Lipids	C ₃₈ H ₇₇ N ₂ O ₆ P	687.5447	-48.4
55	693.4798	PG 30:0	Lipids	C ₃₆ H ₇₁ O ₁₀ P	693.4712	12.4

56	693.4798	PG O-31:0	Lipids	C ₃₇ H ₇₅ O ₉ P	693.5076	−40.1
57	693.4798	PA 36:5	Lipids	C ₃₉ H ₆₇ O ₈ P	693.4501	42.8
58	695.4822	PA 36:4	Lipids	C ₃₉ H ₆₉ O ₈ P	695.4657	23.7
59	697.4876	PA 36:3	Lipids	C ₃₉ H ₇₁ O ₈ P	697.4814	8.9
60	697.4876	PA O-37:3	Lipids	C ₄₀ H ₇₅ O ₇ P	697.5178	−43.3
61	699.5012	PA 36:2	Lipids	C ₃₉ H ₇₃ O ₈ P	699.497	6.0
62	699.5012	CerPE 36:3;O3	Lipids	C ₃₈ H ₇₃ N ₂ O ₇ P	699.5083	−10.1
63	699.5012	PA O-37:2	Lipids	C ₄₀ H ₇₇ O ₇ P	699.5334	−46.0
64	700.5091	PE 33:2	Lipids	C ₃₈ H ₇₂ NO ₈ P	700.4923	24.0
65	700.5091	PE O-34:2	Lipids	C ₃₉ H ₇₆ NO ₇ P	700.5287	−28.0
66	701.5231	CerPE 36:2;O3	Lipids	C ₃₈ H ₇₅ N ₂ O ₇ P	701.5239	−1.1
67	701.5231	PA 36:1	Lipids	C ₃₉ H ₇₅ O ₈ P	701.5127	14.8
68	701.5231	PA O-37:1	Lipids	C ₄₀ H ₇₉ O ₇ P	701.5491	−37.1
69	707.5138	PG O-32:0	Lipids	C ₃₈ H ₇₇ O ₉ P	707.5233	−13.4
70	707.5138	PA O-38:5	Lipids	C ₄₁ H ₇₃ O ₇ P	707.5021	16.5
71	707.5138	PG 31:0	Lipids	C ₃₇ H ₇₃ O ₁₀ P	707.4869	38.0
72	709.52	PA O-38:4	Lipids	C ₄₁ H ₇₅ O ₇ P	709.5178	3.1
73	723.5052	PA 38:4	Lipids	C ₄₁ H ₇₃ O ₈ P	723.497	11.3
74	724.5247	PE O-36:4	Lipids	C ₄₁ H ₇₆ NO ₇ P	724.5287	−5.5
75	724.5247	HexCer 35:3;O3	Lipids	C ₄₁ H ₇₅ NO ₉	724.5369	−16.8
76	724.5247	PE 35:4	Lipids	C ₄₀ H ₇₂ NO ₈ P	724.4923	44.7
77	725.5229	PA 38:3	Lipids	C ₄₁ H ₇₅ O ₈ P	725.5127	14.1
78	726.5438	PE O-36:3	Lipids	C ₄₁ H ₇₈ NO ₇ P	726.5443	−0.7
79	726.5438	HexCer 35:2;O3	Lipids	C ₄₁ H ₇₇ NO ₉	726.5526	−12.1
80	726.5438	PE 35:3	Lipids	C ₄₀ H ₇₄ NO ₈ P	726.5079	49.4
81	727.5434	CerPE 38:3;O3	Lipids	C ₄₀ H ₇₇ N ₂ O ₇ P	727.5396	5.2
82	727.5434	PA 38:2	Lipids	C ₄₁ H ₇₇ O ₈ P	727.5283	20.8
83	727.5434	PA O-39:2	Lipids	C ₄₂ H ₈₁ O ₇ P	727.5647	−29.3
84	727.5434	CerPE 39:2;O2	Lipids	C ₄₁ H ₈₁ N ₂ O ₆ P	727.576	−44.8
85	728.5602	PE O-36:2	Lipids	C ₄₁ H ₈₀ NO ₇ P	728.56	0.3
86	728.5602	CerP 42:1;O2	Lipids	C ₄₂ H ₈₄ NO ₆ P	728.5964	−49.7
87	742.5467	PE 36:2	Lipids	C ₄₁ H ₇₈ NO ₈ P	742.5392	10.1
88	742.5467	PE O-37:2	Lipids	C ₄₂ H ₈₂ NO ₇ P	742.5756	−38.9
89	743.546	PA 39:1	Lipids	C ₄₂ H ₈₁ O ₈ P	743.5596	−18.3
90	743.546	PG O-35:3	Lipids	C ₄₁ H ₇₇ O ₉ P	743.5233	30.5

91	743.546	CerPE 39:2;O3	Lipids	C ₄₁ H ₈₁ N ₂ O ₇ P	743.5709	-33.5
92	744.5573	PE 36:1	Lipids	C ₄₁ H ₈₀ NO ₈ P	744.5549	3.2
93	744.5573	PE O-37:1	Lipids	C ₄₂ H ₈₄ NO ₇ P	744.5913	-45.7
94	745.5579	PA 39:0	Lipids	C ₄₂ H ₈₃ O ₈ P	745.5753	-23.3
95	745.5579	PG O-35:2	Lipids	C ₄₁ H ₇₉ O ₉ P	745.5389	25.5
96	748.536	PE O-38:6	Lipids	C ₄₃ H ₇₆ NO ₇ P	748.5287	9.8
97	748.536	PS O-34:0	Lipids	C ₄₀ H ₈₀ NO ₉ P	748.5498	-18.4
98	748.536	PS 33:0	Lipids	C ₃₉ H ₇₆ NO ₁₀ P	748.5134	30.2
99	750.549	PE O-38:5	Lipids	C ₄₃ H ₇₈ NO ₇ P	750.5443	6.3
100	751.5144	PA 40:4	Lipids	C ₄₃ H ₇₇ O ₈ P	751.5283	-18.5
101	751.5144	PG O-36:6	Lipids	C ₄₂ H ₇₃ O ₉ P	751.492	29.8
102	752.5479	PE O-38:4	Lipids	C ₄₃ H ₈₀ NO ₇ P	752.56	-16.1
103	752.5479	HexCer 37:3;O3	Lipids	C ₄₃ H ₇₉ NO ₉	752.5682	-27.0
104	752.5479	PE 37:4	Lipids	C ₄₂ H ₇₆ NO ₈ P	752.5236	32.3
105	754.5775	PE O-38:3	Lipids	C ₄₃ H ₈₂ NO ₇ P	754.5756	2.5
106	754.5775	HexCer 37:2;O3	Lipids	C ₄₃ H ₈₁ NO ₉	754.5839	-8.5
107	754.5775	CerP 44:2;O2	Lipids	C ₄₄ H ₈₆ NO ₆ P	754.612	-45.7
108	766.5461	PE 38:4	Lipids	C ₄₃ H ₇₈ NO ₈ P	766.5392	9.0
109	766.5461	PE O-38:5;O	Lipids	C ₄₃ H ₇₈ NO ₈ P	766.5392	9.0
110	767.5388	PA 41:3	Lipids	C ₄₄ H ₈₁ O ₈ P	767.5596	-27.1
111	767.5388	PI O-30:0	Lipids	C ₃₉ H ₇₇ O ₁₂ P	767.508	40.1
112	768.5548	PE 38:3	Lipids	C ₄₃ H ₈₀ NO ₈ P	768.5549	-0.1
113	768.5548	PS O-36:4	Lipids	C ₄₂ H ₇₆ NO ₉ P	768.5185	47.2
114	769.509	PG 36:4	Lipids	C ₄₂ H ₇₅ O ₁₀ P	769.5025	8.4
115	769.509	MGDG 36:8	Lipids	C ₄₅ H ₇₀ O ₁₀	769.4896	25.2
116	769.509	PA 42:9	Lipids	C ₄₅ H ₇₁ O ₈ P	769.4814	35.9
117	770.532	PS O-36:3	Lipids	C ₄₂ H ₇₈ NO ₉ P	770.5342	-2.9
118	770.532	PS 35:3	Lipids	C ₄₁ H ₇₄ NO ₁₀ P	770.4978	44.4
119	770.532	PE 38:2	Lipids	C ₄₃ H ₈₂ NO ₈ P	770.5705	-50.0
120	771.5215	PG 36:3	Lipids	C ₄₂ H ₇₇ O ₁₀ P	771.5182	4.3
121	771.5215	MGDG 36:7	Lipids	C ₄₅ H ₇₂ O ₁₀	771.5053	21.0

122	771.5215	PA 42:8	Lipids	C ₄₅ H ₇₃ O ₈ P	771.497	31.8
123	771.5215	PG O-37:3	Lipids	C ₄₃ H ₈₁ O ₉ P	771.5546	-42.9
124	776.52529	PE 39:6	Lipids	C ₄₄ H ₇₆ NO ₈ P	776.5236	2.2
125	776.52529	PS 35:0	Lipids	C ₄₁ H ₈₀ NO ₁₀ P	776.5447	-25.0
126	776.52529	PE O-40:6	Lipids	C ₄₅ H ₈₀ NO ₇ P	776.56	-44.7
127	861.5624	PI 36:2	Lipids	C ₄₅ H ₈₃ O ₁₃ P	861.5499	14.5
128	861.5624	PI O-37:2	Lipids	C ₄₆ H ₈₇ O ₁₂ P	861.5862	-27.6
129	863.5775	PG 43:6	Lipids	C ₄₉ H ₈₅ O ₁₀ P	863.5808	-3.8
130	863.5775	PI 36:1	Lipids	C ₄₅ H ₈₅ O ₁₃ P	863.5655	13.9
131	863.5775	PI O-37:1	Lipids	C ₄₆ H ₈₉ O ₁₂ P	863.6019	-28.3
132	864.5829	PS 42:5	Lipids	C ₄₈ H ₈₄ NO ₁₀ P	864.576	8.0
133	885.5573	PI 38:4	Lipids	C ₄₇ H ₈₃ O ₁₃ P	885.5499	8.4
134	886.5632	PS 44:8	Lipids	C ₅₀ H ₈₂ NO ₁₀ P	886.5604	3.2
135	887.5758	PI 38:3	Lipids	C ₄₇ H ₈₅ O ₁₃ P	887.5655	11.6
136	888.5828	PS 44:7	Lipids	C ₅₀ H ₈₄ NO ₁₀ P	888.576	7.7
137	888.5828	SHexCer 42:2;O2	Lipids	C ₄₈ H ₉₁ NO ₁₁ S	888.624	-46.4
