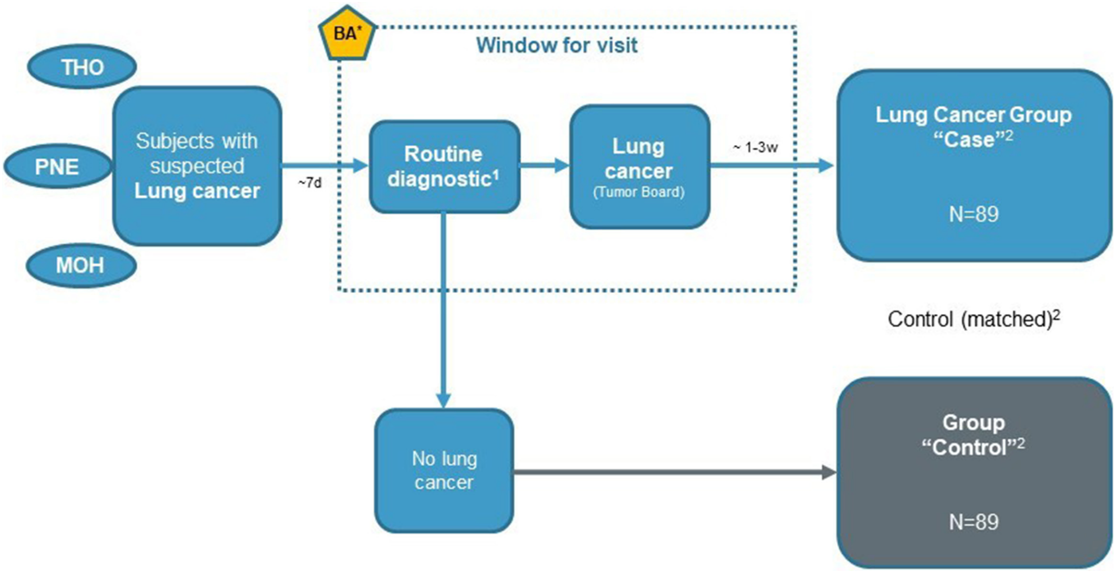

Figure S1 LUCAbreath study design and process. *Breath Analysis by SESI-HRMS (Exhaled breath); 1 Bronchoscopy, broncho-alveolar lavage (BAL), cryobronchoscopy, CT-controlled punction, surgery biopsy or other routine bronchoscopy used to retrieve solid or liquid tissue; 2 Medical history, Lung function testing, Breath analysis by SESI-HRMS; THO = Department of Thoracic Surgery; PNE = Department of Pulmonology; MOH = Department of Medical Oncology and Hematology

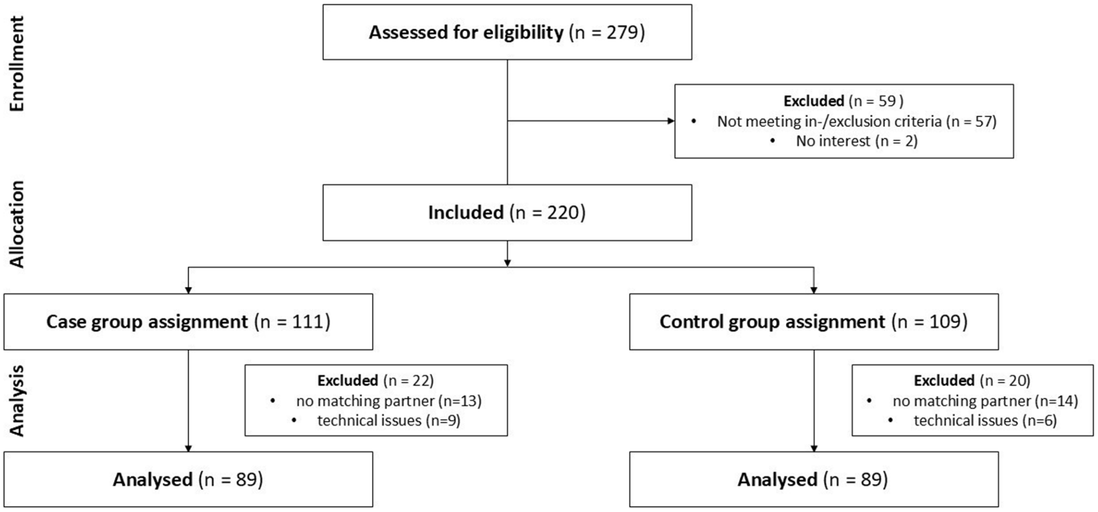

Figure S2 LUCAbreath flowchart of recruitment. Flowchart of participant recruitment, allocation and analysis. In this clinical research project, it was possible to analyse 64% of participants, which were assessed for eligibility.

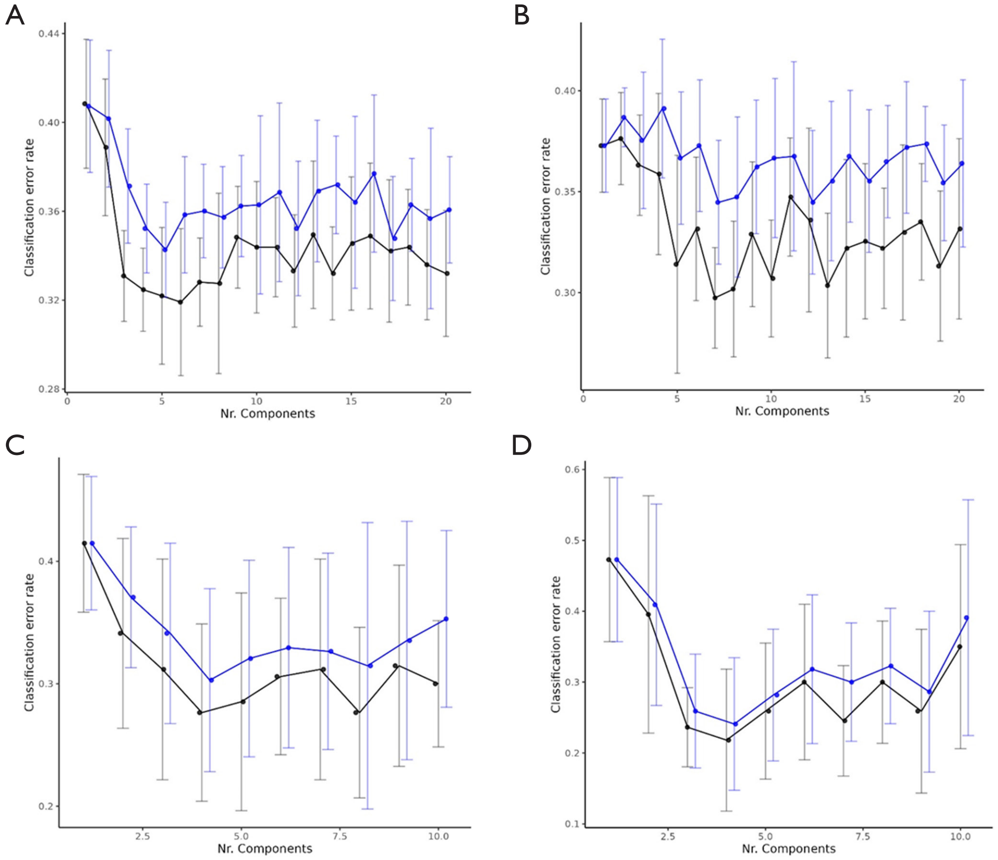

Figure S3 PLS-DA classification error rate. (A) All lung cancer patients vs. Controls (n=178), (B) LUAD *vs*. Controls (n=114), (C) LUSC *vs*. Controls (n=34), (D) SCLC *vs*. Controls (n=22). The plots illustrate the maximum distance to the decision boundary (black) and centroid distance (blue). Black points and lines: These represent the mean maximum distance to the decision boundary (mean.max.dist), which indicates the error rate based on the farthest distance a sample must traverse to reach the correct classification. Blue points and lines: These correspond to the mean centroid distance (mean.centroids.dist), a metric that reflects the classification error rate based on the average distance of samples to the group centroid in the reduced space. LUAD, lung adenocarcinoma; LUSC, lung squamous cell carcinoma; PLS-DA, partial least squares discriminant analysis; SCLC, small cell lung cancer.

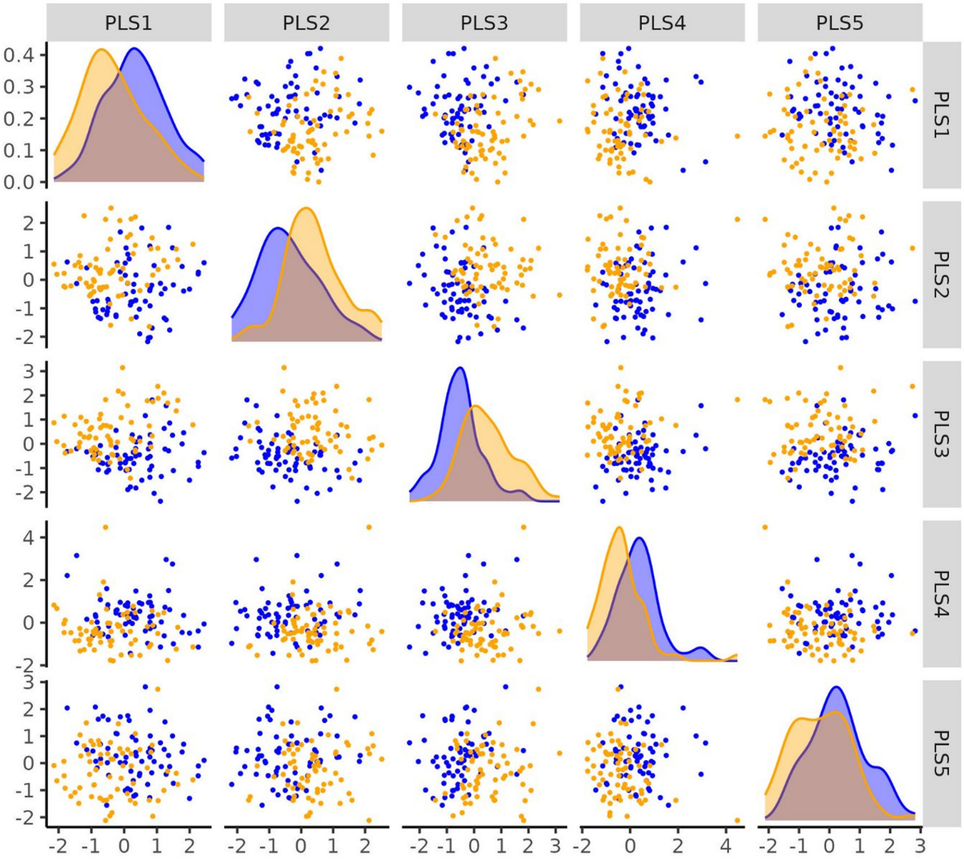

Figure S4 PLS-DA components Cases versus Controls comparison. All LC. The plot illustrates the separation between classes. The position of each point represents the projection into the reduced-dimensional space. LC, lung cancer; PLS-DA, partial least squares discriminant analysis.

https://dx.doi.org/10.21037/tlcr-2025-aw-1187

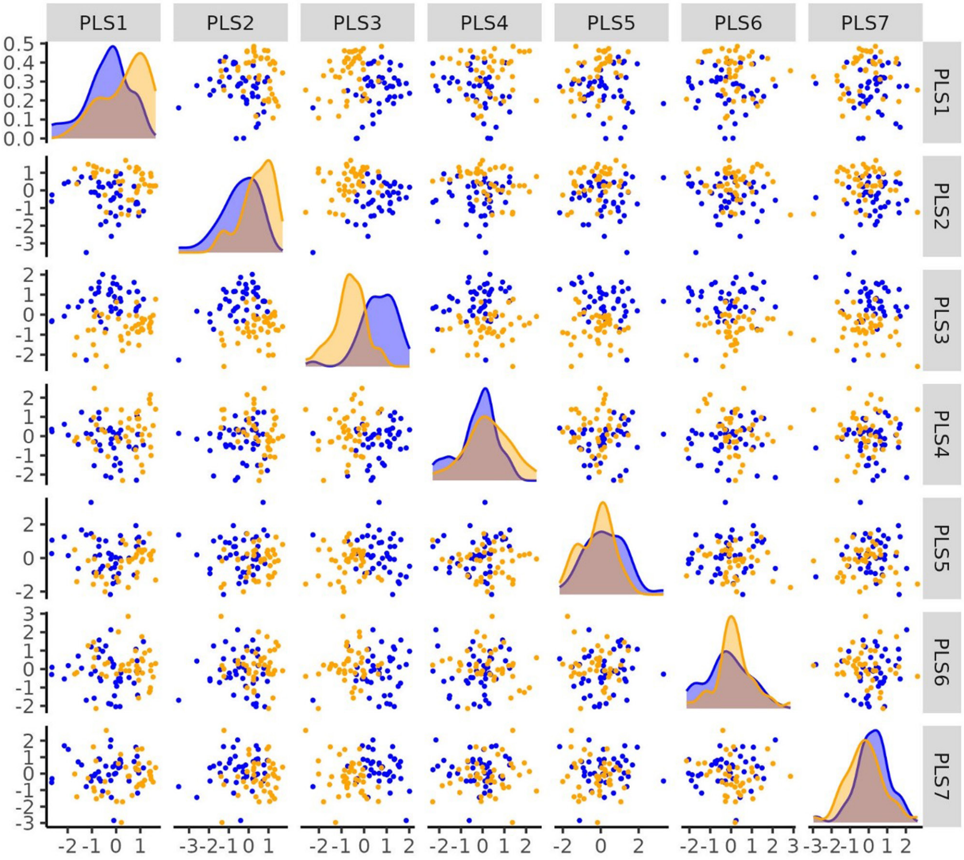

Figure S5 PLS-DA components LUAD versus Controls comparison. LUAD. The plot illustrates the separation between classes. The position of each point represents the projection into the reduced-dimensional space. LUAD, lung adenocarcinoma; PLS-DA, partial least squares discriminant analysis.

https://dx.doi.org/10.21037/tlcr-2025-aw-1187

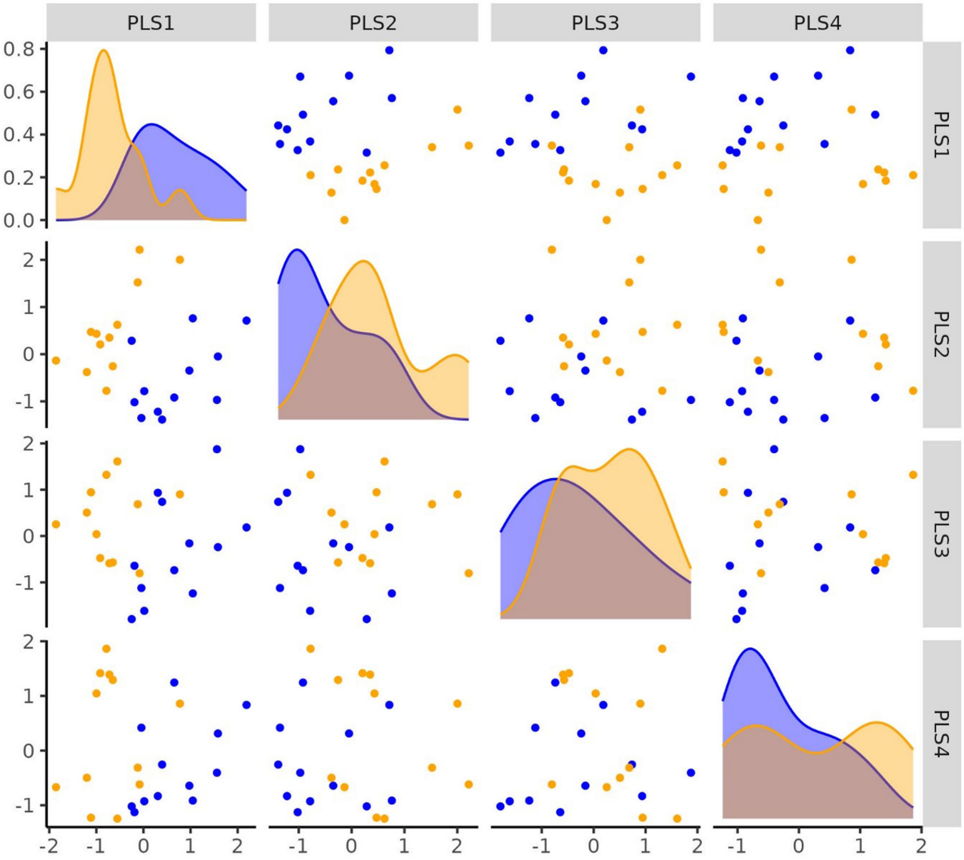

Figure S6 PLS-DA components LUSC versus Controls comparison. LUSC. The plot illustrates the separation between classes. The position of each point represents the projection into the reduced-dimensional space. LUSC, lung squamous cell carcinoma; PLS-DA, partial least squares.

https://dx.doi.org/10.21037/tlcr-2025-aw-1187

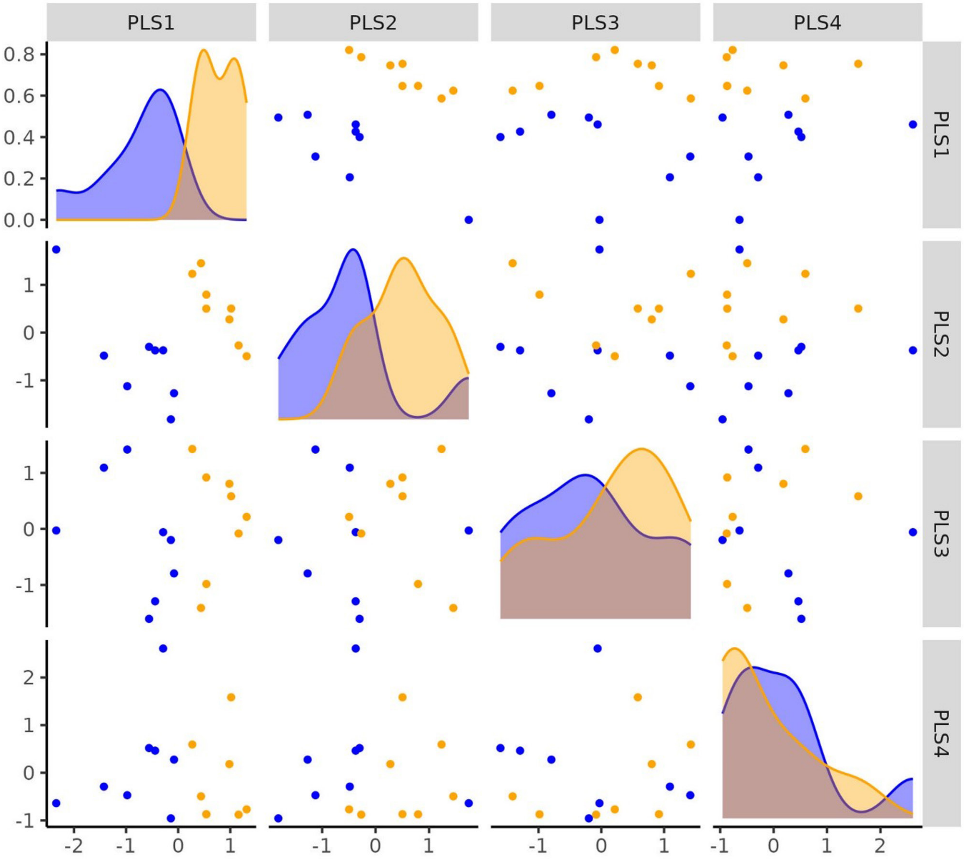

Figure S7 PLS-DA components SCLC versus Controls comparison. SCLC. The plot illustrates the separation between classes. The position of each point represents the projection into the reduced-dimensional space. PLS-DA, partial least squares discriminant analysis; SCLC, small cell lung cancer.

Table S1 SESI-HRMS ionisation adducts

1	$[M+H]^+$
2	$[M-H_2O+H]^+$
3	$[M-H_2O-H]^-$
4	$[M+NH_4]^+$
5	$[M+HCOO]^-$
6	$[M-H]^-$
7	$[M(C^{13})-H]^-$
8	$[M(C^{13})+H]^+$

M: molecule; H: hydrogen; H_2O: water; NH_4: ammoniumion; $HCOO^-$: formiat.

https://dx.doi.org/10.21037/tlcr-2025-aw-1187

Table S2 Total m/z feature list & results group comparison lung cancer *vs.* matched controls

m/z feature	log2FC	P	q	mode	MF	PassIsotopeFilter
257.19405	-0.93583653	6.50E-05	0.04652645			
175.1522	-1.09725372	9.60E-05	0.04652645			
139.13916	1.71920978	1.12E-04	0.04652645			
-178.13184	4.13138226	1.24E-04	0.04652645			
70.01753				1	NA	NaN
70.02874				1	C3H3NO	0
70.03999				1	NA	NaN
70.04132				1	NA	NaN
…						

Table S3 Results group comparison histological subtypes *vs.* matched controls

m/z feature	log2FC	P value	p.adj	q
LUAD				
-141.007	1.37501	1.31E-05	0.049125	0.033538
213.1274	-1.0698	3.88E-05	0.056312	0.038445
-124.02	0.40905	6.74E-05	0.056312	0.038445
257.1941	-1.278	7.96E-05	0.056312	0.038445
LUSC				
113.0346	2.637032	1.87E-04	0.70125	0.591374
150.9914	4.040398	4.67E-04	0.75	0.632485
150.0801	2.150735	6.00E-04	0.75	0.632485
138.9635	1.302043	0.00119	0.825	0.695734
SCLC				
218.1832	-2.73875	5.01E-04	1	1
-150.028	1.545898	0.00297	1	1
141.093	1.787777	0.00515	1	1
-219.051	0.436729	0.00518	1	1
…				

https://dx.doi.org/10.21037/tlcr-2025-aw-1187

Table S4 Results functional pathway enrichment analysis LUAD

Pathway	pathway_ total	hits_ total	P_ gamma	matched_ compound	query_ mass	matched_ form	mass_diff	log2FC	p	p.adj	q	mode	putative compound
De novo fatty acid biosynthesis	106	11	0.03955	C02679	218.2115	M+NH4 [1+]	3.7E-05	-1.025793831	0.000559	0.1040625	0.071045217	positive	Lauric acid
De novo fatty acid biosynthesis	106	11	0.03955	C06427	279.2318	M+H [1+]	4.6E-05	-0.541404269	0.0126	0.197698745	0.134972255	positive	alpha-Linolenic acid
De novo fatty acid biosynthesis	106	11	0.03955	C06426	279.2318	M+H [1+]	4.6E-05	-0.541404269	0.0126	0.197698745	0.134972255	positive	gamma-Linolenic acid
De novo fatty acid biosynthesis	106	11	0.03955	C02679	-200.1737	M(C13)-H [1-]	3.53323E-06	0.831285775	0.0159	0.222481343	0.151891752	negative	Lauric acid
De novo fatty acid biosynthesis	106	11	0.03955	C00712	283.2632	M+H [1+]	1.6E-05	-0.617059922	0.0252	0.267418033	0.182570785	positive	(9Z)-Octadecenoic acid
De novo fatty acid biosynthesis	106	11	0.03955	C00712	265.2526	M-H2O+H [1+]	1.35332E-05	-0.440475033	0.0286	0.281740838	0.192349204	positive	(9Z)-Octadecenoic acid
De novo fatty acid biosynthesis	106	11	0.03955	C02679	202.1882	M(C13)+H [1+]	3.64668E-05	-0.485858682	0.0458	0.332533589	0.227026269	positive	Lauric acid
De novo fatty acid biosynthesis	106	11	0.03955	C02679	-199.1704	M-H [1-]	3.6E-05	0.609830806	0.0699	0.394115442	0.269069235	negative	
De novo fatty acid biosynthesis	106	11	0.03955	C02679	183.1743	M-H2O+H [1+]	6.35332E-05	-0.138440302	0.119	0.468258132	0.319687696	positive	
De novo fatty acid biosynthesis	106	11	0.03955	C02679	201.1849	M+H [1+]	2.4E-05	-0.093570519	0.229	0.597183588	0.407707271	positive	
De novo fatty acid biosynthesis	106	11	0.03955	C06427	-277.2173	M-H [1-]	2.4E-05	-0.656409782	0.327	0.682007786	0.465618177	negative	
De novo fatty acid biosynthesis	106	11	0.03955	C06426	-277.2173	M-H [1-]	2.4E-05	-0.656409782	0.327	0.682007786	0.465618177	negative	
De novo fatty acid biosynthesis	106	11	0.03955	C00712	-282.252	M(C13)-H [1-]	6.35332E-05	-0.227538678	0.478	0.77457956	0.528818482	negative	
De novo fatty acid biosynthesis	106	11	0.03955	C00712	-281.2486	M-H [1-]	2.4E-05	-0.166701188	0.98	0.995637584	0.67973851	negative	
C21-steroid hormone biosynthesis and metabolism	112	6	0.039601	andrstndn	269.19	M-H2O+H [1+]	1.55332E-05	-0.981735496	0.00176	0.120681818	0.082391505	positive	NA
C21-steroid hormone biosynthesis and metabolism	112	6	0.039601	C00280	269.19	M-H2O+H [1+]	1.64668E-05	-0.981735496	0.00176	0.120681818	0.082391505	positive	NA
C21-steroid hormone biosynthesis and metabolism	112	6	0.039601	C02373	118.1226	M+NH4 [1+]	1.7E-05	-1.122921671	0.00638	0.16004902	0.109268155	positive	4-Methylpentanal
…													

Table S5 Results functional pathway enrichment analysis LUSC

Pathway	pathway_ total	hits_ total	p_ gamma	matched_ compound	query_ mass	matched_ form	mass_ diff	log2FC	p	p.adj	q	Mode	putative name
Butanoate metabolism	34	18	0.032689	C00042	119.0339	M+H [1+]	1.4E-05	2.586912	0.0216	0.871439	0.734896	Positive	Succinate
Butanoate metabolism	34	18	0.032689	C00109	85.0284	M-H2O+H [1+]	3.35E-05	0.740854	0.0217	0.871439	0.734896	Positive	2-Oxobutanoate
Butanoate metabolism	34	18	0.032689	C06144	85.0284	M+H [1+]	3.4E-05	0.740854	0.0217	0.871439	0.734896	Positive	3-Butynoate
Butanoate metabolism	34	18	0.032689	C00232	85.0284	M-H2O+H [1+]	3.35E-05	0.740854	0.0217	0.871439	0.734896	Positive	Succinate semialdehyde
Butanoate metabolism	34	18	0.032689	C00164	85.0284	M-H2O+H [1+]	3.35E-05	0.740854	0.0217	0.871439	0.734896	Positive	Acetoacetate
Butanoate metabolism	34	18	0.032689	C06144	86.0318	M(C13)+H [1+]	2.65E-05	1.445542	0.0297	0.871439	0.734896	Positive	3-Butynoate
Butanoate metabolism	34	18	0.032689	C00246	90.0631	M(C13)+H [1+]	6.47E-06	1.457495	0.036	0.871439	0.734896	Positive	Butanoic acid
Butanoate metabolism	34	18	0.032689	C00246	89.0597	M+H [1+]	2.4E-05	1.239639	0.0421	0.871439	0.734896	Positive	Butanoic acid
Butanoate metabolism	34	18	0.032689	C06010	115.039	M-H2O+H [1+]	6.47E-06	0.426589	0.0483	0.871439	0.734896	Positive	2-Oxobutanoate
Butanoate metabolism	34	18	0.032689	C00109	120.0655	M+NH4 [1+]	3E-06	0.254492	0.0595	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C00232	120.0655	M+NH4 [1+]	3E-06	0.254492	0.0595	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C00164	120.0655	M+NH4 [1+]	3E-06	0.254492	0.0595	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C00246	71.0491	M-H2O+H [1+]	6.35E-05	0.632262	0.062	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C01089	-104.043	M(C13)-H [1-]	1.65E-05	1.114277	0.0696	0.871439	0.734896	Negative	
Butanoate metabolism	34	18	0.032689	C05984	-104.043	M(C13)-H [1-]	1.65E-05	1.114277	0.0696	0.871439	0.734896	Negative	
Butanoate metabolism	34	18	0.032689	C01089	105.0546	M+H [1+]	5.4E-05	-0.32994	0.116	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C05984	105.0546	M+H [1+]	5.4E-05	-0.32994	0.116	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C06010	133.0495	M+H [1+]	3.6E-05	1.076886	0.121	0.871439	0.734896	Positive	
Butanoate metabolism	34	18	0.032689	C00042	-118.023	M(C13)-H [1-]	2.35E-05	0.592924	0.142	0.871439	0.734896	Negative	
Butanoate metabolism	34	18	0.032689	C00042	-117.019	M-H [1-]	1.6E-05	0.473969	0.148	0.871439	0.734896	Negative	
Butanoate metabolism	34	18	0.032689	C00246	106.0863	M+NH4 [1+]	2.7E-05	-0.18443	0.157	0.872812	0.736054	Positive	
Butanoate metabolism	34	18	0.032689	C01089	-103.04	M-H [1-]	5.6E-05	0.854556	0.163	0.872812	0.736054	Negative	
Butanoate metabolism	34	18	0.032689	C05984	-103.04	M-H [1-]	5.6E-05	0.854556	0.163	0.872812	0.736054	Negative	
Butanoate metabolism	34	18	0.032689	C00042	101.0233	M-H2O+H [1+]	3.35E-05	1.530464	0.167	0.872812	0.736054	Positive	
Butanoate metabolism	34	18	0.032689	C06144	102.055	M+NH4 [1+]	3.7E-05	0.107741	0.225	0.872812	0.736054	Positive	
Butanoate metabolism	34	18	0.032689	C00109	103.039	M+H [1+]	4E-06	0.059004	0.286	0.885632	0.746865	Positive	
Butanoate metabolism	34	18	0.032689	C00232	103.039	M+H [1+]	4E-06	0.059004	0.286	0.885632	0.746865	Positive	
Butanoate metabolism	34	18	0.032689	C00164	103.039	M+H [1+]	4E-06	0.059004	0.286	0.885632	0.746865	Positive	
Butanoate metabolism	34	18	0.032689	C01089	87.0441	M-H2O+H [1+]	8.35E-05	-0.38796	0.349	0.90411	0.762448	Positive	
Butanoate metabolism	34	18	0.032689	C05984	87.0441	M-H2O+H [1+]	8.35E-05	-0.38796	0.349	0.90411	0.762448	Positive	
Butanoate metabolism	34	18	0.032689	C00246	-88.0485	M(C13)-H [1-]	3.53E-06	-0.54451	0.358	0.906649	0.764589	Negative	
Butanoate metabolism	34	18	0.032689	C06010	-131.035	M-H [1-]	4.4E-05	0.074017	0.462	0.931169	0.785267	Negative	
Butanoate metabolism	34	18	0.032689	C06144	-84.0172	M(C13)-H [1-]	2.35E-05	-0.34044	0.514	0.936268	0.789567	Negative	
Butanoate metabolism	34	18	0.032689	C00109	-102.028	M(C13)-H [1-]	6.35E-05	-0.06027	0.526	0.936268	0.789567	Negative	
Butanoate metabolism	34	18	0.032689	C00232	-102.028	M(C13)-H [1-]	6.35E-05	-0.06027	0.526	0.936268	0.789567	Negative	
Butanoate metabolism	34	18	0.032689	C00164	-102.028	M(C13)-H [1-]	6.35E-05	-0.06027	0.526	0.936268	0.789567	Negative	
Butanoate metabolism	34	18	0.032689	C06010	150.0761	M+NH4 [1+]	3.3E-05	-0.37401	0.795	0.971091	0.818934	Positive	
Butanoate metabolism	34	18	0.032689	C00109	-101.024	M-H [1-]	4E-06	-0.16002	0.928	0.987065	0.832405	Negative	
Butanoate metabolism	34	18	0.032689	C00232	-101.024	M-H [1-]	4E-06	-0.16002	0.928	0.987065	0.832405	Negative	
Butanoate metabolism	34	18	0.032689	C00164	-101.024	M-H [1-]	4E-06	-0.16002	0.928	0.987065	0.832405	Negative	
Butanoate metabolism	34	18	0.032689	C00246	-87.0452	M-H [1-]	3.6E-05	-0.17129	0.938	0.987779	0.833008	Negative	
Butanoate metabolism	34	18	0.032689	C06144	-83.0139	M-H [1-]	3.6E-05	-0.14382	0.954	0.989627	0.834565	Negative	
Butanoate metabolism	34	18	0.032689	C06010	-132.038	M(C13)-H [1-]	3.53E-06	-0.02926	0.988	0.997319	0.841053	Negative	
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00160	-76.0121	M(C13)-H [1-]	2.35E-05	2.456151	0.00436	0.871439	0.734896	Negative	Glycolate
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00160	-75.0088	M-H [1-]	3.6E-05	2.266551	0.00908	0.871439	0.734896	Negative	Glycolate
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00109	85.0284	M-H2O+H [1+]	3.35E-05	0.740854	0.0217	0.871439	0.734896	Positive	2-Oxobutanoate
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C03508	-116.035	M-H [1-]	4E-06	1.195486	0.0255	0.871439	0.734896	Negative	L-2-Amino-3-oxobutanoic acid
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00048	-73.9965	M(C13)-H [1-]	4.35E-05	1.370331	0.0322	0.871439	0.734896	Negative	Glyoxylate
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00048	-72.9931	M-H [1-]	4E-06	0.941698	0.0354	0.871439	0.734896	Negative	Glyoxylate
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00109	120.0655	M+NH4 [1+]	3E-06	0.254492	0.0595	0.871439	0.734896	Positive	
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C05519	120.0655	M+H [1+]	4.4E-05	0.254492	0.0595	0.871439	0.734896	Positive	
Glycine, serine, alanine and threonine metabolism	88	29	0.032712	C00188	120.0655	M+H [1+]	4.4E-05	0.254492	0.0595	0.871439	0.734896	Positive	
…													

Table S6 Results functional pathway enrichment analysis SCLC

Pathway	pathway_ total	hits_ total	p_ gamma	matched_ compound	query_ mass	matched_ form	mass_ diff	log2FC	p	p.adj	q	Mode	putative name
Arginine and Proline Metabolism	45	22	0.033023	C01157	-130.051	M-H [1-]	3.6E-05	-0.74112	0.00897	1	1	Negative	Hydroxyproline
Arginine and Proline Metabolism	45	22	0.033023	C01165	-130.051	M-H [1-]	3.6E-05	-0.74112	0.00897	1	1	Negative	L-Glutamate 5-semialdehyde
Arginine and Proline Metabolism	45	22	0.033023	C02714	113.1073	M-H2O+H [1+]	5.35E-05	1.798593	0.011	1	1	Positive	N-Acetylputrescine
Arginine and Proline Metabolism	45	22	0.033023	C00148	-114.056	M-H [1-]	5.6E-05	-0.30466	0.0368	1	1	Negative	L-Proline
Arginine and Proline Metabolism	45	22	0.033023	C00763	-114.056	M-H [1-]	5.6E-05	-0.30466	0.0368	1	1	Negative	D-Proline
Arginine and Proline Metabolism	45	22	0.033023	C01127	-161.009	M-H [1-]	3.6E-05	-0.56244	0.0756	1	1	Negative	4-Hydroxy-2-oxoglutarat
Arginine and Proline Metabolism	45	22	0.033023	C03912	-112.04	M-H [1-]	2.4E-05	-0.37499	0.0825	1	1	Negative	(S)-1-Pyrroline-5-carboxylate;
Arginine and Proline Metabolism	45	22	0.033023	C03564	-112.04	M-H [1-]	2.4E-05	-0.37499	0.0825	1	1	Negative	1-Pyrroline-2-carboxylate
Arginine and Proline Metabolism	45	22	0.033023	C02946	-144.067	M-H [1-]	4E-06	-0.69022	0.0945	1	1	Negative	4-Acetamidbutanoate
Arginine and Proline Metabolism	45	22	0.033023	C00122	-116.007	M(C13)-H [1-]	8.35E-05	-0.4571	0.099	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C04281	-128.035	M-H [1-]	4E-06	-0.33962	0.0997	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C00022	-88.0121	M(C13)-H [1-]	2.35E-05	-0.26766	0.138	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C03912	114.055	M+H [1+]	1.6E-05	-0.30838	0.145	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C03564	114.055	M+H [1+]	1.6E-05	-0.30838	0.145	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C01157	114.055	M-H2O+H [1+]	8.35E-05	-0.30838	0.145	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C01165	114.055	M-H2O+H [1+]	8.35E-05	-0.30838	0.145	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00026	-146.018	M(C13)-H [1-]	2.35E-05	-0.97385	0.149	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C00148	98.06	M-H2O+H [1+]	6.35E-05	-0.50867	0.162	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00763	98.06	M-H2O+H [1+]	6.35E-05	-0.50867	0.162	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00022	-87.0088	M-H [1-]	3.6E-05	-0.18793	0.309	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C00026	-145.014	M-H [1-]	1.6E-05	-0.22625	0.313	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C01157	132.0655	M+H [1+]	3.4E-05	-0.02644	0.323	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C01165	132.0655	M+H [1+]	3.4E-05	-0.02644	0.323	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00122	-115.004	M-H [1-]	4.4E-05	-0.19933	0.388	1	1	Negative	
Arginine and Proline Metabolism	45	22	0.033023	C03564	96.0444	M-H2O+H [1+]	3.53E-06	0.236724	0.497	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00022	106.0499	M+NH4 [1+]	5.7E-05	1.803864	0.548	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00122	134.0448	M+NH4 [1+]	2.3E-05	1.959867	0.599	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C04281	130.0499	M+H [1+]	6E-06	0.41429	0.605	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00122	99.0077	M-H2O+H [1+]	3.53E-06	-0.20524	0.635	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C02946	146.0812	M+H [1+]	4E-06	-0.15234	0.728	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C02946	128.0706	M-H2O+H [1+]	2.35E-05	0.201224	0.805	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00022	71.0128	M-H2O+H [1+]	7.35E-05	0.29045	0.843	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C04281	112.0393	M-H2O+H [1+]	3.35E-05	0.132545	0.845	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00148	116.0706	M+H [1+]	2.4E-05	-0.04739	0.865	1	1	Positive	
Arginine and Proline Metabolism	45	22	0.033023	C00763	116.0706	M+H [1+]	2.4E-05	-0.04739	0.865	1	1	Positive	
Histidine metabolism	33	11	0.03312	C00099	-88.0404	M-H [1-]	4.4E-05	-1.93412	0.0332	1	1	Negative	beta-Alanine
Histidine metabolism	33	11	0.03312	C02835	-125.036	M-H [1-]	1.6E-05	-1.29267	0.0518	1	1	Negative	
Histidine metabolism	33	11	0.03312	C05827	125.0709	M+H [1+]	3.6E-05	0.541999	0.112	1	1	Positive	
Histidine metabolism	33	11	0.03312	C05130	-109.041	M-H [1-]	4E-06	-1.69863	0.13	1	1	Negative	
Histidine metabolism	33	11	0.03312	C00785	-137.036	M-H [1-]	3.6E-05	-0.85818	0.132	1	1	Negative	
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