

SUPPLEMENTARY TABLES

Table S1 Differential bacteria between smoking PDAC and non-smoking PDAC groups of tumor tissue from surgical samples

Species name	Group	Mean	LDA value	<i>P</i>
o__Gaiellales	PDAC_non-smoking	2.307637	2.929493	0.017001
p__unclassified_k__norank_d__Bacteria	PDAC_smoking	4.595560	4.195179	0.039318
g__Slackia	PDAC_smoking	2.369785	3.263086	0.047912
c__Thermoleophilia	PDAC_non-smoking	2.307637	2.913857	0.017001
o__unclassified_k__norank_d__Bacteria	PDAC_smoking	4.595560	4.195179	0.039318
c__unclassified_k__norank_d__Bacteria	PDAC_smoking	4.595560	4.195179	0.039318
g__Aeromonas	PDAC_non-smoking	1.953362	3.386388	0.004373
g__Aeromicrobium	PDAC_smoking	1.816943	3.385643	0.047912
g__Turicibacter	PDAC_non-smoking	2.743922	2.900026	0.017001
f__Aeromonadaceae	PDAC_non-smoking	1.953362	3.382760	0.004373
g__Faecalibacterium	PDAC_non-smoking	2.890487	2.863061	0.012222
g__unclassified_k__norank_d__Bacteria	PDAC_smoking	4.595560	4.195179	0.039318
f__unclassified_k__norank_d__Bacteria	PDAC_smoking	4.595560	4.195179	0.039318
g__Bradyrhizobium	PDAC_non-smoking	2.625058	3.017654	0.023870
g__Selenomonas	PDAC_non-smoking	2.798460	2.958753	0.034856
o__Aeromonadales	PDAC_non-smoking	1.953362	3.390673	0.004373
f__Xanthobacteraceae	PDAC_non-smoking	2.761896	2.904319	0.042611
g__Faecalibaculum	PDAC_non-smoking	2.478125	3.421223	0.046133

Table S2 Differential metabolites between smoking PDAC and non-smoking PDAC groups of tumor tissue from surgical samples

Metabolite	Regulate	VIP	FC(smoking_PDAC/non-smoking_PDAC)	P	FDR	smoking_PDA C (mean±SD)	non-smoking_PD AC (mean±SD)
PGP(16:0/TXB2)	down	3.8694	0.6558	0.01877	0.6188	2.925±1.287	4.46±1.57
PGP(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/5-iso PGF2VI)	down	4.0378	0.6319	0.000925 4	0.9995	3.315±1.045	5.246±0.5221
Lumirubin	up	3.8688	1.2758	0.03958	0.9995	6.106±0.4647	4.786±1.779
Demethylated antipyrine	down	3.5842	0.7317	0.01563	0.7536	3.074±0.4118	4.201±1.207
Nalmefene	down	3.3661	0.8065	0.02084	0.9995	4.321±0.7311	5.358±0.8385
Ile-Ile-Ala-Glu-Lys	down	3.114	0.6632	0.004551	0.9995	2.4±0.3123	3.619±1.094
5-Hydroxy-L-tryptophan	down	2.9877	0.8796	0.01698	0.9995	4.91±0.3704	5.582±0.6322
LysoPC(P-18:1(9Z)/0:0)	down	2.9871	0.8483	0.002007	0.9995	4.781±0.3115	5.636±0.6007
Oxalic Acid	down	2.9775	0.8274	0.01359	0.7536	3.678±0.4982	4.445±0.574
17-methylnonadecanoylcarnitine	down	2.9402	0.7992	0.01525	0.7536	4.315±0.7183	5.399±0.8295
Kinetensin 1-8	down	2.8989	0.8153	0.02209	0.9995	3.934±0.5435	4.825±0.8511
Ile Ile	down	2.6493	0.7426	0.03158	0.9995	3.831±1.268	5.159±0.5926
Asn Ala Glu Val Leu	down	2.4866	0.8893	0.04071	0.9995	5.124±0.6374	5.762±0.3291
Hydroxyrepaglinide	down	2.2196	0.8909	0.04946	0.9995	4.901±0.4895	5.501±0.6215
Val Asn Leu	down	2.107	0.8359	0.0387	0.9995	3.896±0.5677	4.661±0.7747
Trp Ile	down	2.0379	0.8588	0.04813	0.9995	4.487±0.7728	5.225±0.3786
PG(18:1(12Z)-2OH(9,10)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	down	2.0304	0.8301	0.04156	0.9995	4.12±0.817	4.963±0.5301
N-Acetyl-L-methionine	up	2.0109	1.0888	0.03831	0.9995	5.589±0.3611	5.133±0.4287
Humilixanthin	down	2.0049	0.8865	0.03728	0.9995	4.265±0.4644	4.811±0.4508
Naphthoxylactic acid	up	1.971	1.1444	0.02671	0.7536	4.415±0.3933	3.858±0.5036

Zedoarondiol	up	1.9304	1.179	0.03642	0.9995	4.848±0.2639	4.112±0.9681
Guanosine 3'-monophosphate	up	1.928	1.0922	0.0216	0.7536	6.004±0.2408	5.497±0.5482
Cetyl recinoleate	down	1.892	0.9267	0.02781	0.9995	5.258±0.3187	5.674±0.344
METHACHOLINE	up	1.8713	1.0841	0.01233	0.9995	5.609±0.3068	5.174±0.2685
Diaminopimelic acid	down	1.8434	0.8741	0.04963	0.9995	4.095±0.4995	4.685±0.5837
N-Acetyl-DL-Methionine	up	1.8386	1.0561	0.03286	0.7536	6.27±0.2977	5.937±0.2172
PI(PGJ2/20:1(11Z))	down	1.771	0.777	0.03773	0.9995	3.175±0.8333	4.086±0.6363
Uridine-5'-Monophosphate	up	1.7629	1.1082	0.029	0.7536	5.573±0.3291	5.029±0.5755
(9S,10S)-9,10-dihydroxyoctadecanoate	down	1.7474	0.9525	0.02833	0.7536	5.369±0.1229	5.637±0.3158
Homo-L-arginine	down	1.7446	0.9018	0.04456	0.9995	4.694±0.4932	5.205±0.3535
Prostratin	down	1.6708	0.923	0.03481	0.9995	4.302±0.2886	4.661±0.3144
8-Azaspiro[4.5]decane-7,9-dione	up	1.5809	1.0869	0.009585	0.9995	5.705±0.3341	5.249±0.204
Neotussilagine	down	1.5526	0.8552	0.04395	0.9995	3.249±0.4143	3.799±0.5823
Citramalic Acid	up	1.492	1.0593	0.02789	0.7536	5.463±0.2821	5.157±0.1442
(12R)-12-Hydroxyoctadec-9-enoic acid	up	1.4515	1.1106	0.04317	0.9995	4.981±0.3231	4.485±0.5778
Lys-Lys-OH	down	1.4497	0.961	0.01488	0.7536	5.393±0.1544	5.612±0.1505
Asiaticoside	up	1.4273	1.1686	0.0464	0.9995	4.74±0.4944	4.056±0.769
2-Hydroxypyridine	up	1.195	1.0586	0.01608	0.7536	4.354±0.1759	4.113±0.1596
Phthalic Acid	down	1.1867	0.9741	0.03602	0.7536	6.082±0.1564	6.244±0.08384
L-Lactic acid	up	1.173	1.0174	0.01477	0.7536	8.206±0.07917	8.066±0.1229
2,6-Dimethylocta-3,7-diene-1,6-diol	up	1.1701	1.1578	0.01934	0.9995	3.58±0.2584	3.092±0.4866
N-Nervonoyl Tryptophan	up	1.1607	1.044	0.04872	0.9995	6.456±0.2676	6.184±0.1943
Dinoterb	up	1.1249	1.0237	0.04222	0.7536	5.443±0.09391	5.317±0.1322
2-Hydroxy-3-Methylbutyric Acid	up	1.0202	1.0327	0.03458	0.7536	5.899±0.1758	5.712±0.1071

Table S3 Altered metabolic pathways between smoking PDAC and non-smoking PDAC groups of tumor tissue from surgical samples

Pathway Description	Ratio in study	Ratio in pop	<i>P</i>
HIF-1 signaling pathway	1/8	15/4407	0.02693
Glucagon signaling pathway	1/8	26/4407	0.04627
Choline metabolism in cancer	1/8	11/4407	0.01981
cAMP signaling pathway	1/8	25/4407	0.04453
Purine metabolism	2/8	101/4407	0.01331

Table S4 Differential bacteria between smoking PDAC and non-smoking PDAC groups of paracancerous tissue from surgical samples

Species name	Group	Mean	LDA value	<i>P</i>
o__Deinococcales	PDAC_smoking	2.256276	3.083655	0.047913
g__Romboutsia	PDAC_non-smoking	2.424143	3.078833	0.024968
f__Nocardioideaceae	PDAC_non-smoking	2.616940	3.119963	0.023870
g__Veillonella	PDAC_smoking	4.430748	4.315691	0.036454
g__Aeromicrobium	PDAC_non-smoking	2.573906	3.069251	0.046134
g__Deinococcus	PDAC_smoking	2.256276	3.083712	0.047913
g__Enterococcus	PDAC_smoking	4.664164	4.533765	0.027670
f__Deinococcaceae	PDAC_smoking	2.256276	3.083738	0.047913
g__Streptomyces	PDAC_non-smoking	2.214884	3.375907	0.017002
f__Enterococcaceae	PDAC_smoking	4.664164	4.533789	0.027670
f__Nocardiaceae	PDAC_non-smoking	2.698844	2.871430	0.023870
f__Streptomycetaceae	PDAC_non-smoking	2.214884	3.282668	0.017002
p__Deinococcota	PDAC_smoking	2.487057	3.101904	0.012074
o__Streptomycetales	PDAC_non-smoking	2.214884	3.319216	0.017002
c__Deinococci	PDAC_smoking	2.487057	3.101913	0.012074
g__Novosphingobium	PDAC_smoking	2.610335	3.15903	0.025922
o__Deinococcales	PDAC_smoking	2.256276	3.083655	0.047913

Table S5 Differential metabolites between smoking PDAC and non-smoking PDAC groups of paracancerous tissue from surgical samples

Metabolite	Regulate	VI P	FC(smoking_PDA C/non-smoking_P DAC)	P	FD R	smoking_PDA C (mean±SD)	non-smoking_PDA C (mean±SD)
Schizandrin	down	3.5308	0.2872	9.44E-05	0.02375	1.493±1.376	5.199±1.245
Cromakalim	up	3.1184	2.2012	0.0005478	0.02392	5.043±0.4784	2.291±1.897
Dermorphin	down	3.0754	0.3542	0.005024	0.06558	1.881±2.426	5.311±0.7707
MG(14:1(9Z)/0:0/0:0)	down	2.9205	0.5169	0.01178	0.04997	3.067±2.295	5.934±0.9112
BUTHIONINE SULFOXIMINE	down	2.8773	0.4823	0.001466	0.03871	2.535±1.587	5.256±0.6785
Bempedoic acid	down	2.86	0.6257	5.41E-05	0.02185	3.723±0.7594	5.95±0.7483
Glucosaminylmuramyl-2-alanine-D-isoglutamine	down	2.858	0.4988	0.00497	0.06558	2.814±2.006	5.642±0.58

		4		2			
PGP(16:0/TXB2)	dow n	2.8 44	0.5353	0.00 018 59	0.02 425	2.891± 1.068	5.401±0. 7514
21-Desacetyl Deflazacort	dow n	2.8 37 4	0.4509	0.00 517 4	0.06 635	2.651± 2.288	5.88±0.7 635
MG(5-iso PGF2VI/0:0/0:0)	dow n	2.8 15	0.6164	5.18 E-0 5	0.02 185	3.907± 0.6484	6.338±1. 064
L-Theanine	dow n	2.7 93 7	0.5211	0.00 038 06	0.02 694	2.396± 0.6106	4.598±1. 301
Allysine	dow n	2.7 79 1	0.5614	0.00 071 57	0.02 962	3.21±1. 338	5.718±0. 5732
Ile Asp Val	dow n	2.6 76 1	0.5847	0.01 253	0.09 18	3.462± 2.059	5.921±0. 3427
Pro Val Ala	dow n	2.6 66	0.5503	0.00 298 7	0.05 354	3.051± 1.67	5.544±0. 2431
Val Thr Leu	dow n	2.6 62 8	0.6094	0.00 019 4	0.02 425	3.47±1. 039	5.694±0. 3665
PS(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	dow	2.6	0.5276	0.00	0.03	2.468±	4.678±0.

	n	53 4		110 3	51	1.269	4085
Leu His Ile	dow n	2.6 18 4	0.565	0.00 161 6	0.03 888	2.756± 1.237	4.878±0. 6013
Bersimoside I	dow n	2.5 99 6	0.4015	0.00 366 6	0.05 927	1.86±1. 903	4.633±0. 3731
Carboprost	dow n	2.5 74 3	0.7601	5.76 E-0 6	0.01 188	5.747± 0.3639	7.561±0. 6759
Heliotridine	dow n	2.5 23 5	0.6065	0.00 519 9	0.06 635	3.486± 1.643	5.748±0. 2368
Nalmefene	dow n	2.5 22 1	0.7002	0.00 033 3	0.02 694	4.444± 0.8295	6.347±0. 6878
Gly Leu Leu	dow n	2.5 21 4	0.6141	0.00 121 8	0.03 596	3.407± 1.248	5.548±0. 3819
Bms-275183	dow n	2.5 10 9	0.6567	0.00 487	0.06 534	3.872± 1.452	5.896±0. 2592
Oxypinnatanine	dow n	2.4 97 4	0.6818	0.00 134 1	0.03 709	4.096± 1.144	6.008±0. 2284

Nandrolone	dow n	2.4 73 6	0.7145	8.56 E-0 5	0.02 375	4.398± 0.6839	6.155±0. 4996
9-(2,3-dihydroxypropoxy)-9-Oxononanoic Acid	dow n	2.4 64 2	0.7038	0.00 083 05	0.02 392	4.049± 0.648	5.753±0. 9711
Hypromellose	dow n	2.4 62 7	0.6315	0.00 107 1	0.03 501	3.384± 1.054	5.359±0. 6548
Lumirubin	up	2.4 48 7	1.4431	0.00 162 2	0.03 888	5.957± 0.6163	4.128±1. 278
Ser Thr Pro Asp Ala	dow n	2.4 37 3	0.6004	0.04 503	0.13 99	3.324± 2.317	5.536±0. 9681
14-Deoxy-11,12-Didehydroandrographolide	dow n	2.4 12 4	0.7038	0.00 116 4	0.03 577	4.374± 0.6485	6.215±1. 183
Epsilon-Caprolactone	dow n	2.3 83 3	0.7155	0.00 041 65	0.02 694	4.149± 0.4482	5.799±0. 996
Phe Pro His	dow n	2.3 80 2	0.7002	0.00 069 57	0.02 962	4.297± 0.9533	6.137±0. 5126
Ganglioside GM3 (d18:0/14:0)	dow n	2.3 65	0.7602	0.00 040	0.02 694	4.959± 0.6446	6.523±0. 677

		9		2			
Thr Glu Ile	dow n	2.3 58 7	0.6376	0.01 737	0.10 05	3.551± 1.785	5.569±0. 3771
Arginylasparagine	dow n	2.3 34 1	0.7209	0.00 049 89	0.02 694	4.078± 0.7391	5.657±0. 5569
4-Fluoro-N-methyl-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N-ethyl-L-tyrosinamide	dow n	2.3 27 1	0.6886	0.00 132 9	0.03 709	3.922± 0.9696	5.696±0. 6147
9-Oxo-nonanoic acid	dow n	2.3 13 1	0.6796	0.00 260 2	0.02 67	3.39±0. 7215	4.988±1. 035
Histidylleucine	dow n	2.3 11 1	0.7644	0.00 106 6	0.03 501	5.087± 0.8483	6.655±0. 4852
9-F1-phytoprostane	dow n	2.2 95 9	0.7363	0.00 134 1	0.03 709	4.44±0. 5981	6.03±1.0 11
Ser Asp Ile	dow n	2.2 93 7	0.7236	0.00 345 4	0.05 811	4.367± 1.068	6.035±0. 5613
Cinnassiol D2	dow n	2.2 92 5	0.6133	0.02 39	0.10 92	3.236± 1.425	5.276±1. 776
Trp Thr Gln	dow	2.2	0.5586	0.02	0.10	2.694±	4.823±0.

	n	84		138	62	1.931	6142
		9					
Val Ile Leu	dow	2.2	0.6737	0.01	0.08	3.915±	5.811±0.
	n	77		064	684	1.48	6406
		3					
PGP(i-22:0/6 keto-PGF1 alpha)	dow	2.2	0.5135	0.00	0.08	2.306±	4.491±0.
	n	71		859	251	1.641	7311
		9		5			
Valylisoleucine	dow	2.2	0.7577	0.00	0.02	4.321±	5.703±0.
	n	63		194	589	0.725	6641
		5		6			
Agavasaponin D	dow	2.2	0.6482	0.00	0.07	3.027±	4.67±0.7
	n	62		690	626	1.123	515
		7		4			
Gly Asp Leu	dow	2.2	0.7447	0.00	0.04	4.302±	5.777±0.
	n	60		2	456	0.8796	4475
		9					
His Ser Val Glu	dow	2.2	0.6218	0.01	0.09	3.265±	5.251±0.
	n	48		453	575	1.688	4476
		3					
Gln Ala Phe	dow	2.2	0.4571	0.03	0.12	1.663±	3.638±2.
	n	47		537	67	1.264	163
		8					
6-Hydroxymelatonin	dow	2.2	0.7309	0.00	0.02	3.909±	5.348±0.
	n	39		030	392	0.6267	5051
		7		81			

Asparaginylisoleucine	dow n	2.2 38 7	0.7431	0.00 455 1	0.03 282	3.997± 0.8912	5.379±0. 5773
5-Deoxydiplosporin	dow n	2.2 32 6	0.5837	0.02 413	0.10 95	2.311± 1.442	3.959±0. 8485
Valylglutamine	dow n	2.2 30 1	0.7541	0.00 011 5	0.02 375	4.308± 0.5922	5.713±0. 3323
Isoguvacine	dow n	2.2 27 4	0.6634	0.01 153	0.08 971	3.66±1. 524	5.517±0. 3323
6-n-Octylaminouracil	dow n	2.2 27 2	0.7708	0.00 420 7	0.03 139	4.133± 0.8117	5.362±0. 4188
Imazapyr	dow n	2.2 21 4	0.7504	0.00 053 36	0.02 694	4.308± 0.7017	5.741±0. 4413
(11E,15Z)-9,10,13-Trihydroxy-11,15-octadecadienoic acid	dow n	2.2 11 6	0.7493	0.00 261 4	0.04 942	4.728± 0.7137	6.31±1.0 27
PIP(20:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))	dow n	2.2 08 8	0.5938	0.00 502 7	0.06 558	2.74±1. 209	4.614±0. 8439
10-(2,3-Dihydroxypropoxy)-10-oxodecanoic acid	dow n	2.2 01	0.7184	0.00 265	0.04 965	3.9±0.9 968	5.429±0. 2431

				5			
S-(PGA2)-glutathione	dow n	2.1 86 5	0.7499	0.00 071 07	0.02 962	4.33±0. 7471	5.774±0. 413
4-Oxododecanedioic acid	dow n	2.1 85 8	0.7337	0.00 785 4	0.04 105	4.186± 0.9368	5.705±0. 9716
13-HODE	dow n	2.1 81 4	0.7148	0.00 417 8	0.06 179	3.937± 0.5098	5.508±1. 324
PG(18:1(12Z)-2OH(9,10)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	dow n	2.1 81 3	0.7105	0.00 053 87	0.02 694	3.952± 0.7929	5.562±0. 4858
PGP(20:3(8Z,11Z,14Z)/6 keto-PGF1alpha)	dow n	2.1 79 3	0.6706	0.00 164 2	0.03 912	3.619± 1.061	5.397±0. 4163
Val-pro-pro	dow n	2.1 59 1	0.7872	0.00 105 3	0.03 501	5.017± 0.7315	6.373±0. 4202
Aspartyl-Valine	dow n	2.1 52 3	0.788	0.03 067	0.07 918	4.694± 1.206	5.957±0. 5332
Val Ala Ser	dow n	2.1 45 1	0.6722	0.01 588	0.09 835	4.002± 1.666	5.954±0. 5648
LysoPC(20:3(8Z,11Z,14Z)/0:0)	dow	2.1	0.7749	0.01	0.09	4.946±	6.383±0.

	n	42		189	023	1.197	1293
		8					
Gly His	dow	2.1	0.6845	0.00	0.07	3.454±	5.046±0.
	n	41		605	258	1.07	6984
		7		7			
Pro Ser Ile	dow	2.1	0.7073	0.00	0.06	3.892±	5.503±0.
	n	40		39	007	1.11	2648
		3					
9,10-Epoxystearic acid	dow	2.1	0.7207	0.00	0.02	3.452±	4.79±0.6
	n	38		041	694	0.5304	205
		1		81			
Demethylated antipyrine	dow	2.1	0.7294	0.00	0.02	3.903±	5.351±0.
	n	35		091	392	0.5618	8298
		8		88			
Lyciumoside I	dow	2.1	0.7133	0.00	0.08	3.98±1.	5.58±0.1
	n	25		897	337	269	561
		6		1			
Leu Pro Arg	dow	2.1	0.7161	0.00	0.08	4.144±	5.787±0.
	n	24		892	337	1.118	9113
				2			
(9Z,11E,13S,15Z)-13-Hydroxyoctadeca-9,11,15-trienoic acid	dow	2.1	0.7955	0.00	0.03	5.177±	6.508±0.
	n	15		144	87	0.6239	7
		3		6			
Prostaglandin A2	dow	2.1	0.7025	0.00	0.02	3.856±	5.489±0.
	n	12		137	419	0.7565	86
		5		3			

Ferulic acid	dow n	2.1 01 2	0.714	0.00 524 4	0.06 671	3.195± 0.3814	4.475±1. 147
Uric Acid	up	2.1 00 3	1.3353	0.01 69	0.05 932	6.774± 0.3227	5.073±1. 987
Thr Ile Ala	dow n	2.0 99 2	0.7779	0.00 17	0.03 981	4.897± 0.8257	6.295±0. 3774
Ser Val Gln Leu Leu	dow n	2.0 98 5	0.7545	0.00 136 9	0.03 738	4.478± 0.7844	5.935±0. 5479
Leu Val Ala	dow n	2.0 97 3	0.6979	0.00 041 97	0.02 694	3.636± 0.6587	5.21±0.6 74
Gly Val Leu	dow n	2.0 89 1	0.682	0.03 732	0.12 86	4.012± 1.935	5.883±0. 4569
Bis(4-methoxybenzoyl)-3a,29-dihydroxy-8-multifloren-7-one	dow n	2.0 83 4	0.7056	0.00 010 07	0.02 375	3.385± 0.5543	4.797±0. 4197
Isoleucyl-Valine	dow n	2.0 69 1	0.7707	0.00 269 9	0.02 68	4.338± 0.7402	5.629±0. 5801
Citric Acid	up	2.0 64	1.2823	0.01 844	0.06 205	6.5±0.9 867	5.069±1. 127

		2					
11'-Carboxy-gamma-tocotrienol	dow n	2.0 55 3	0.6306	0.01 791	0.10 13	3.344± 1.71	5.303±0. 5819
13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	dow n	2.0 46	0.7825	0.00 051 74	0.02 694	5.097± 0.5863	6.514±0. 6573
Cilomilast	dow n	2.0 45 5	0.7764	0.00 414 2	0.03 118	4.271± 0.8134	5.501±0. 4095
Milbemycin alpha10	dow n	2.0 43 2	0.739	0.00 029 94	0.02 694	3.984± 0.4154	5.391±0. 7761
9-OxoODE	dow n	2.0 42	0.8033	0.00 156 1	0.03 888	5.241± 0.5484	6.524±0. 7662
Etimicin	dow n	2.0 35 2	0.7129	6.14 E-0 5	0.02 185	3.698± 0.5679	5.187±0. 3902
9,12,13-TriHOME	dow n	2.0 34 6	0.8055	0.00 665 5	0.07 562	5.59±0. 6952	6.94±1.0 1
12-OPDA	dow n	2.0 34 2	0.8169	0.00 212 2	0.04 594	5.564± 0.3749	6.811±0. 9503
Lys Leu Ile	dow	2.0	0.7695	0.00	0.02	4.519±	5.873±0.

	n	30		010	375	0.3459	6784
		2		47			
Val Gly Val	dow	2.0	0.7543	0.00	0.04	4.267±	5.657±0.
	n	19		243	763	0.8822	3013
		3		8			
Thr-Leu	dow	2.0	0.7589	0.00	0.02	4.072±	5.366±0.
	n	15		199	589	0.6506	6808
		9		8			
L-Aspartyl-L-Phenylalanine	dow	2.0	0.7971	0.01	0.05	4.44±0.	5.57±0.2
	n	14		425	573	9589	427
		6					
13(S)-HOTrE	dow	2.0	0.8322	0.00	0.03	5.976±	7.181±0.
	n	04		161	888	0.337	8947
		3		4			
PGP(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/5-iso PGF2VI)	dow	2.0	0.7383	0.02	0.10	4.206±	5.697±0.
	n	02		272	81	1.389	3073
		4					
Avocadyne 1-acetate	dow	1.9	0.844	6.36	0.02	6.14±0.	7.275±0.
	n	71		E-0	185	32	4941
		2		5			
Anhydrocinnzeylanine	dow	1.9	0.7738	0.02	0.10	5.008±	6.472±0.
	n	7		039	5	1.261	6541
Corchorifatty acid F	dow	1.9	0.8161	0.00	0.03	5.441±	6.667±0.
	n	64		470	318	0.5352	9405
		6		4			
2-Cyclohexylidencyclohexanone	dow	1.9	0.7185	0.01	0.08	3.598±	5.008±1.

	n	62 8		126	91	0.7203	233
14,15-DiHETrE	dow n	1.9 56 4	0.8248	0.00 710 6	0.03 982	4.75±0. 5654	5.759±0. 7094
N-(p-Hydroxyphenethyl)actinidine	dow n	1.9 49 8	0.7075	0.00 218	0.04 61	3.425± 0.8755	4.841±0. 3508
Leu Glu Gly	dow n	1.9 43 8	0.7913	0.00 101 2	0.03 501	4.581± 0.6236	5.789±0. 4428
Arg-3-hyp-7-phe-bradykinin	dow n	1.9 43 5	0.5795	0.03 344	0.12 33	2.88±2. 064	4.97±0.7 584
Val His Ile	dow n	1.9 40 2	0.7941	0.00 223 8	0.04 613	4.475± 0.5327	5.635±0. 7104
Ligusticide	dow n	1.9 37 9	0.7266	0.00 905 9	0.08 354	3.538± 0.5044	4.869±1. 255
4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	dow n	1.9 34 7	0.7142	0.00 804 7	0.08 09	3.641± 1.061	5.098±0. 5609
Trimethobenzamide	dow n	1.9 34 2	0.726	0.00 658	0.07 555	3.94±1. 072	5.427±0. 4649

Biocytin	dow n	1.9 30 1	0.8101	0.00 638 1	0.07 43	4.483± 0.6778	5.534±0. 5504
Dethiobiotin	dow n	1.9 28	0.7403	0.00 260 6	0.02 67	4.017± 0.6626	5.426±0. 8779
Ile Glu Ser	dow n	1.9 26 3	0.7545	0.00 032 56	0.02 694	4.124± 0.5189	5.466±0. 6013
Kifunensine	dow n	1.9 15 7	0.7531	0.01 248	0.09 18	3.487± 0.6533	4.63±0.9 503
Sinomenine	dow n	1.9 15 1	0.8135	0.01 039	0.04 662	4.721± 0.839	5.803±0. 3731
Glycyl-Phenylalanine	dow n	1.9 14 4	0.7818	0.00 387	0.03 073	4.024± 0.7323	5.147±0. 3806
Ile Pro Ile	dow n	1.9 13 7	0.7622	0.00 913 2	0.08 365	4.326± 1.068	5.676±0. 2001
Elaidic Acid	dow n	1.9 13 6	0.8055	0.00 141 2	0.02 421	3.942± 0.5471	4.894±0. 2578
THYMOPENTIN	dow n	1.9 13	0.706	0.02 793	0.11 63	3.41±1. 328	4.83±0.5 935

		4					
Bolasterone	dow n	1.9 13 2	0.7711	0.00 866 5	0.04 231	3.814± 0.6283	4.946±0. 8588
Ala Val Ile	dow n	1.9 12 2	0.786	0.00 430 5	0.06 246	4.547± 0.7149	5.785±0. 6857
Humilixanthin	dow n	1.8 98 5	0.7966	0.00 151 7	0.03 888	4.093± 0.6071	5.138±0. 2826
ALANYL-dl-LEUCINE	dow n	1.8 88 8	0.7935	0.00 668 7	0.03 865	4.658± 0.7655	5.87±0.6 87
3,5-Dichloro-2,6-dihydroxybenzoic acid	up	1.8 88 8	1.2746	0.00 578 7	0.03 58	5.848± 0.4425	4.588±1. 106
Thr Asp Phe	dow n	1.8 88 7	0.7795	0.00 039 96	0.02 694	4.077± 0.5849	5.23±0.1 978
Arg Leu	dow n	1.8 87 5	0.8277	0.00 038	0.02 694	5.265± 0.4514	6.361±0. 4665
N-(N-(3-Amino-3-carboxypropyl)-3-amino-3-carboxypropyl)azetidine-2-carboxylic acid	dow n	1.8 87 4	0.7294	0.00 178 9	0.02 486	3.661± 0.7381	5.019±0. 5743
Kukoamine D	dow	1.8	0.6929	0.03	0.12	3.913±	5.647±0.

	n	84 1		474	51	1.768	3802
9,10,13-TriHOME	dow n	1.8 82 2	0.8514	0.00 422 5	0.03 139	6.297± 0.5036	7.396±0. 7954
PIP(18:1(12Z)-O(9S,10R)/20:1(11Z))	dow n	1.8 79 2	0.75	0.00 059 38	0.02 75	3.958± 0.7011	5.277±0. 2337
Serylisoleucine	dow n	1.8 71 8	0.7796	0.00 390 1	0.03 073	4.202± 0.6904	5.39±0.6 216
Astacin	dow n	1.8 68 2	0.722	0.01 329	0.09 374	4.057± 1.221	5.619±0. 7138
Ala Val Thr	dow n	1.8 67 8	0.7944	0.00 939 7	0.08 416	4.603± 0.9192	5.794±0. 3536
1,2-Dihydroxy-3-keto-5-methylthiopentene	dow n	1.8 33	0.7602	0.01 331	0.09 374	3.494± 0.5071	4.596±1. 062
Ile Ile	dow n	1.8 31 3	0.7521	0.01 774	0.10 07	4.169± 1.156	5.543±0. 5843
Asparaginylnl-Phenylalanine	dow n	1.8 25 6	0.7745	0.02	0.06 396	4.139± 0.7615	5.344±1. 082
Ile Gly Leu	dow	1.8	0.7298	0.02	0.10	3.473±	4.759±1.

	n	14		409	95	0.8671	167
Kinetensin 1-8	dow n	1.8 11 4	0.7718	0.00 36	0.05 911	4.146± 0.6243	5.372±0. 7706
12-Hydroxyheptadeca-5,8,10-trienoic acid	dow n	1.8 06	0.8009	0.03 384	0.12 42	4.388± 0.9651	5.479±0. 7642
(R)-Laudanidine	dow n	1.8 02 5	0.8303	0.00 291 4	0.02 751	4.609± 0.5296	5.551±0. 4638
Asn Phe	dow n	1.7 96 6	0.727	0.02 793	0.11 63	4.147± 1.434	5.704±0. 7325
Val Val	dow n	1.7 92 9	0.7963	0.01 931	0.10 35	4.668± 0.9507	5.862±0. 7191
Arabinofuranosylguanine	dow n	1.7 86 4	0.8443	0.03 862	0.08 967	5.033± 0.8594	5.961±0. 6379
9(S)-HpOTrE	dow n	1.7 71 7	0.8467	0.00 557 6	0.03 517	5.646± 0.2702	6.668±0. 9454
9(S)-HpODE	dow n	1.7 69	0.853	0.00 258 1	0.02 67	6.087± 0.3442	7.136±0. 8064
4-ene-Valproic acid	dow n	1.7 67	0.8303	0.00 115	0.02 392	5.134± 0.3915	6.183±0. 6499

				3			
Ser Ala Val Thr Ala	dow n	1.7 58 7	0.8184	0.00 055 67	0.02 694	4.502± 0.4062	5.501±0. 4836
Meclizine	dow n	1.7 57 9	0.8302	0.00 374 2	0.05 961	5.157± 0.7036	6.212±0. 2816
D-Glucono-1,4-lactone	up	1.7 57 9	1.2681	0.01 632	0.09 862	5.118± 0.8325	4.036±0. 6344
Tryptophyl-Glutamine	dow n	1.7 52	0.8088	0.01 456	0.09 575	4.365± 0.6687	5.397±0. 7965
8-Epi pgf1 alpha	dow n	1.7 48 6	0.7814	0.04 668	0.10 02	4.026± 0.7803	5.152±1. 304
Cinnassiol D3	dow n	1.7 42 7	0.6891	0.00 756 8	0.04 029	3.403± 0.9657	4.938±0. 9306
(2-Naphthalenyloxy)acetic acid	dow n	1.7 40 7	0.8108	0.02 494	0.11 06	4.238± 0.3118	5.227±1. 206
Nopalinic acid	dow n	1.7 34 4	0.8252	0.00 830 5	0.08 249	4.943± 0.7843	5.99±0.3 346
Thromboxane B2	dow n	1.7 27	0.7836	0.00 294	0.05 326	3.671± 0.5571	4.685±0. 5275

		3		6			
Citramide	up	1.7 25 4	1.2449	0.00 515 8	0.03 438	5.175± 0.5356	4.157±0. 6906
5-Hydroxy-L-tryptophan	dow n	1.7 24 3	0.8519	0.00 482 7	0.06 534	5.246± 0.3241	6.158±0. 769
Dihydrojasmone	dow n	1.7 21	0.7686	0.01 983	0.10 44	3.69±0. 6183	4.801±1. 09
(R)-2-Hydroxysterculic acid	dow n	1.7 10 9	0.8375	0.01 157	0.08 977	5.395± 0.8643	6.442±0. 1487
4-Ethyl-7,11-dimethyldodeca-trans-2-trans-6-1-o-trien-1-al	up	1.7 09 6	1.2658	0.00 669	0.07 562	5.072± 0.3162	4.007±0. 9999
Tyr Leu	dow n	1.7 06 9	0.8237	0.00 342 2	0.05 804	4.593± 0.6269	5.576±0. 3368
Lys Ile Leu	dow n	1.6 91	0.7839	0.00 249 7	0.04 856	4.32±0. 2771	5.511±0. 9818
Isoleucyl-Serine	dow n	1.6 90 4	0.8367	0.00 781 3	0.07 972	5.267± 0.6161	6.295±0. 6855
Val Ala Leu	dow n	1.6 88	0.759	0.04 485	0.13 99	4.138± 1.354	5.452±0. 6607

		3					
3-O-Demethylfortimicin A	dow n	1.6 83 8	0.7217	0.01 541	0.09 757	3.84±1. 206	5.321±0. 639
D-Glucosamine-6-phosphate	dow n	1.6 79 3	0.8341	0.02 293	0.06 825	4.237± 0.7636	5.08±0.3 056
Sphinganine (C20)	up	1.6 73 5	1.2575	0.00 515 9	0.06 635	5.362± 0.7332	4.264±0. 4324
LysoPC(P-18:1(9Z)/0:0)	dow n	1.6 68	0.8486	0.01 042	0.08 621	5.032± 0.7038	5.93±0.2 757
Cimifugin	up	1.6 6	1.1701	0.02 141	0.10 62	6.267± 0.533	5.356±0. 8877
Pelargonidin 3-sophoroside	up	1.6 58 4	1.1448	0.01 969	0.10 44	7.188± 0.4146	6.279±0. 9715
(6E)-8-hydroxygeraniol	dow n	1.6 55 4	0.7547	0.00 797 9	0.04 157	2.822± 0.3701	3.739±0. 8244
PA(20:2(11Z,14Z)/22:5(7Z,10Z,13Z,16Z,19Z))	dow n	1.6 53 5	0.7326	0.01 178	0.09 023	3.989± 1.009	5.445±0. 9087
Dapta	dow n	1.6 52 6	0.753	0.02 271	0.10 81	3.924± 1.113	5.211±0. 6505

Val Asn Leu	dow n	1.6 50 8	0.8031	0.00 384	0.05 996	4.324± 0.5359	5.384±0. 6841
Lamprey gonadotropin-releasing hormone-I	dow n	1.6 49 9	0.7553	0.00 239 2	0.04 714	3.763± 0.6579	4.982±0. 6035
CDP-DG(PGF1alpha/18:1(9Z))	dow n	1.6 48 1	0.7397	0.01 431	0.09 539	3.444± 0.5982	4.656±1. 154
4-(2-((7-Amino-2-(furan-2-yl)-[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino)ethyl)phenol	dow n	1.6 47	0.7583	0.04 826	0.14 35	3.502± 0.9239	4.618±1. 12
Acetylsoyasaponin A6	dow n	1.6 42 7	0.8164	0.00 212 9	0.04 594	4.363± 0.6297	5.344±0. 06224
11(R)-HEDE	dow n	1.6 39 1	0.865	0.03 693	0.08 74	4.356± 0.6109	5.036±0. 4914
Cholecystokinin (10-20)	dow n	1.6 37 3	0.8065	0.00 414 7	0.06 179	4.156± 0.4881	5.153±0. 6797
Corchorifatty acid A	dow n	1.6 36 8	0.8493	0.02 239	0.10 81	5.195± 0.3175	6.117±1. 083
Gln Asp Ile	dow n	1.6 35 7	0.7669	0.03 564	0.12 68	4.432± 1.373	5.779±0. 3645

His Met Arg	dow n	1.6 35 7	0.7665	0.01 229	0.09 142	3.909± 0.9062	5.1±0.57 13
Metronidazole	up	1.6 14	1.2679	0.00 097 66	0.02 392	5.282± 0.3453	4.166±0. 737
Glycohyocholic Acid	dow n	1.6 09 4	0.7618	0.03 579	0.12 68	3.62±0. 9789	4.752±0. 8776
L-Leucyl-L-Alanine	dow n	1.6 05 2	0.8271	0.02 956	0.07 781	4.45±0. 7059	5.38±0.8 069
PE(22:1/0:0)	dow n	1.6 04 6	0.8623	0.00 438 4	0.03 212	4.698± 0.4857	5.448±0. 2978
(+)-Lysergic acid	up	1.6 01 9	1.2586	0.02 532	0.07 152	5.392± 0.5178	4.284±1. 254
Mayzent	dow n	1.6 00 8	0.8001	0.00 996 1	0.08 518	4.48±0. 8096	5.599±0. 5505
Phe Val	dow n	1.5 99 3	0.8113	0.02 21	0.10 78	4.532± 0.937	5.586±0. 4265
L-cis-Cyclo(aspartylphenylalanyl)	dow n	1.5 97	0.8486	0.00 287	0.05 247	4.766± 0.5023	5.616±0. 3605

		2		3			
(Z)-7-[(1R,2R,3R,5S)-2-(1,2-Dihydroxy-3-oxooctyl)-3,5-dihydroxycyclopentyl]hept-5-enoic acid	dow n	1.5 92 7	0.8105	0.01 611	0.05 842	4.487± 0.7914	5.536±0. 6457
N-Carbamoylsarcosine	dow n	1.5 89 8	0.8006	0.00 692 7	0.03 941	4.204± 0.6022	5.251±0. 7054
Epothilone D	dow n	1.5 85 5	0.5707	0.02 315	0.10 85	2.183± 1.498	3.825±0. 5644
Monic acid	dow n	1.5 83	0.8248	0.02 22	0.10 78	4.083± 0.1286	4.95±1.0 79
LysoPC(14:0/0:0)	dow n	1.5 81 2	0.8217	0.01 984	0.10 44	4.416± 0.815	5.374±0. 4477
Alpha-Cyperol	dow n	1.5 76 1	0.7057	0.01 368	0.09 395	2.643± 0.8083	3.745±0. 6543
1-Stearoylglycerophosphoglycerol	up	1.5 76	1.1962	0.04 404	0.09 675	5.919± 0.2945	4.948±1. 365
(+)-Erysotrine	dow n	1.5 72	0.8152	0.00 216 2	0.04 61	3.939± 0.2925	4.832±0. 6649
Pro Asn Leu	dow n	1.5 71 8	0.8287	0.02 123	0.10 59	4.606± 0.8809	5.558±0. 1337

Araloside S1	dow n	1.5 69 2	0.7943	0.00 927 5	0.08 416	4.322± 0.5792	5.441±0. 9179
Protodegalactotigonin	dow n	1.5 67 3	0.8482	0.00 121 5	0.03 596	4.431± 0.4508	5.224±0. 1957
D-Glycerate 2-phosphate	up	1.5 67 1	1.1623	0.00 844 5	0.04 163	5.752± 0.375	4.949±0. 6838
11(S)-HEDE	dow n	1.5 66 7	0.779	0.01 06	0.04 717	3.866± 0.6251	4.963±0. 8672
4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanol	up	1.5 65 5	1.1871	0.01 388	0.05 543	4.923± 0.1892	4.147±0. 858
Pro Asp Phe	dow n	1.5 65 2	0.8328	0.01 684	0.09 989	4.263± 0.7421	5.119±0. 2341
7-Isopropyl-5-methylbicyclo[2.2.2]oct-5-en-2-one	dow n	1.5 55 1	0.8235	0.01 348	0.09 379	4.058± 0.3846	4.928±0. 8544
N-Acetyl-DL-Aspartic Acid	dow n	1.5 50 1	0.8841	0.00 839 8	0.04 163	5.301± 0.5263	5.996±0. 2034
Tyrosyl-Valine	dow n	1.5 48	0.8682	0.00 254	0.04 882	5.705± 0.4763	6.571±0. 4218

		8		6			
(2S,3S,4R,5R)-5-(6-Aminopurin-9-yl)-N-cyclopropyl-3,4-dihydroxyoxolane-2-carboxamide	down	1.5 47 2	0.8398	0.00 779 4	0.07 971	4.219± 0.5019	5.024±0. 5033
Arachidyl carnitine	up	1.5 41 2	1.2141	0.02 367	0.10 88	6.318± 0.6336	5.204±1. 139
(3R)-3-Hydroxy-N-[(3S)-2-oxoxolan-3-yl]butanamide	down	1.5 35 6	0.8224	0.02 202	0.06 709	3.562± 0.2249	4.331±0. 9205
Midodrine	up	1.5 35 3	1.2809	0.01 126	0.08 91	5.896± 0.6258	4.603±1. 167
Glycylvaline	down	1.5 28 5	0.7892	0.01 406	0.09 483	4.459± 0.8557	5.65±0.7 579
5alpha-Androstane-3beta,7alpha,17beta-triol	down	1.5 26 2	0.8106	0.04 437	0.13 94	5.787± 1.442	7.139±0. 436
Glycerylphosphorylcholine	down	1.5 24 4	0.8801	0.02 496	0.07 107	5.351± 0.6903	6.08±0.1 686
Isokobusone	down	1.5 22 9	0.8274	0.00 832 9	0.08 251	4.362± 0.5373	5.272±0. 6363
Phenol sulphate	up	1.5	1.1578	0.04	0.09	5.68±0.	4.906±0.

		22 4		051	243	7235	5403
(3b,6a,12b,17a,20S)-Dammar-24-ene-3,6,12,17,20-pentol 20-[glucosyl-(1->2)-[rhamnosyl-(1->6)]-glucoside] 3-[glucosyl-(1->6)-glucoside] 6-xyloside	dow n	1.5 21 8	0.8364	0.00 64	0.07 431	5.027± 0.5602	6.01±0.6 523
Asparaginyln-Proline	dow n	1.5 18 2	0.8534	0.02 063	0.06 471	4.478± 0.5405	5.247±0. 6205
3-Carboxy-4-Methyl-5-Propyl-2-Furanpropanoic Acid	up	1.5 16 3	1.2375	0.00 951 5	0.04 395	5.174± 0.534	4.181±0. 797
Met Phe	dow n	1.5 12 3	0.7927	0.02 712	0.11 5	4.145± 0.6745	5.229±1. 097
14-(Hydroxymethyl)-5,9-dimethyltetracyclo[11.2.1.0~1,10~.0~4,9~]hexadecan-5-ol	dow n	1.5 10 3	0.8473	0.00 301 8	0.05 38	4.583± 0.3624	5.409±0. 5684
Riboprine	dow n	1.5 08 5	0.8443	0.04 25	0.13 72	4.397± 0.7879	5.208±0. 52
13Z-Docosenamide	up	1.5 06 3	1.1586	0.00 128	0.03 677	6.106± 0.2849	5.27±0.5 563
Hordatine A glucoside	dow n	1.5 02 8	0.8164	0.01 509	0.09 708	4.563± 0.8785	5.589±0. 228

N-Nonanoylglycine	dow n	1.4 96 9	0.8152	0.04 294	0.13 78	4.174± 1.008	5.12±0.2 636
Morph	dow n	1.4 89 2	0.8486	0.01 935	0.10 35	5.028± 0.7156	5.925±0. 5385
Threonylisoleucine	dow n	1.4 87 7	0.8479	0.00 292 2	0.05 306	4.472± 0.2885	5.274±0. 6099
Naxagolide	up	1.4 83 5	1.2137	0.01 035	0.08 617	4.442± 0.1687	3.66±0.8 261
Phe Phe	dow n	1.4 82 2	0.8308	0.01 858	0.10 23	4.374± 0.6435	5.265±0. 6566
LysoPE(20:0/0:0)	dow n	1.4 80 8	0.8884	0.04 887	0.10 29	5.575± 0.7598	6.275±0. 2567
Lycopersiconolide	dow n	1.4 80 6	0.8764	0.00 923	0.04 347	4.99±0. 4981	5.694±0. 3531
N-acetylaspartate	dow n	1.4 71 7	0.89	0.02 939	0.07 751	5.569± 0.6704	6.257±0. 1893
Dmap-ethyl-paf	up	1.4 70	1.2081	0.01 579	0.09 835	5.851± 0.5761	4.843±0. 9046

		2					
N'-nitrosoanabasine	up	1.4 67 9	1.1643	0.00 085 38	0.02 392	4.889± 0.1118	4.199±0. 5083
Glu Ile Leu	dow n	1.4 67 4	0.7311	0.04 589	0.14 04	3.905± 1.506	5.341±0. 6534
PA(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/18:4(6Z,9Z,12Z,15Z))	dow n	1.4 65 9	0.8281	0.00 124 4	0.03 637	4.722± 0.2473	5.702±0. 7144
Methyl-[12]-gingerdiol	dow n	1.4 63 1	0.8503	0.03 351	0.08 301	4.395± 0.681	5.169±0. 5447
Homo-L-arginine	dow n	1.4 62 3	0.869	0.00 518 9	0.06 635	4.572± 0.4707	5.261±0. 2393
Blumealactone C	dow n	1.4 60 6	0.8069	0.02 437	0.10 95	3.886± 0.6286	4.816±0. 8443
PE(P-16:0/16:0)	up	1.4 58 4	1.1503	0.00 097 25	0.03 501	6.283± 0.2776	5.462±0. 5211
2,3-Dimethyl-2-cyclohexen-1-one	up	1.4 47 4	1.282	0.01 159	0.08 977	4.06±0. 6042	3.167±0. 5813
Alpha-Dimorphecolic acid	dow	1.4	0.9071	0.00	0.02	6.33±0.	6.978±0.

	n	43		241	67	1761	5167
		3		7			
Subaphylline	dow	1.4	0.833	0.00	0.04	4.016±	4.821±0.
	n	41		193	33	0.4703	2693
		4		3			
Ile Leu	dow	1.4	0.8719	0.01	0.09	5.276±	6.051±0.
	n	40		456	575	0.5458	5252
		9					
Neurotensin 1-10	up	1.4	1.1994	0.01	0.10	5.142±	4.287±0.
		39		911	29	0.5502	7429
		5					
Dinoterb	up	1.4	1.1267	0.00	0.02	5.435±	4.824±0.
		39		095	392	0.119	448
				85			
Cyclopentolate	dow	1.4	0.8465	0.00	0.06	4.567±	5.395±0.
	n	38		459	395	0.5555	28
		5		1			
PC(2:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))	dow	1.4	0.8227	0.03	0.12	3.897±	4.737±0.
	n	37		335	33	0.7623	5336
		5					
Imidazole-4-Acetic Acid	up	1.4	1.2134	0.03	0.12	4.612±	3.801±0.
		29		11		0.6904	5875
		4					
N-Nervonoyl Tryptophan	up	1.4	1.1349	0.00	0.03	6.454±	5.687±0.
		27		076	03	0.2847	4375
		7		74			

Leucyl-Aspartate	dow n	1.4 25 3	0.8126	0.03 96	0.09 121	4.461± 0.7282	5.49±1.0 97
Ganglioside GD3 (d18:0/18:1(9Z))	dow n	1.4 23 4	0.8628	0.02 014	0.10 49	4.992± 0.5274	5.786±0. 6788
Phe Leu	dow n	1.4 23 2	0.857	0.00 866 7	0.08 251	4.829± 0.4419	5.635±0. 6187
Ser Leu Val Asn Ala	dow n	1.4 18 4	0.8107	0.01 182	0.09 023	4.481± 0.6661	5.527±0. 7576
Biliverdin	up	1.4 14 5	1.1347	0.02 062	0.10 53	5.906± 0.2674	5.205±0. 7944
Glucosamine	dow n	1.4 12 8	0.911	0.01 118	0.04 862	5.853± 0.4552	6.425±0. 1735
2-Aminoacrylic acid	dow n	1.4 09 8	0.8651	0.02 508	0.07 107	4.426± 0.5494	5.116±0. 5004
4-(Glutamylamino) butanoate	dow n	1.4 06 2	0.8608	0.04 41	0.13 94	5.354± 0.8924	6.22±0.4 205
PA(20:4(8Z,11Z,14Z,17Z)-2OH(5S,6R)/P-16:0)	up	1.4 05	1.2217	0.02 958	0.11 76	4.745± 0.7031	3.884±0. 6617

		3					
O-Aminoazotoluene	dow n	1.4 04	0.7766	0.03 859	0.13 03	3.177± 0.6744	4.091±0. 9307
Allylestrenol	dow n	1.4 02 7	0.8634	0.03 577	0.08 537	4.645± 0.5567	5.38±0.7 025
Ser Val Val	dow n	1.4 01 8	0.7515	0.03 866	0.13 03	3.704± 1.224	4.929±0. 5721
(1R,2R,4S)-p-Menthane-1,2,8-triol 8-glucoside	up	1.4 00 1	1.1749	0.02 843	0.11 65	5.152± 0.4602	4.385±0. 8089
Epioxylubimin	dow n	1.3 94 6	0.8609	0.01 809	0.10 19	4.907± 0.69	5.7±0.25 86
Tyr-ile-gly-ser-arg	dow n	1.3 92 6	0.7855	0.02 146	0.10 63	4.608± 0.9767	5.866±0. 8754
N-Acetylserotonin	dow n	1.3 91 1	0.7961	0.00 045 51	0.02 694	3.12±0. 2471	3.919±0. 4631
Guanidineacetic acid	dow n	1.3 89 5	0.8969	0.01 601	0.09 839	6.01±0. 5561	6.701±0. 3343
Xi-3-Nonenoic acid	dow n	1.3 88	0.8977	0.01 999	0.10 48	5.88±0. 2374	6.55±0.7 637

		5					
N-Nervonoyl Valine	up	1.3 88	1.3162	0.03 886	0.09 011	4.354± 0.9667	3.308±0. 7263
Histamine	up	1.3 82 8	1.1215	0.01 893	0.10 29	6.122± 0.4014	5.459±0. 6055
Asn Ala Glu Val Leu	dow n	1.3 82 2	0.8799	0.01 742	0.10 05	4.965± 0.5551	5.643±0. 3306
Ile Phe Gln	dow n	1.3 79 3	0.7895	0.04 934	0.14 49	3.904± 1.135	4.945±0. 3708
Ecgonine	dow n	1.3 67 3	0.8673	0.03 212	0.08 144	4.633± 0.1402	5.342±0. 9461
Glu Val Lys	dow n	1.3 55 1	0.8704	0.00 461 4	0.06 395	4.628± 0.3523	5.317±0. 4649
3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	up	1.3 50 6	1.1591	0.00 939 2	0.04 362	6.383± 0.1685	5.507±0. 9157
8-Azaspiro[4.5]decane-7,9-dione	up	1.3 48	1.1301	0.00 099 54	0.03 501	5.662± 0.3215	5.01±0.2 72
4-O-(Indole-3-acetyl)-D-glucopyranose	dow n	1.3 45	0.8582	0.03 302	0.08 262	3.97±0. 6219	4.626±0. 3366

		5					
PA(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/i-15:0)	dow n	1.3 38 1	0.8298	0.03 763	0.12 9	3.943± 0.625	4.752±0. 7752
Oxalic Acid	dow n	1.3 37 6	0.8755	0.03 325	0.08 287	4.157± 0.5985	4.748±0. 112
Butyl (S)-3-hydroxybutyrate [arabinosyl-(1->6)-glucoside]	dow n	1.3 34 9	0.8447	0.00 692 2	0.07 626	4.427± 0.5697	5.241±0. 3346
Dilept	dow n	1.3 34 9	0.8685	0.02 117	0.10 59	4.478± 0.5479	5.156±0. 4204
Leu Ile	dow n	1.3 34 1	0.8839	0.00 641 8	0.07 431	5.472± 0.3574	6.191±0. 5472
Trp Ile	dow n	1.3 30 6	0.8856	0.00 050 73	0.02 694	5.014± 0.2881	5.662±0. 2632
Thiodiacetic acid	up	1.3 30 5	1.1679	0.04 19	0.13 64	5.587± 0.7311	4.784±0. 6215
Asp Leu	dow n	1.3 28 8	0.9008	0.00 431 7	0.06 246	5.905± 0.4241	6.555±0. 2445
Phe Ile	dow	1.3	0.892	0.00	0.08	5.623±	6.304±0.

	n	22		945 8	416	0.2677	6405
Asn Ile Phe	dow n	1.3 20 8	0.7004	0.00 812 8	0.08 132	2.843± 0.4072	4.059±1. 155
Arginyl-prolyl-proline	dow n	1.3 20 3	0.8168	0.01 393	0.05 544	4.266± 0.5694	5.223±0. 7963
2-n-Propyl-4-oxopentanoic acid	up	1.3 17 5	1.1663	0.00 633 2	0.07 422	4.853± 0.1394	4.161±0. 6733
Caprylic acid	dow n	1.3 17	0.8984	0.00 790 1	0.07 989	5.104± 0.1893	5.681±0. 5476
5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	dow n	1.3 06 4	0.8951	0.01 405	0.05 559	5.257± 0.1562	5.873±0. 6804
Thr Glu Phe	dow n	1.3 05 8	0.8481	0.04 156	0.13 56	4.058± 0.677	4.785±0. 5256
12-Hydroxydodecanoic acid	up	1.3 04 3	1.1283	0.01 782	0.06 096	5.206± 0.1096	4.614±0. 6988
2-(1,2,3,4-Tetrahydroxybutyl)thiazolidine-4-carboxylic acid	up	1.3 03 5	1.178	0.00 941 1	0.08 416	4.433± 0.3778	3.763±0. 5139

N-NITROSOMORPHOLINE	dow n	1.3 01 6	0.8664	0.02 255	0.06 763	4.059± 0.461	4.685±0. 494
Diocetyl phthalate	up	1.2 99 1	1.2038	0.04 388	0.13 91	5.76±0. 7614	4.785±0. 9956
1-(11Z,14Z-eicosadienoyl)-glycero-3-phosphate	dow n	1.2 97 1	0.9247	0.04 951	0.10 33	6.253± 0.5194	6.762±0. 3186
Tolmetin	up	1.2 95 9	1.2181	0.03 411	0.12 46	4.636± 0.7976	3.806±0. 4105
Neoporrigenin B	dow n	1.2 93	0.8866	0.03 331	0.12 33	5.224± 0.6785	5.892±0. 111
3-Methyl-5-pentyl-2-furanundecanoic acid	dow n	1.2 91 8	0.931	0.00 026 42	0.02 694	6.343± 0.1833	6.813±0. 1974
Azithromycin	up	1.2 90 1	1.1925	0.03 863	0.13 03	5.228± 0.7213	4.384±0. 709
N1-Methyl-4-pyridone-3-carboxamide	up	1.2 85 5	1.1261	0.00 342 6	0.05 804	5.652± 0.3031	5.019±0. 4185
Ser Leu Ser Gly Leu	dow n	1.2 85	0.7875	0.03 38	0.12 42	3.639± 0.8619	4.621±0. 7019
Asp Asn Leu	dow	1.2	0.8592	0.03	0.12	4.997±	5.816±0.

	n	85		572	68	0.7498	5383
LysoPC(P-18:0/0:0)	dow n	1.2 81 3	0.9031	0.01 983	0.10 44	6.097± 0.5729	6.751±0. 2421
Gamma-Undecalactone	dow n	1.2 81 2	0.8797	0.02 277	0.10 81	4.411± 0.517	5.014±0. 3184
Cis-Zeatin-7-N-glucoside	dow n	1.2 80 3	0.8206	0.00 479 3	0.06 534	3.289± 0.4442	4.008±0. 3606
PS(20:3(5Z,8Z,11Z)/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))	dow n	1.2 76 3	0.8653	0.00 635 3	0.07 422	3.637± 0.3672	4.203±0. 2911
Dihydrojasmonic acid	dow n	1.2 68 6	0.8937	0.00 679 7	0.03 898	4.866± 0.1127	5.445±0. 5715
4-Amino-1-[5-(hydroxymethyl)oxolan-2-yl]pyrimidin-2-one	dow n	1.2 68 1	0.896	0.00 233 5	0.04 695	4.883± 0.2648	5.45±0.3 448
Ala Leu Leu	dow n	1.2 67 2	0.8462	0.03 261	0.12 26	4.65±0. 7449	5.495±0. 5775
Betavulgarin	up	1.2 64 4	1.1348	0.01 268	0.05 212	5.201± 0.1206	4.583±0. 6827
KIRENOL	dow	1.2	0.8847	0.03	0.12	5.04±0.	5.697±0.

	n	61 9		473	51	4979	6194
Pro Pro Gln	dow n	1.2 58 5	0.8674	0.01 506	0.09 708	4.437± 0.5569	5.115±0. 2647
Lys Leu Gln	up	1.2 58 2	1.1151	0.00 484 6	0.06 534	5.811± 0.3482	5.211±0. 3482
LysoPE(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	up	1.2 56 4	1.213	0.03 548	0.12 67	5.7±0.7 191	4.699±1. 005
PC(P-16:0/0:0)	dow n	1.2 42 3	0.9251	0.02 984	0.11 8	7.344± 0.5688	7.939±0. 2351
PI(22:2(13Z,16Z)/TXB2)	dow n	1.2 38 1	0.8747	0.03 303	0.12 31	4.571± 0.6558	5.226±0. 1728
Ile Val	dow n	1.2 36 8	0.8962	0.03 126	0.12 02	5.309± 0.4575	5.924±0. 5637
Geranylcitronellol	up	1.2 33 4	1.1031	0.00 730 6	0.07 823	7.081± 0.2096	6.419±0. 6236
Ethanone, 1-(4-butylphenyl)-	dow n	1.2 21 6	0.8998	0.01 561	0.09 808	4.761± 0.2947	5.291±0. 4827

Cytarabine	dow n	1.2 08 8	0.8772	0.02 243	0.10 81	4.772± 0.5028	5.44±0.5 061
Leu Gln Ala	dow n	1.2 08 4	0.8433	0.02 834	0.11 65	4.504± 0.7062	5.341±0. 5788
PC(P-18:0/0:0)	up	1.2 05 6	1.125	0.01 247	0.09 18	6.632± 0.5469	5.895±0. 3942
Pentaethylene glycol	up	1.2 01 7	1.1104	0.00 514	0.06 635	5.433± 0.2463	4.893±0. 412
Nerolidol	up	1.1 99 7	1.1622	0.00 684 5	0.07 613	4.923± 0.2734	4.236±0. 6001
Foropafant	up	1.1 99 2	1.1497	0.01 85	0.10 23	5.1±0.3 765	4.436±0. 6301
Stearoylcarnitine	up	1.1 95 9	1.0993	0.01 255	0.09 18	7.57±0. 3676	6.886±0. 5972
LysoPC(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	dow n	1.1 94 8	0.8915	0.04 82	0.14 35	5.489± 0.6641	6.157±0. 4522
Linoleic Acid	dow n	1.1 94	0.9443	0.00 921	0.04 347	6.107± 0.2791	6.467±0. 0966

		2		8			
Gentamicin C	up	1.1 88 2	1.1029	0.01 484	0.09 673	5.876± 0.3844	5.328±0. 3789
(5Z)-7-[(1R,2R,3R,5S)-3,5-Dihydroxy-2-[(1E,3S,5Z)-3-hydroxyocta-1,5-dien-1-yl]cyclopentyl]hept-5-enoylcarnitine	up	1.1 80 4	1.1339	0.01 978	0.06 392	5.675± 0.4475	5.005±0. 5658
3,4-Di-O-caffeoylquinic acid	down	1.1 77 4	0.9091	0.03 542	0.12 67	5.151± 0.4565	5.666±0. 3723
Dodecatrienoic acid	down	1.1 71 4	0.9036	0.02 262	0.10 81	4.581± 0.3141	5.07±0.4 541
Butylate	up	1.1 68 3	1.1063	0.01 669	0.09 983	5.892± 0.3776	5.326±0. 447
D-Galactose	up	1.1 67 1	1.0908	0.00 246 6	0.02 67	5.9±0.1 809	5.409±0. 3569
(E)-6,10-Dimethyl-9-methylene-5-undecen-2-one	up	1.1 66 6	1.1569	0.00 633 4	0.07 422	5±0.25 28	4.322±0. 5952
Anispermus	up	1.1 61 8	1.1461	0.00 895 6	0.08 337	5.664± 0.2352	4.942±0. 704
Serylhydroxyproline	down	1.1	0.9118	0.01	0.05	5.137±	5.634±0.

	n	59 1		331	376	0.3048	3953
Leu Val	dow n	1.1 58	0.878	0.03 568	0.12 68	4.916± 0.5466	5.599±0. 6082
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone	up	1.1 50 6	1.1313	0.00 355 7	0.05 911	4.998± 0.1671	4.418±0. 4887
2-Hydroxy-3-Methylbutyric Acid	up	1.1 45 5	1.0908	0.00 014 99	0.02 392	5.839± 0.1292	5.353±0. 252
PC(18:4(6Z,9Z,12Z,15Z)/20:0)	up	1.1 44	1.099	0.03 167	0.12 09	7.335± 0.2125	6.674±0. 8521
11-Aminoundecanoic Acid	up	1.1 43 6	1.1231	0.01 675	0.09 983	4.698± 0.1617	4.183±0. 5762
Citreoviridin C	up	1.1 40 6	1.1228	0.01 707	0.10 04	4.581± 0.2168	4.08±0.5 246
7a,12a-Dihydroxy-3-oxo-4-cholenoic acid	up	1.1 37 2	1.1481	0.02 909	0.11 74	6.194± 0.4901	5.395±0. 8385
D-(+)-dihydrocarvone	up	1.1 36 9	1.1475	0.00 581 2	0.07 088	4.917± 0.2166	4.285±0. 5594
Prolylhydroxyproline	dow n	1.1 35	0.9158	0.00 119	0.02 392	5.622± 0.2757	6.139±0. 1854

		7		1			
LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z))	up	1.1 34 2	1.1121	0.01 435	0.09 539	6.319± 0.3821	5.682±0. 5334
9,10-Dihome	dow n	1.1 33 2	0.9247	0.01 969	0.06 385	6.028± 0.2659	6.519±0. 4883
Z-LLNle-CHO	up	1.1 32 9	1.0933	0.02 49	0.11 06	6.049± 0.426	5.533±0. 3417
(23S)-23,25-dihydroxy-24-oxovitamin D3 23-(beta-glucuronide)	dow n	1.1 30 8	0.7839	0.04 308	0.13 8	3.592± 0.8481	4.582±0. 8858
Cysteinylglycine	up	1.1 3	1.1358	0.04 529	0.14 01	5.009± 0.4444	4.41±0.6 513
Antipyrine	up	1.1 28 9	1.2012	0.03 438	0.12 49	3.117± 0.4879	2.595±0. 3032
Benzocaine	dow n	1.1 27 5	0.8988	0.00 744 5	0.07 906	4.618± 0.3555	5.138±0. 2517
4-Vinylcyclohexene	dow n	1.1 27 2	0.9032	0.02 348	0.10 86	4.572± 0.298	5.062±0. 4798
(R)-Pterosin B	dow n	1.1 16	0.9364	0.03 194	0.12 11	6.71±0. 4505	7.166±0. 1365

		1					
Beta-Citryl-L-glutamic acid	up	1.1 11	1.0855	0.01 349	0.09 379	6.707± 0.2087	6.179±0. 537
Glutamylleucine	dow n	1.1 10 5	0.9011	0.02 58	0.11 25	5.039± 0.3931	5.592±0. 4895
Iniparib	up	1.1 09 6	1.1395	0.02 256	0.06 763	4.901± 0.1077	4.301±0. 7449
Sulindac	up	1.1 08 1	1.067	0.00 197	0.02 589	6.244± 0.1113	5.852±0. 2988
LysoPC(16:0/0:0)	up	1.1 04 6	1.1669	0.01 565	0.05 815	4.628± 0.4528	3.966±0. 4908
Polidocanol	up	1.1 04 3	1.0845	0.00 988 5	0.08 514	6.057± 0.2831	5.585±0. 3439
3,4-Pyrrolidinediol, 2-(p-methoxybenzyl)-, 3-acetate, (2S,3R,4R)-	up	1.1 02 2	1.1036	0.02 117	0.10 59	6.339± 0.3155	5.744±0. 61
Epsilon-(Carboxyethyl)lysine	dow n	1.0 94 2	0.9189	0.00 602 3	0.07 238	5.089± 0.274	5.538±0. 2613
Val Tyr	dow n	1.0 94	0.8997	0.03 782	0.12 93	4.789± 0.5115	5.323±0. 3152

		1					
Indolelactic acid	up	1.0 88 6	1.074	0.00 019 79	0.02 392	5.196± 0.1467	4.838±0. 1245
Cis-Quinceoxepane	up	1.0 79 7	1.1484	0.00 981 2	0.08 514	5.014± 0.1894	4.366±0. 6547
LysoPS(18:0/0:0)	up	1.0 78 8	1.0906	0.03 558	0.08 515	6.032± 0.3055	5.531±0. 5649
Arachidonoyl Ethanolamide	up	1.0 73	1.1577	0.02 598	0.11 29	5.711± 0.3342	4.933±0. 9074
Ibuprofen glucuronide	up	1.0 7	1.1151	0.03 317	0.08 287	5.938± 0.0885 8	5.325±0. 8329
Sulfonamidoethanol	up	1.0 62 5	1.1107	0.02 332	0.10 86	6.171± 0.2752	5.556±0. 6893
Gemfibrozil	up	1.0 59	1.1098	0.01 261	0.05 207	5.315± 0.0850 6	4.789±0. 5849
9,10-Epoxy-18-hydroxy-octadecanoic acid	dow n	1.0 58 2	0.9308	0.02 676	0.11 41	5.943± 0.2383	6.385±0. 4821
Ambrosonide	up	1.0 56	1.1014	0.00 965	0.08 468	6.085± 0.1621	5.525±0. 5655

		4		5			
Ile Gly	dow n	1.0 55	0.9071	0.03 069	0.11 94	5.351± 0.3541	5.899±0. 5658
Galaxolide	up	1.0 48 9	1.1466	0.02 064	0.10 53	4.887± 0.3179	4.262±0. 6477
P-Dichlorobenzene	up	1.0 47 9	1.0781	0.00 199 1	0.02 589	5.229± 0.1299	4.85±0.2 732
Palmitic amide	up	1.0 47 7	1.0795	0.00 687 1	0.07 613	6.804± 0.1865	6.303±0. 4474
Maniladiol	up	1.0 45	1.0707	0.02 633	0.11 37	5.661± 0.2394	5.287±0. 3672
2-(L-Menthoxy)ethanol	up	1.0 42 9	1.0922	0.03 71	0.12 84	5.842± 0.1114	5.349±0. 6766
Asp-Phe	dow n	1.0 38 6	0.9046	0.01 185	0.09 023	5.412± 0.4111	5.983±0. 3258
Trihexyphenidyl	up	1.0 36 9	1.0988	0.01 453	0.09 575	5.05±0. 1599	4.596±0. 4819
ALANYL-dl-PHENYLALANINE	dow n	1.0 33 7	0.893	0.03 862	0.13 03	4.69±0. 4603	5.252±0. 5049

3-Hydroxybutanoic Acid	up	1.0 31 5	1.0522	0.00 227 8	0.02 67	7.034± 0.1546	6.685±0. 2219
Antcin K	dow n	1.0 30 2	0.9259	0.03 649	0.12 75	6.961± 0.453	7.518±0. 4905
Behenic acid	up	1.0 28 4	1.0721	0.01 06	0.08 684	7.168± 0.3232	6.686±0. 3038
N-Methyl-L-glutamate	up	1.0 28 3	1.1222	0.03 608	0.12 71	5.08±0. 1562	4.527±0. 7449
(2S,3S,5S,8R,9S,10S,13S,14S,16S,17R)-17-Acetyloxy-10,13-dimethyl-2-morpholin-4-yl-16-(1-prop-2-enylpyrrolidin-1-ium-1-yl)-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-olate	up	1.0 23 4	1.0481	0.02 28	0.10 81	7.8±0.2 261	7.442±0. 336
Morphinone	dow n	1.0 22 7	0.8725	0.03 415	0.12 46	3.9±0.4 802	4.47±0.4 543
Cinobufagin	up	1.0 22	1.0625	0.04 525	0.14 01	7.348± 0.1727	6.916±0. 5926
(1R,4E,6S,7S,17R)-4-Ethylidene-7-hydroxy-7-(hydroxymethyl)-6-methyl-2,9-dioxo-14-azatricyclo[9.5.1.0 ^{14,17}]heptadec-11-ene-3,8-dione	dow n	1.0 20 7	0.9128	0.04 027	0.13 33	5.121± 0.4661	5.61±0.3 171
METHACHOLINE	up	1.0 20 6	1.1211	0.01 257	0.09 18	5.423± 0.3342	4.837±0. 4889

2-Butyne-1,4-diol	up	1.0 16 8	1.1251	0.03 075	0.11 95	5.001± 0.1976	4.445±0. 7021
Zeranol	up	1.0 14 8	1.1132	0.03 243	0.12 24	6.253± 0.2835	5.617±0. 78
Oleamide	up	1.0 13 7	1.0629	0.00 963 7	0.08 468	7.98±0. 1624	7.508±0. 462
L-Proline, 1-(2-methyl-3-(methylthio)-1-oxopropyl)-, (S)-	dow n	1.0 12 1	0.8629	0.03 261	0.12 26	3.771± 0.3376	4.37±0.6 823
Eplerenone	up	1.0 05 1	1.0814	0.01 114	0.08 88	6.312± 0.1735	5.837±0. 4715
Beta-Aminopropionitrile	up	1.0 04 7	1.1065	0.01 358	0.09 379	5.247± 0.3047	4.742±0. 4119
Ethyl Myristate	dow n	1.0 02	0.9396	0.03 519	0.08 471	5.596± 0.3627	5.956±0. 1166

Table S6 Altered metabolic pathways between smoking PDAC and non-smoking PDAC groups of paracancerous tissue from surgical samples

Pathway Description	Ratio in study	Ratio in pop	<i>P</i>
Pancreatic cancer	1/63	2/4407	0.02839
Systemic lupus erythematosus	1/63	3/4407	0.04229
PPAR signaling pathway	2/63	5/4407	0.001956
Retrograde endocannabinoid signaling	2/63	19/4407	0.02942
cAMP signaling pathway	2/63	25/4407	0.04887
Ether lipid metabolism	2/63	25/4407	0.04887
Alanine, aspartate and glutamate metabolism	3/63	28/4407	0.007071
Glycine, serine and threonine metabolism	3/63	48/4407	0.03052
Neuroactive ligand-receptor interaction	3/63	52/4407	0.03746
Serotonergic synapse	4/63	42/4407	0.002826
Arginine and proline metabolism	4/63	69/4407	0.01639
Arachidonic acid metabolism	4/63	75/4407	0.02163
alpha-Linolenic acid metabolism	5/63	44/4407	0.0003595
Linoleic acid metabolism	9/63	28/4407	7.72E-11
Choline metabolism in cancer	4/63	11/4407	1.16E-05
Glycerophospholipid metabolism	5/63	56/4407	0.001108

Table S7 Differential bacteria between smoking PDAC and non-smoking PDAC groups from FNA samples

Species name	Group	Mean	LDA value	<i>P</i>
f__Saccharimonadaceae	PDAC_smoking	3.60037	3.258046	0.033246
o__Streptosporangiales	PDAC_smoking	2.367495	2.980661	0.046852
g__norank_f__Bacteroidetes_BD2-2	PDAC_non-smoking	2.129596	3.100606	0.032976
f__Weeksellaceae.g__Soonwooa	PDAC_smoking	2.022999	3.359299	0.027012
p__Proteobacteria	PDAC_non-smoking	5.877802	5.018821	0.030041
g__Pseudolabrys	PDAC_non-smoking	1.376268	3.494831	0.032905
g__Bradyrhizobium	PDAC_non-smoking	2.744245	2.98733	0.040517
g__Thalassotalea	PDAC_non-smoking	1.677298	3.359313	0.046852
g__Acholeplasma	PDAC_non-smoking	1.899147	2.872176	0.004519
g__Ellin6055	PDAC_non-smoking	2.45545	2.999585	0.034187
f__Bacteroidetes_BD2-2	PDAC_non-smoking	2.129596	3.122892	0.032976
c__AD3	PDAC_non-smoking	2.075238	3.426935	0.032905
g__Turicibacter	PDAC_smoking	2.451815	3.003183	0.027207
g__Eubacterium_brachy_group	PDAC_smoking	2.066465	3.204207	0.046852
f__Frankiaceae	PDAC_non-smoking	1.376268	3.691745	0.032905
f__Acholeplasmataceae	PDAC_non-smoking	1.899147	2.909901	0.004519
o__norank_c__AD3	PDAC_non-smoking	2.075238	3.110999	0.032905
f__Peptococcaceae	PDAC_smoking	2.964353	2.819522	0.046852
f__Muribaculaceae	PDAC_non-smoking	3.322393	3.032627	0.041271
o__Acholeplasmatales	PDAC_non-smoking	1.899147	2.97838	0.004519
f__norank_o__norank_c__AD3	PDAC_non-smoking	2.075238	3.350075	0.032905
g__Polynucleobacter	PDAC_non-smoking	1.85339	3.591186	0.032905
g__TM7x	PDAC_smoking	3.504668	3.180837	0.033015
g__norank_f__norank_o__norank_c__AD3	PDAC_non-smoking	2.075238	3.537623	0.032905
g__Simiduia	PDAC_non-smoking	1.677298	3.771282	0.032905
p__Patescibacteria	PDAC_smoking	4.021625	3.687101	0.030941
g__norank_f__Muribaculaceae	PDAC_non-smoking	3.319103	3.03649	0.041271
o__Peptococcales	PDAC_smoking	2.964353	2.838272	0.046852
g__Aggregatibacter	PDAC_smoking	3.708033	3.44933	0.026767
c__Gammaproteobacteria	PDAC_non-smoking	5.867695	5.028827	0.038964
g__norank_f__Lentimicrobiaceae	PDAC_non-smoking	1.376268	3.622662	0.032905
c__Saccharimonadia	PDAC_smoking	4.005508	3.674639	0.023107
o__Saccharimonadales	PDAC_smoking	4.005508	3.674639	0.023107
g__Jatrophihabitans	PDAC_non-smoking	1.376268	3.697893	0.032905
f__Colwelliaceae	PDAC_non-smoking	1.677298	3.360323	0.046852
g__Peptococcus	PDAC_smoking	2.964353	2.81783	0.046852
o__Burkholderiales	PDAC_non-smoking	5.845462	5.092689	0.015757

Community barplot analysis

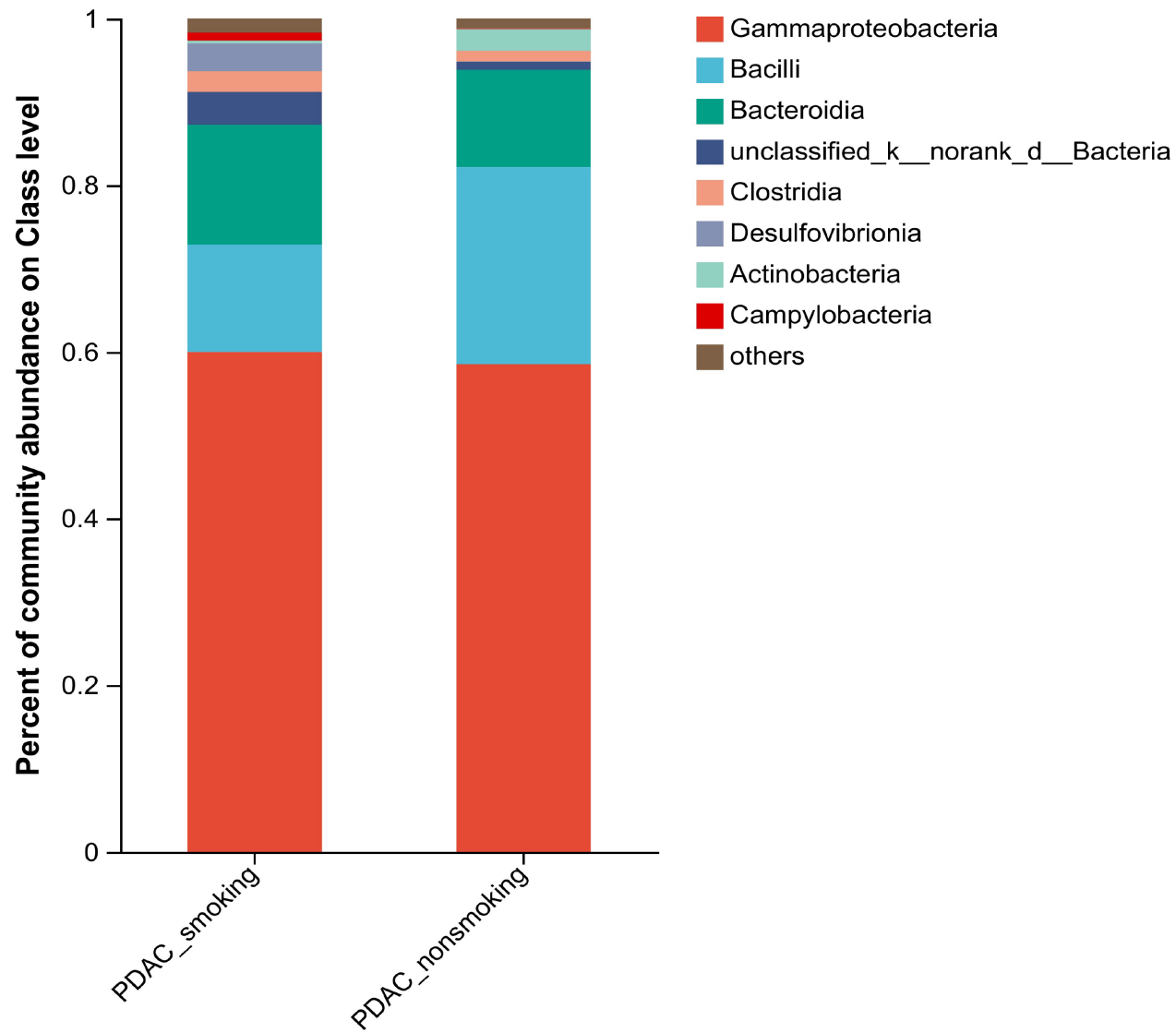


Fig. S1 Bacterial composition at the class level of subjects in tumor tissue of surgical samples.

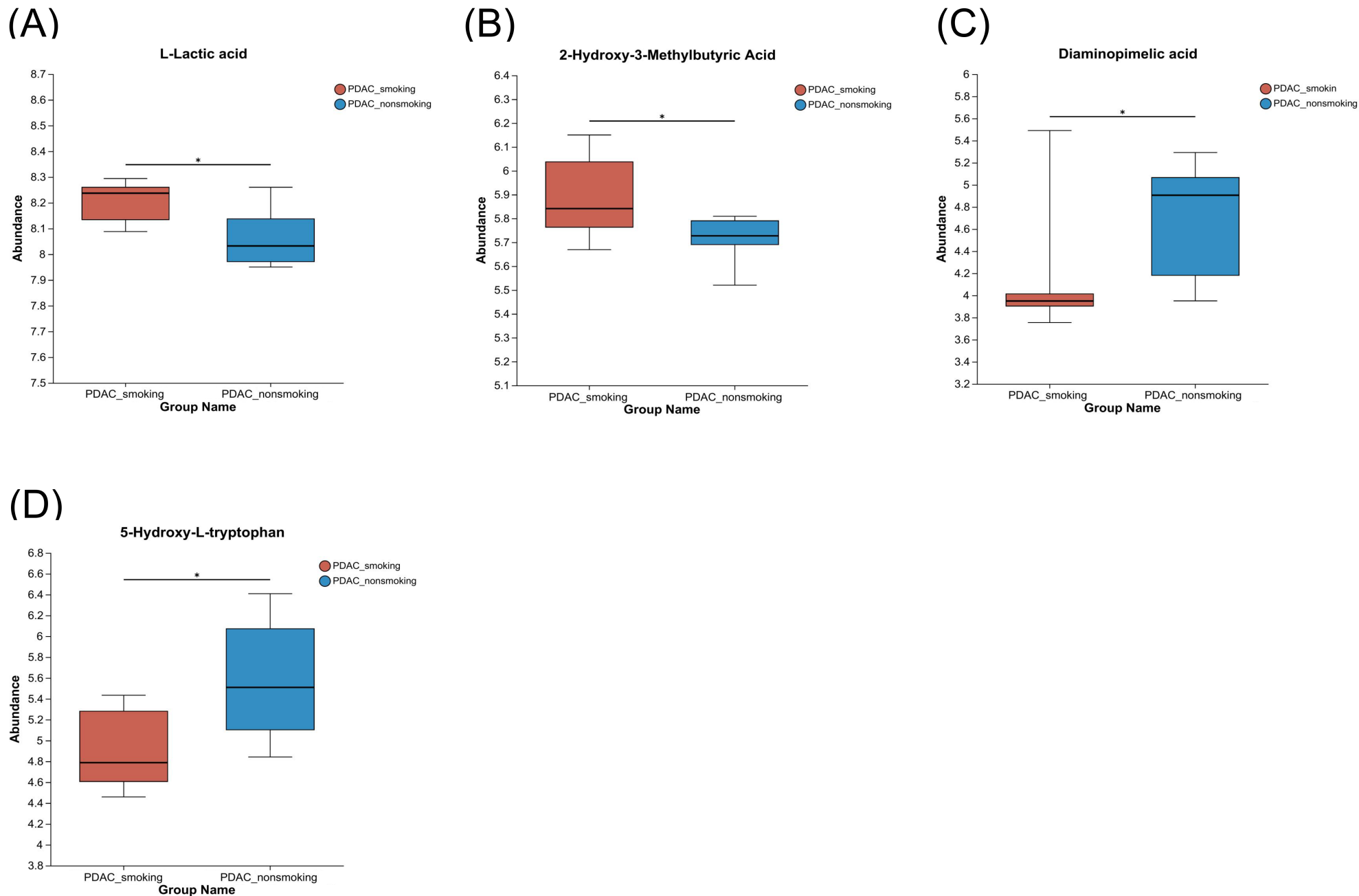


Fig. S2 Partial differential metabolites in tumor tissue of surgical samples from smoking vs. non-smoking PDAC. L-lactic acid (A), 2-hydroxy-3-methylbutyric acid (B), diaminopimelic acid (C), 5-hydroxy-L-tryptophan (D). $P < 0.05$ is marked as *.

Community barplot analysis

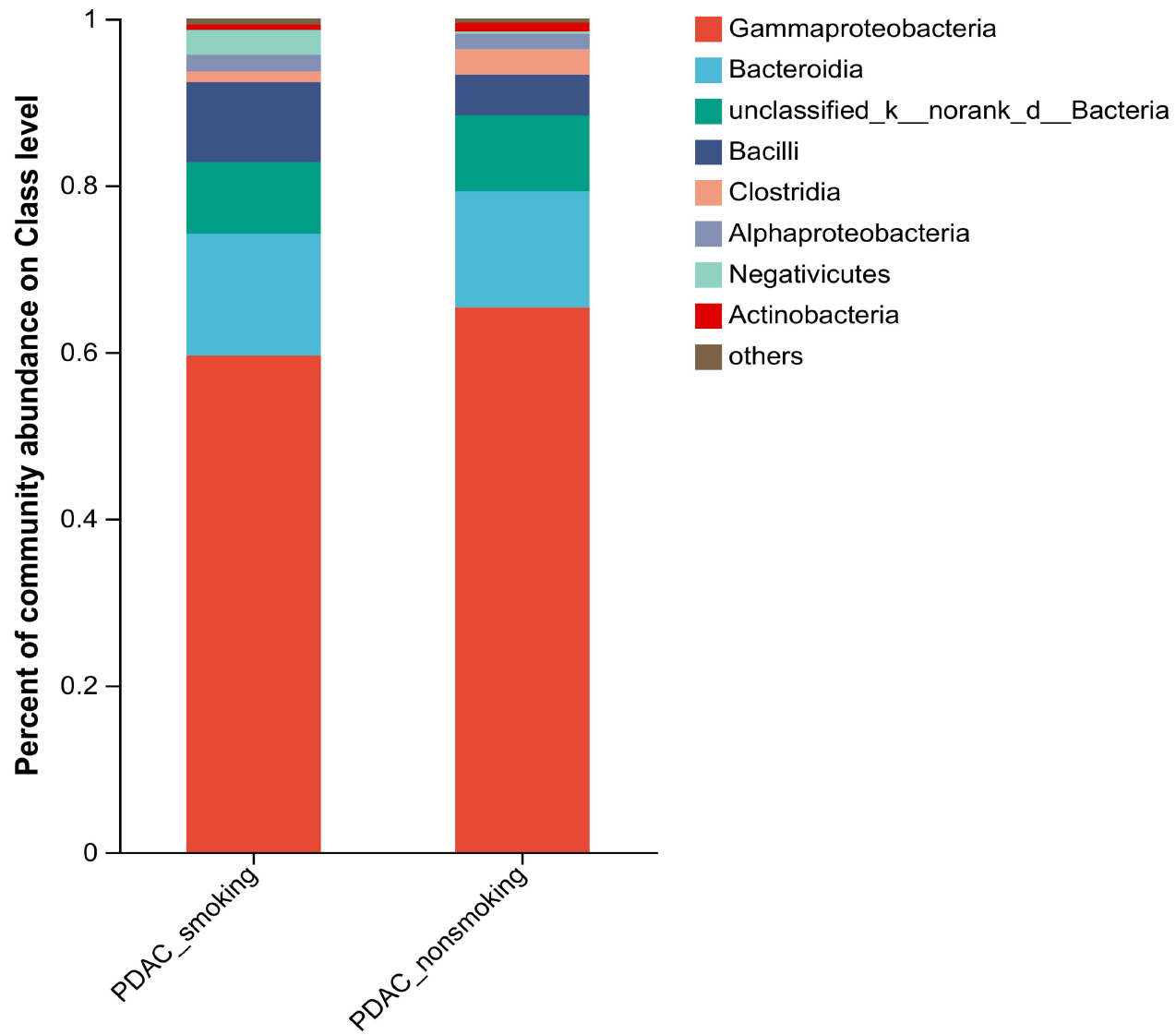


Fig. S3 Bacterial composition at the class level of subjects between the smoking PDAC group and non-smoking PDAC group in the paracancerous tissue of surgical samples.

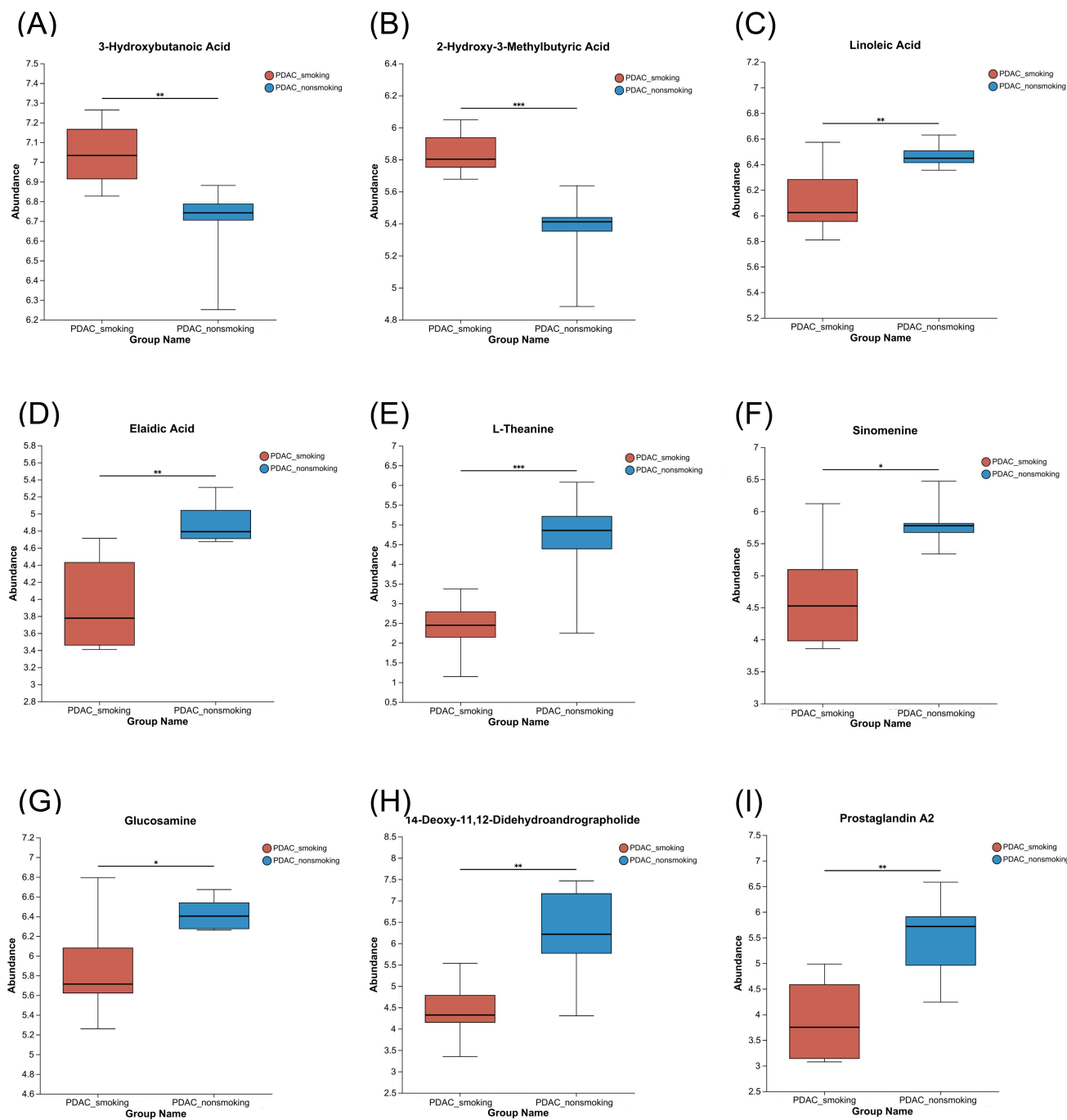


Fig. S4 Partial differential metabolites in paracancerous tissue of surgical samples from smoking vs. non-smoking PDAC. 3-hydroxybutanoic acid (A), 2-hydroxy-3-methylbutyric acid (B), linoleic acid (C), elaidic acid (D), L-theanine (E), sinomenine (F), glucosamine (G), 14-deoxy-11, 12-didehydroandrographolide (H), prostaglandin A2 (I). $P < 0.001$ is marked as ***, $P < 0.01$ is marked as **, $P < 0.05$ is marked as *.

Community barplot analysis

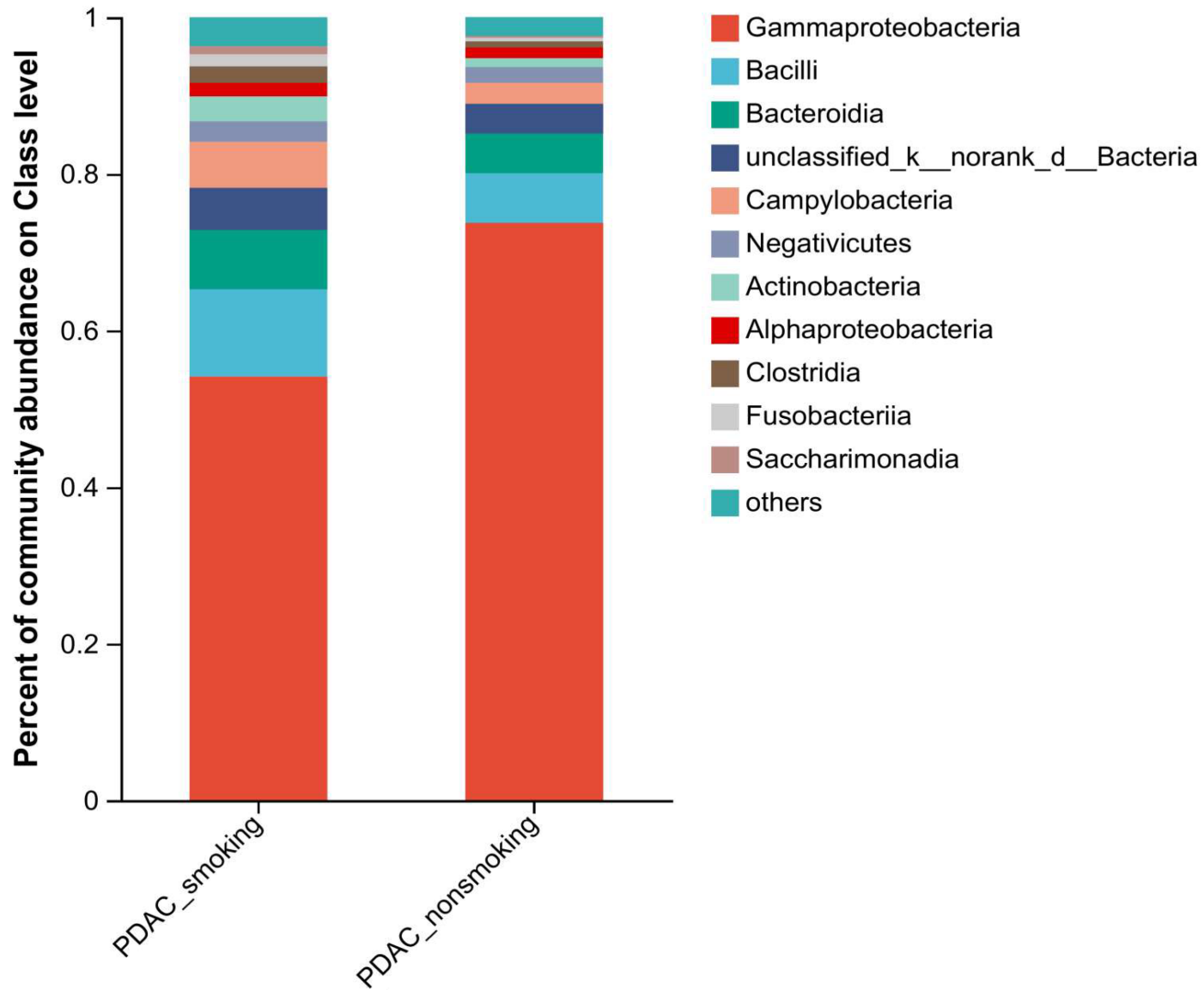


Fig. S5 Bacterial composition at the class level of subjects in FNA samples.