

Support information

Compositional Analysis of Archaeological Leather and Simulated Leather and Their Degradation Research Based on HRMS

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Table S1. Chemical Components in Degraded Leather

Compound number	Compound name	Molecular formula	Relative molecular weight	Calculated [M+H] ⁺	Measured [M+H] ⁺	Mass error $\delta/10^{-6}$
1	Glycine	C ₂ H ₆ O ₂ N	75.032	76.0394	76.0399	7.9
2	Alanine	C ₃ H ₈ O ₂ N	89.094	90.0550	90.0556	7.3
3	Serine	C ₃ H ₈ O ₃ N	105.093	106.0499	106.0507	7.4
4	Proline	C ₅ H ₁₀ O ₂ N	115.132	116.0707	116.0715	7.2
5	Valine	C ₅ H ₁₂ O ₂ N	117.148	118.0863	118.0871	7.3
6	Threonine	C ₄ H ₁₀ O ₃ N	119.120	120.0656	120.0664	7.4
7	Cysteine	C ₃ H ₈ O ₂ NS	121.154	122.0271	122.0259	-9.5
8	Pyroglutamic acid	C ₅ H ₈ O ₃ N	129.115	130.0499	130.0508	7.3
9	Cycloleucine	C ₆ H ₁₂ O ₂ N	129.159	130.0863	130.0872	7.3
10	Hydroxyproline	C ₅ H ₁₀ O ₃ N	131.131	132.0656	132.0665	7.3
11	Leucine/Isoleucine	C ₆ H ₁₄ O ₂ N	131.175	132.1020	132.1029	7.2
12	Aspartate	C ₄ H ₈ O ₄ N	133.103	134.0448	134.0458	7.2
13	N-Methylformanilide	C ₈ H ₁₀ ON	135.166	136.0757	136.0768	7.7
14	Lysine	C ₆ H ₁₅ O ₂ N ₂	146.190	147.1129	147.1139	7.1
15	Glutamate	C ₅ H ₁₀ O ₄ N	147.130	148.0605	148.0615	7.1
16	Histidine	C ₆ H ₁₀ O ₂ N ₃	155.157	156.0768	156.0779	7.4
17	L-Amido-L-Proline	C ₆ H ₁₂ O ₂ N ₃	157.173	158.0925	158.0936	7.5
18	Phenylalanine	C ₉ H ₁₂ O ₂ N	165.192	166.0863	166.0875	7.3
19	Arginine	C ₆ H ₁₅ O ₂ N ₄	174.204	175.1190	175.1202	7.2
20	Glycyl-D-Threonine	C ₆ H ₁₃ O ₄ N ₂	176.172	177.0870	177.0882	7.0
21	Tyrosine	C ₉ H ₁₂ O ₃ N	181.191	182.0812	182.0826	7.7
	N-					
22	Tertbutoxycarbonyl beta alanine	C ₈ H ₁₆ O ₄ N	189.211	190.1074	190.1088	7.604
23	L-Alanyl-L-leucine	C ₉ H ₁₉ O ₃ N ₂	202.254	203.1391	203.1405	7.340
24	Tryptophan	C ₁₁ H ₁₃ O ₂ N ₂	204.229	205.0972	205.0987	7.391

Table S2. Potential Chemical Components in XINJIANG Archaeological leather

Compound number	Compound name	Molecular formula	Relative molecular weight	Calculated [M+H] ⁺	Ionization mode	Measured [M+H] ⁺	Mass error $\delta/10^{-6}$	MS/MS matching score
1	2-Pyrroline	C ₄ H ₇ N	69.057	70.0646	Positive	70.0650	-1.8	6.57
2	Glycine	C ₂ H ₅ NO ₂	75.032	76.0394	Positive	76.0920	-2.0	6.26
3	L-Serine	C ₃ H ₇ NO ₃	105.043	104.0353	Negative	104.0352	-1.1	8.09
4	L-Proline	C ₅ H ₉ NO ₂	115.063	116.0707	Positive	116.0702	-3.2	7.72
5	L-Valine	C ₅ H ₁₁ NO ₂	117.079	118.0863	Positive	118.0858	-3.7	6.98
6	Succinic acid	C ₄ H ₆ O ₄	118.027	117.0193	Negative	117.0192	-1.1	7.24
7	L-Threonine	C ₄ H ₉ NO ₃	119.058	118.0508	Negative	118.0509	0.6	6.93
8	Indoline	C ₈ H ₉ N	119.074	120.0808	Positive	120.0804	-3.1	5.15
9	4-Hydroxyproline	C ₅ H ₉ NO ₃	131.058	132.0656	Positive	132.0651	-3.5	7.31
10	L-Aspartic acid	C ₄ H ₇ NO ₄	133.038	134.0448	Positive	134.0446	-1.4	6.72
11	2-Phenylacetamide	C ₈ H ₉ NO	135.068	136.0757	Positive	136.0752	-3.8	5.69
12	4-Guanidinobutanoic acid	C ₅ H ₁₁ N ₃ O ₂	145.085	146.0925	Positive	146.0925	0.5	6.47
13	L-Lysine	C ₆ H ₁₄ N ₂ O ₂	146.106	147.1129	Positive	147.1117	-7.5	6.86
14	L-Glutamic acid	C ₅ H ₉ NO ₄	147.053	148.0605	Positive	148.0601	-2.1	6.92
15	L-Glutamic acid	C ₅ H ₉ NO ₄	147.053	146.0455	Negative	146.0457	1.2	7.60
16	Triethanolamine	C ₆ H ₁₅ NO ₃	149.105	150.1124	Positive	150.1119	-3.5	5.25
17	L-Histidine	C ₆ H ₉ N ₃ O ₂	155.070	156.0768	Positive	156.0764	-2.1	6.86
18	N-Acetylproline	C ₇ H ₁₁ NO ₃	157.074	158.0812	Positive	158.0800	-7.3	6.12
19	L-Carnitine	C ₇ H ₁₅ NO ₃	161.105	162.1124	Positive	162.1119	-3.2	6.77
20	L-Phenylalanine	C ₉ H ₁₁ NO ₂	165.079	166.0863	Positive	166.0857	-3.4	7.20
21	1-Deoxy-D-glucitol	C ₆ H ₁₄ O ₅	166.084	167.0914	Positive	167.0899	-9.2	5.47
22	L-Arginine	C ₆ H ₁₄ N ₄ O ₂	174.112	175.1190	Positive	175.1186	-2.0	7.48
23	L-Tyrosine	C ₉ H ₁₁ NO ₃	181.074	182.0808	Positive	182.0789	-10.6	7.09
24	3-Methyl-octahydro-1H-[1,4]diazino[1,2-a]pyrazine-1,4-dione	C ₈ H ₁₃ N ₃ O ₂	183.101	184.1081	Positive	184.1078	-0.7	5.07
25	10-Hydroxy-9-methyl-3H,4H,6H-pyrido[4,3-f][1,4]oxazocin-4-one	C ₈ H ₁₄ O ₄ S	206.069	207.0687	Positive	207.0705	8.6	5.05

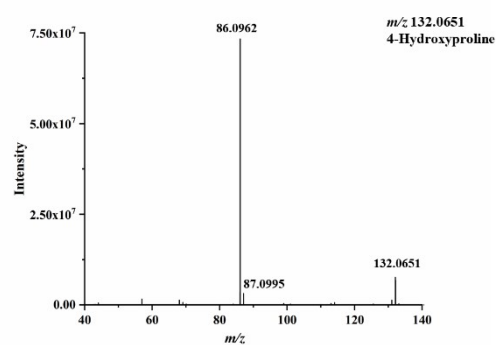
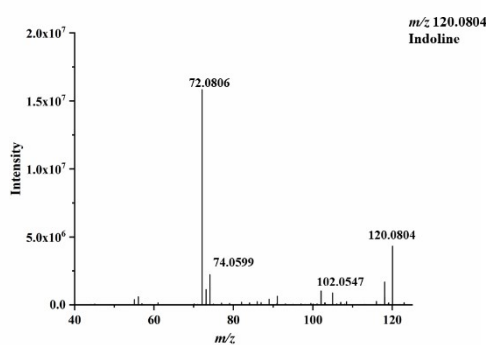
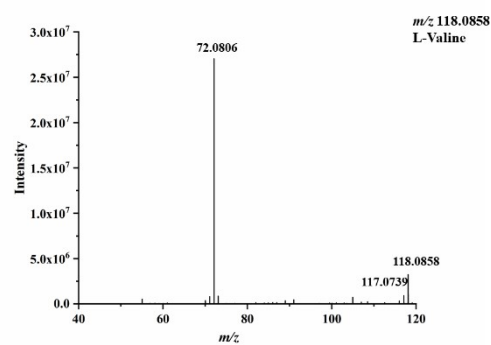
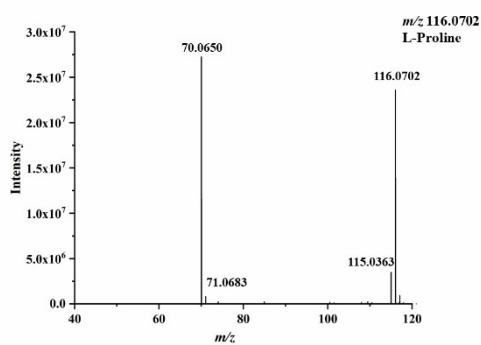
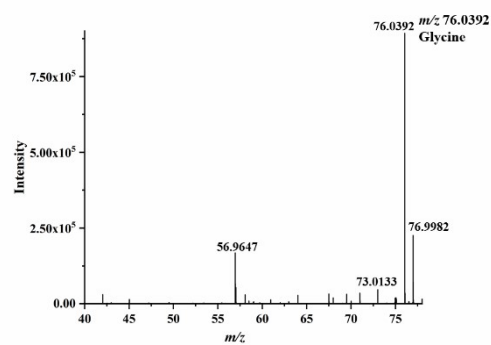
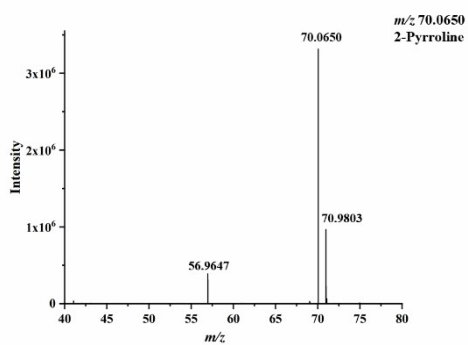
Table S3. Potential Chemical Components in Wuwangdun Archaeological leather

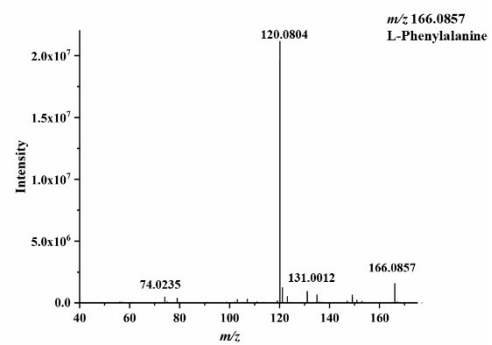
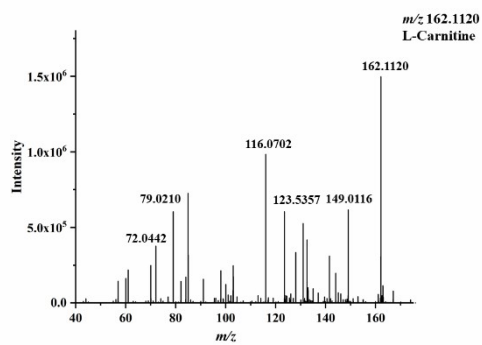
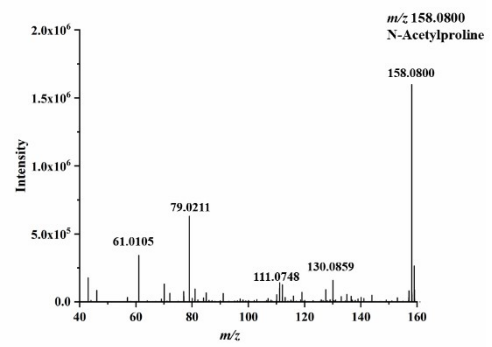
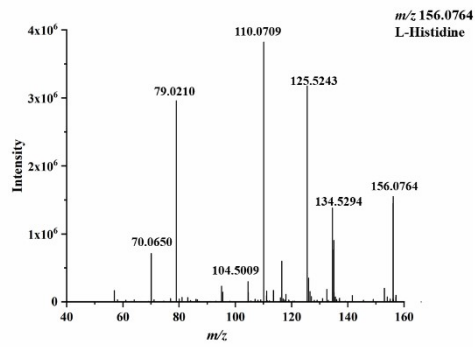
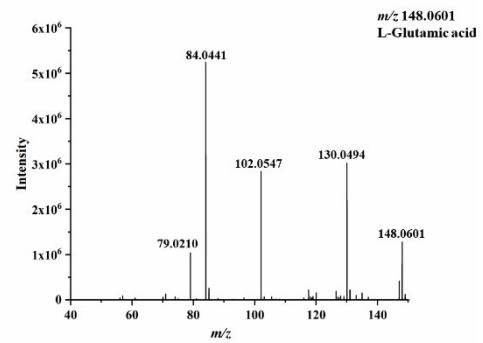
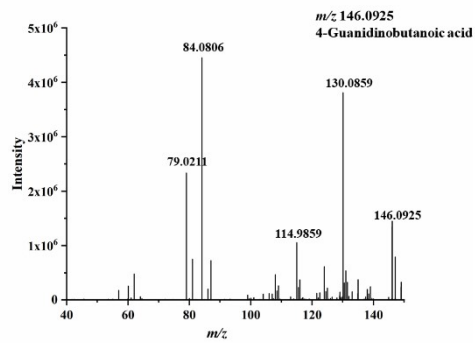
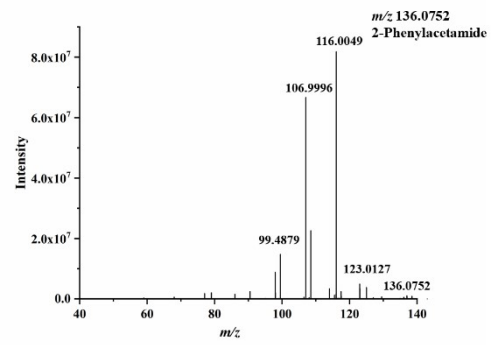
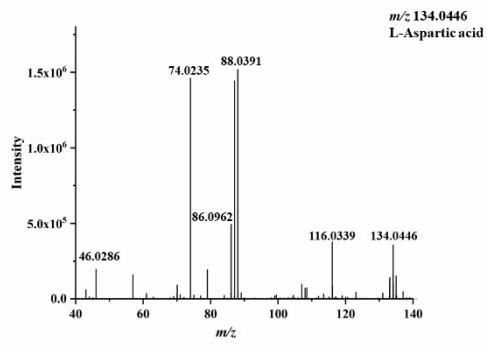
Compound number	Compound name	Molecular formula	Relative molecular weight	Calculated [M+H] ⁺	Ionization mode	Measured [M+H] ⁺	Mass error $\delta/10^{-6}$	MS/MS matching score
1	L-Lactic acid	C ₃ H ₆ O ₃	90.032	89.0244	Negative	89.0242	2.2	8.33
2	(Z)-4-oxopent-2-enoic acid	C ₅ H ₆ O ₃	114.032	115.0390	Positive	115.0389	0.9	5.24
3	Succinic acid	C ₄ H ₆ O ₄	118.027	119.0339	Positive	119.0343	-3.4	6.35
4	3-Hydroxy-4,5-dimethyl-2(5H)-furanone	C ₆ H ₈ O ₃	128.047	129.0547	Positive	129.0549	-1.5	5.64
5	Triethanolamine	C ₆ H ₁₅ N O ₃	149.105	150.1125	Positive	150.1120	3.3	6.08
6	Phthalic acid	C ₈ H ₆ O ₄	166.027	165.0193	Negative	165.0189	2.4	5.98
7	N-Acetylornithine	C ₇ H ₁₄ N ₂ O ₃	174.100	173.0932	Negative	173.0927	2.9	6.72
8	Tetrahydro-2,5-furan-diacetic acid	C ₈ H ₁₂ O ₅	188.069	189.0758	Positive	189.0759	-0.5	5.85
9	5-(2-ethyltetrazol-5-yl)-1-methyl-3,6-dihydro-2H-pyridine	C ₉ H ₁₅ N ₅	193.133	194.1401	Positive	194.1405	-2.1	5.39
10	6-Phosphonoglucono-D-lactone	C ₆ H ₁₁ O ₉ P	258.014	259.0248	Positive	259.0249	-0.4	6.42

Table S4. Potential Chemical Components in Xinyang Archaeological leather

Compound number	Compound name	Molecular formula	Relative molecular weight	Calculated [M+H] ⁺	ionization mode	Measured [M+H] ⁺	Mass error $\delta/10^{-6}$	MS/MS matching score
1	Acrolein	C ₃ H ₄ O	56.026	57.0337	Positive	57.0335	3.3	5.61
2	Propionic acid	C ₃ H ₆ O ₂	74.037	75.0441	Positive	75.0441	-0.6	6.55
3	Dimethyl sulfoxide	C ₂ H ₆ OS	78.014	79.0212	Positive	79.0212	0.2	5.91
4	Dimethylethanola mine	C ₄ H ₁₁ NO	89.084	90.0913	Positive	90.0913	0.5	5.84
5	(S)-3-Hydroxyisobutyric acid	C ₄ H ₈ O ₃	104.047	103.0401	Negative	103.0397	3.5	6.91
6	L-Serine	C ₃ H ₇ NO ₃	105.043	104.0353	Negative	104.0351	2.1	7.59
7	1-(dimethylamino)propan-2-ol	C ₅ H ₁₃ NO	103.100	104.1070	Positive	104.1069	0.9	5.29
8	Epsilon-caprolactam	C ₆ H ₁₁ NO	113.084	114.0914	Positive	114.0913	0.4	5.59
9	L-Proline	C ₅ H ₉ NO ₂	115.063	116.0707	Positive	116.0706	0.0	6.71
10	L-Valine	C ₅ H ₁₁ NO ₂	117.079	118.0863	Positive	118.0861	1.3	7.04
11	indoline	C ₈ H ₉ N	119.074	120.0808	Positive	120.0806	1.5	4.85
12	L-leucine	C ₆ H ₁₃ NO ₂	131.095	132.1019	Positive	132.1017	1.6	7.00
13	2-[2-(dimethylamino)ethoxy]ethanol	C ₆ H ₁₅ NO ₂	133.110	134.1176	Positive	134.1174	1.2	5.54
14	Triethanolamine	C ₆ H ₁₅ NO ₃	149.105	150.1125	Positive	150.1123	1.1	5.91
15	3-aminobutyl(methyl)phosphinic acid	C ₅ H ₁₄ NO ₂ P	151.076	152.0835	Positive	152.0834	0.6	5.00
16	Vanillin	C ₈ H ₈ O ₃	152.047	153.0546	Positive	153.0542	2.8	6.69
17	N-Acetylproline	C ₇ H ₁₁ NO ₃	157.074	158.0812	Positive	158.0810	1.1	6.29
18	3-methyl-5-phenyl-3H-pyrazole	C ₁₀ H ₁₀ N ₂	158.084	159.0917	Positive	159.0916	0.5	5.38
19	N-Acetylvaline	C ₇ H ₁₃ NO ₃	159.090	160.0968	Positive	160.0967	0.8	6.01
20	L-Arginine	C ₆ H ₁₄ N ₄ O ₂	174.112	175.1190	Positive	175.1186	2.0	8.06
21	4',5'-Dihydropsoralen	C ₁₁ H ₈ O ₃	188.047	187.0401	Negative	187.0395	3.0	5.74
22	(-)-Salsoline	C ₁₁ H ₁₅ NO ₂	193.110	194.1176	Positive	194.1172	1.8	6.37
23	Xanthone	C ₁₃ H ₈ O ₂	196.052	197.0597	Positive	197.0595	1.1	5.18
24	5-(2-phenylethynyl)fur	C ₁₅ H ₈ O	212.047	211.0401	Negative	211.0395	2.7	5.27

	an-2-carboxylic acid							
	N,N-							
25	dimethyltetradecy lamine N-oxide	$C_{16}H_{35}NO$	257.272	258.2791	Positive	258.2789	0.9	5.34





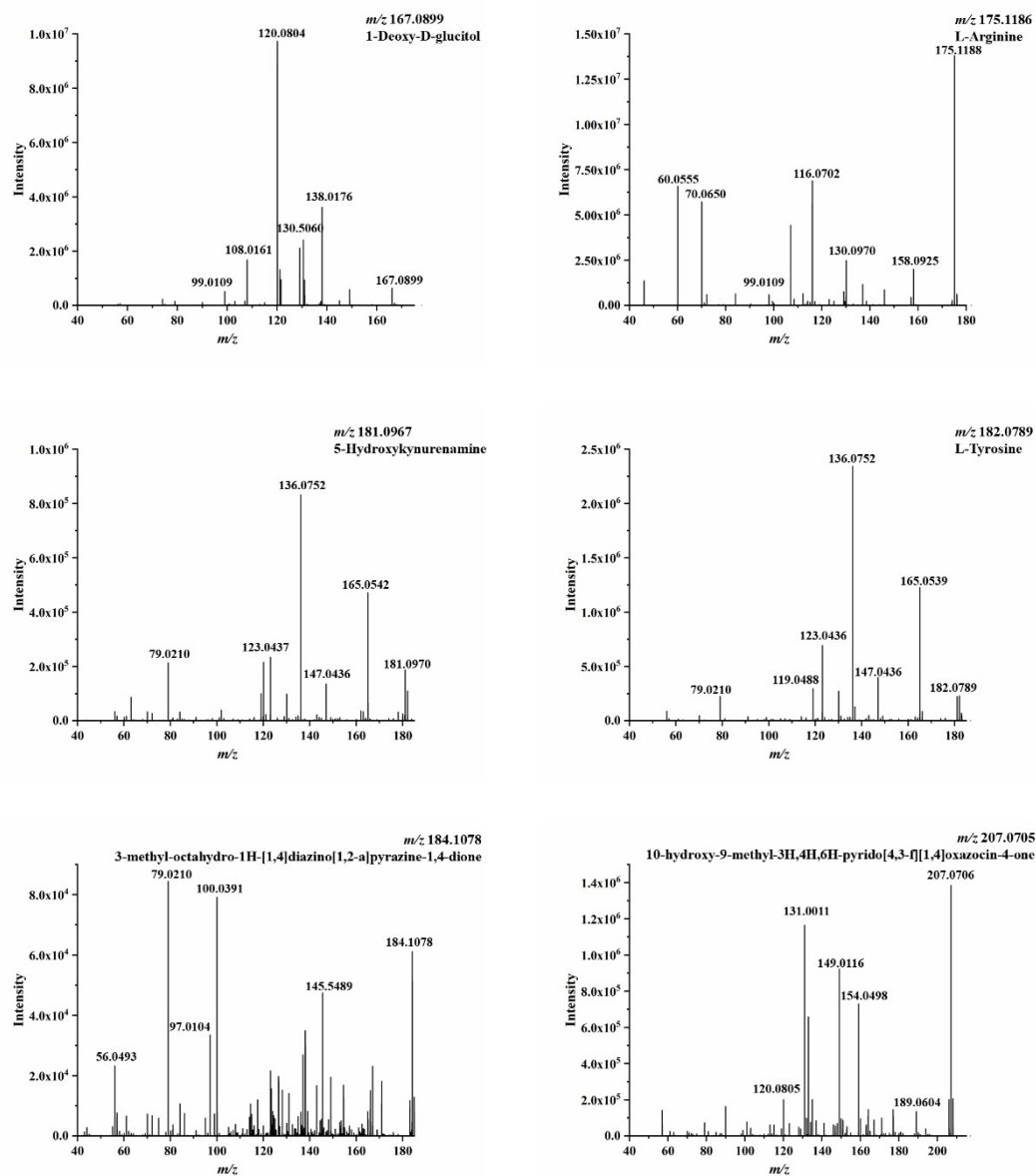
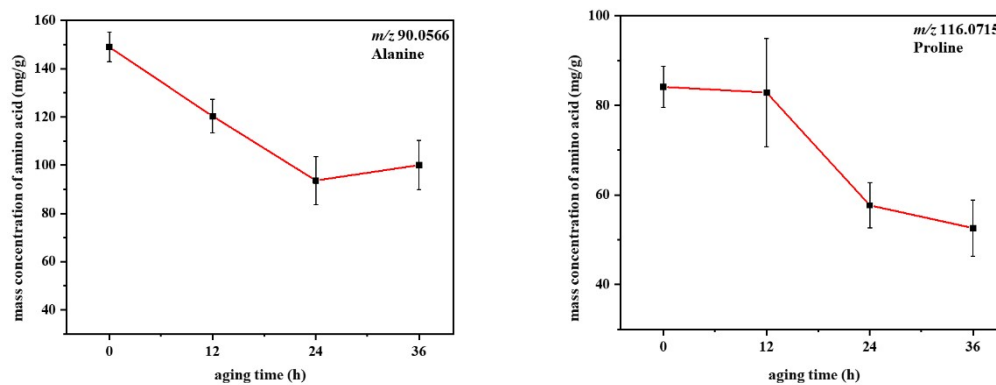


Figure S1. MS/MS of Archaeological leather



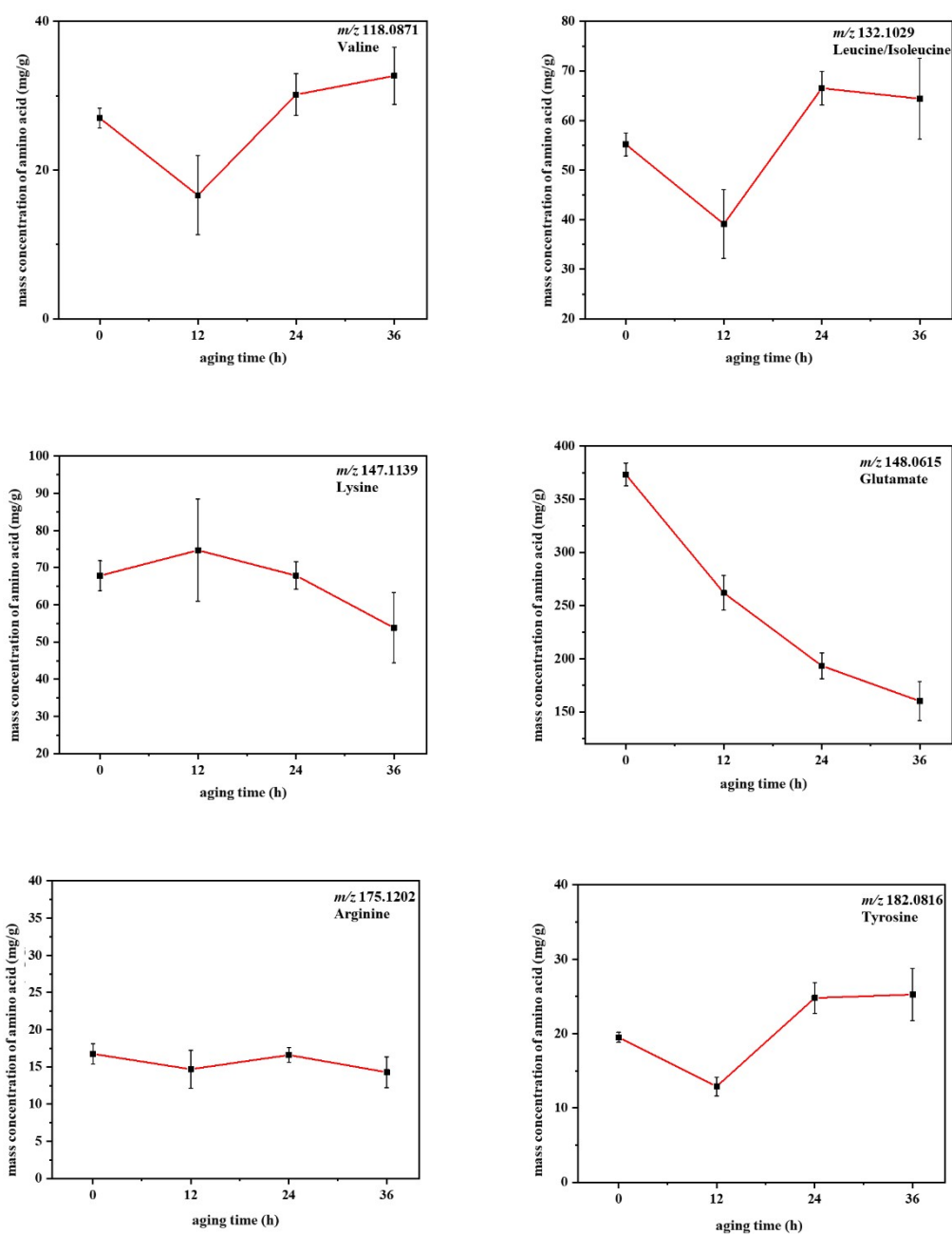


Figure S2. The degradation time of simulated leather samples alongside the mass concentration