

## **Zinc treatment reverses and anti-Zn-regulated miRs suppress esophageal carcinomas in vivo**

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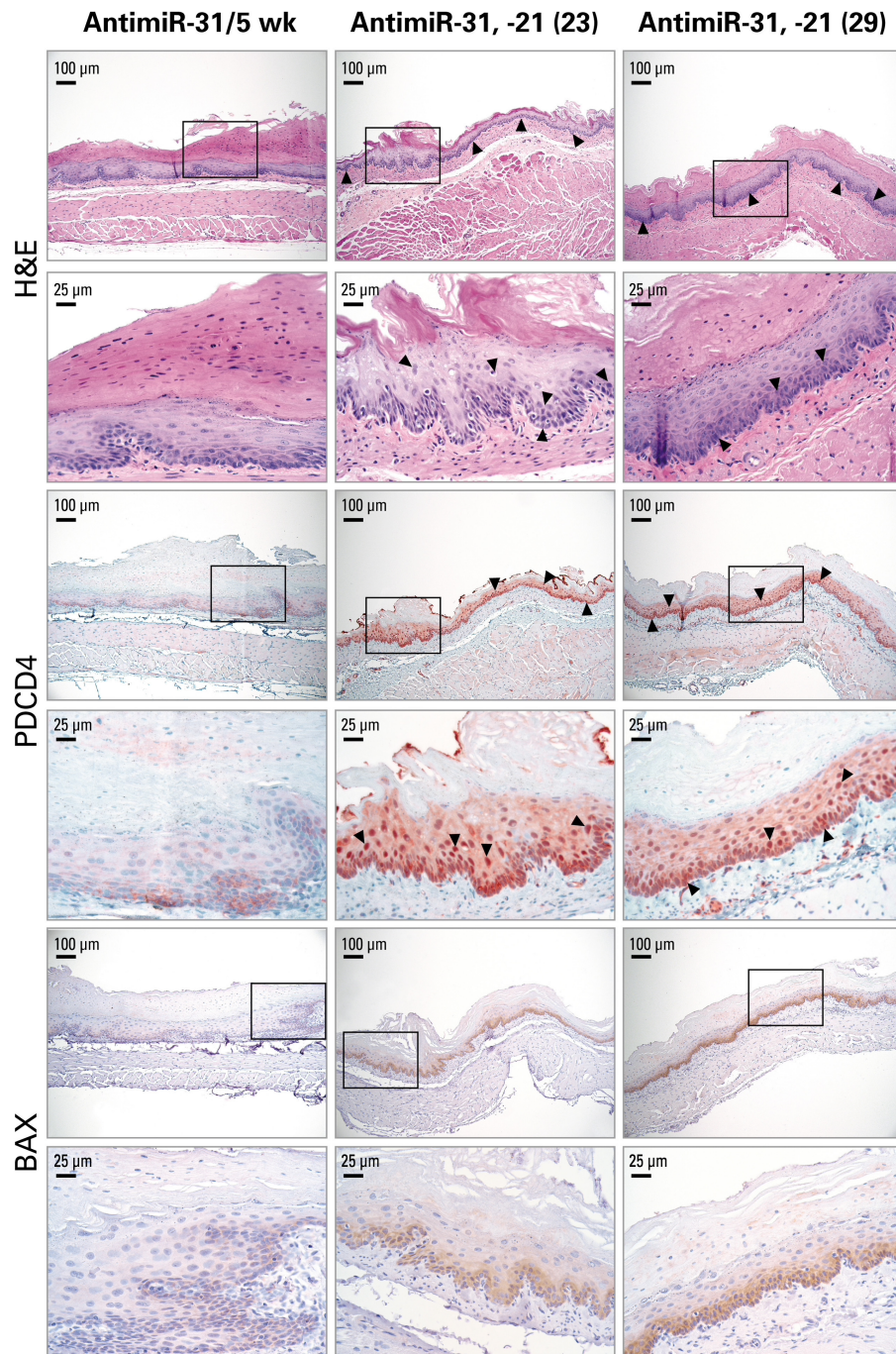
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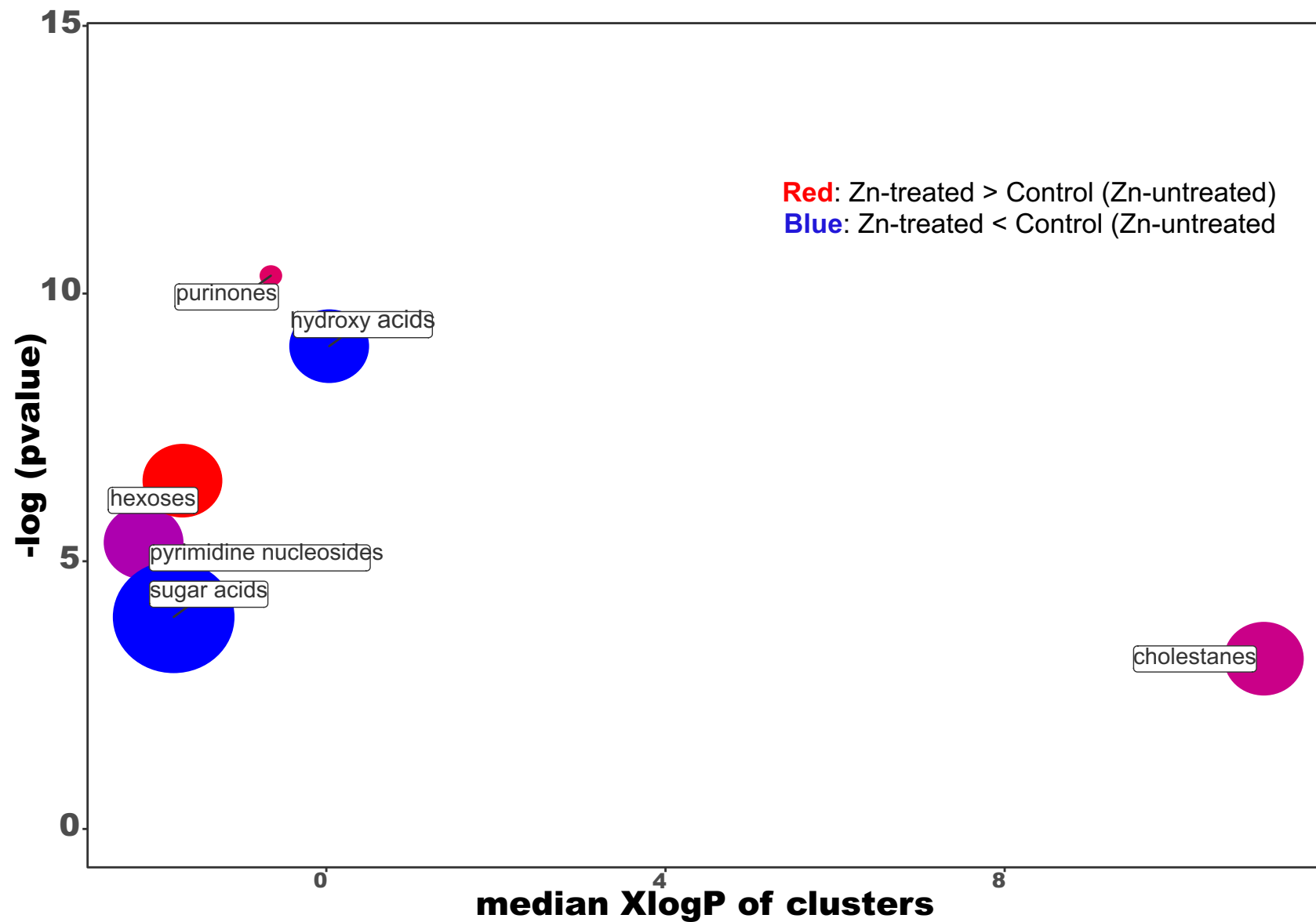
Figure S1 and S2

Table S1 and S2



**Fig. S1.** Sequential delivery of antimiR-31 (5-wk) followed by antimiR-21 (15-wk) induces apoptosis in esophagus.

Representative photos of hematoxylin & eosin (H&E)-stained, antimiR-31, -21 rat esophageal epithelium (rat 23 & 29). Arrowheads indicate numerous suprabasal & basal cells undergoing apoptosis, shrunken apoptotic cells with condensed cytoplasm. PDCD4-IHC: near serial sections showing abundant cells that were undergoing apoptosis with intense nuclear overexpression of PDCD4 (tumor suppressor target of miR-21). BAX-IHC: near serial sections showing abundant cells that were undergoing apoptosis with strong cytoplasmic expression of BAX protein. Conversely, antimiR-31/5-wk rat esophageal epithelium showing lack of apoptosis (H&E-stained section) and absence of PDCD4 nuclear expression (PDCD4-IHC) and BAX protein expression (BAX-IHC).



**Fig. S2.** ChemRICH set enrichment statistics plot on Zn-treated vs Zn untreated rat esophagus metabolites. Enrichment p-values are given by the Kolmogorov-Smirnov-test. The plot y-axis shows the most significantly altered clusters on the top. Node sizes represent the total number of metabolites in each cluster set. The node color scale shows the proportion of increased (**red**), decreased (**blue**) metabolites; purple nodes have both increased & decreased metabolites.

**Table S1.** Zn intervention reverses ESCC metabolome phenotype in Zn-treated versus Zn-untreated rats<sup>a</sup>

Metabolite name	InChI Key	Fold change (Zn-treated vs. Zn-untreated)	P-value	Biological process
<b>24 down-regulated</b>				
Thymine	RWQNBRDOKXIBIVUHFFFAOYSA-N	-5.43	0.01	Pyrimidine metabolism
<b>Putrescine</b>	KIDHWZJUCRJVML-UHFFFAOYSA-N	-3.96	0.02	Polyamine biosynthesis
<b>3-Phenyllactic acid</b>	VOXXWSYKYCBWHO-UHFFFAOYSA-N	-3.86	0.01	Phenylalanine metabolism
Indole-3-lactate	XGILAAAMKEQUXLS-UHFFFAOYSA-N	-3.73	0.00	Tryptophan metabolism
<b>Glyceric acid</b>	RBNPOMFGQQGHHO-UHFFFAOYSA-N	-3.02	0.00	Pentose phosphate pathway
Hexadecylglycerol	OOWQBDFWEXAPB-UHFFFAOYSA-N	-2.88	0.02	---
Alpha-ketoglutarate	KPGXRSRHYNQIFN-UHFFFAOYSA-N	-2.35	0.01	Pentose phosphate pathway
p-Tolyl glucuronide	JPAUCQAJHLSMQW-XPORZQOISA-N	-2.30	0.01	---
<b>Phenylpyruvate</b>	BTNMPGBKDVTSJY-UHFFFAOYSA-N	-2.24	0.02	Amino acid metabolism
Pseudo-uridine	PTJWIQPHWPFNBW-GBNDHIKLSA-N	-2.22	0.00	Pyrimidine metabolism
Lanosterol	CAHGCLMLTWQZJN-BQNIITSRSA-N	-2.09	0.03	Steroid biosynthesis
2-Hydroxyglutaric acid	HWXBTVNAVRSUOJR-UHFFFAOYSA-N	-2.01	0.01	Butanoate metabolism
Uric acid	LEHOTFFKMJEONL-UHFFFAOYSA-N	-1.96	0.01	Purine metabolism
Succinic acid	KDYFGRWQOYBRFD-UHFFFAOYSA-N	-1.87	0.01	Citrate cycle (TCA cycle)
2-Aminobutyric acid	QWCKQJZIFLGMSD-UHFFFAOYSA-N	-1.84	0.01	---
<b>Saccharic acid</b>	DSLZVSRJTYRBFB-LLEIAEIESA-N	-1.81	0.02	Ascorbate & aldarate metabolism
Octadecylglycerol	OGBUMNBNEWYMNJ-UHFFFAOYSA-N	-1.77	0.04	---
Thymidine	IQFYKMKMVGJFEH-XLPZGREQSA-N	-1.77	0.00	Pyrimidine metabolism
Xylonic acid isomer	QXKAIJAYHKCRRRA-UHFFFAOYSA-N	-1.55	0.00	---
Glycerol-alpha-phosphate	AWUCVROLDVIAJX-UHFFFAOYSA-N	-1.51	0.02	Glycerolipid metabolism (e.g. Plasmalogens)
2-Ketoisocaproic acid	BKAJNAXTPSGJCU-UHFFFAOYSA-N	-1.51	0.04	Amino acid metabolism
Threonic acid	JPIJQSOTBSSVTP-STHAYSLISA-N	-1.48	0.04	Ascorbate & aldarate metabolism
Oxoproline	ODHCTXKNWHXJC-VKHMVHEASA-N	-1.16	0.02	Glutathione metabolism
Pyruvic acid	LCTONWCANYUPML-UHFFFAOYSA-N	-1.14	0.04	Citrate cycle; glycine, serine & threonine metabolism
<b>14 up-regulated</b>				
Guanosine	NYHBQMYGNKIUIF-UUOKFMHZSA-N	3.58	0.00	Purine metabolism
<b>Glucose</b>	WQZGKKKJIFFOK-VFUOTHLCSA-N	3.38	0.02	Glycolysis/gluconeogenesis
<b>Isomaltose</b>	DLRVLDZNNYCBX-RTPHMHGBSA-N	2.45	0.04	Starch and sucrose metabolism
Inosine	UGQMRVRMYASKQ-KQYNXXCUSA-N	2.42	0.00	Purine metabolism
5-Hydroxy-3-indoleacetic acid	DUUGKQCEGZLZNO-UHFFFAOYSA-N	2.35	0.04	Tryptophan metabolism
Uridine	DRTQHJPVMGBUFC-XVFCMESISA-N	2.19	0.01	Pyrimidine metabolism
Hypoxanthine	FDGQSTZJBFJUBT-UHFFFAOYSA-N	1.98	0.03	Purine metabolism
Ribonic acid	QXKAIJAYHKCRRRA-BXXZVTAOSA-N	1.92	0.00	---
Xanthine	LRFVTYWOQMYALW-UHFFFAOYSA-N	1.77	0.02	Purine metabolism
<b>Fructose</b>	RFSUNEUAIZKAJO-ARQDHWQXSA-N	1.70	0.01	Starch & sucrose metabolism
<b>Myo-inositol</b>	CDAISMWEOUEBRE-UHFFFAOYSA-N	1.58	0.02	Galactose metabolism
Tocopherol gamma-	QUEDXNHFTDJVIY-DQCZWHMSA-N	1.50	0.02	Ubiquinone/terpenoid-quinone biosynthesis
Beta-sitosterol	KZJWDPNRJALLNS-VJSFXXLFSA-N	1.49	0.00	Steroid biosynthesis
<b>Mannose</b>	WQZGKKKJIFFOK-QTVWNMPRSA-N	1.29	0.04	Fructose & mannose metabolism

<sup>a</sup>ESCC (esophageal squamous cell carcinoma)-bearing Zn-deficient rats were given Zn treatment for 33 days (25 ppm Zn gluconate in drinking water) or untreated. Nontargeted metabolomic profiling (GC-TOF MS) on esophageal mucosa was performed at Zn-treatment endpoint ( $n = 10$  rats per group). A total of 39 significantly altered metabolites were identified (24 down- 14 up-regulated,  $P < 0.05$ ). In

particular, levels of hexoses (glucose, fructose, mannose) were increased, and levels of polyamine (putrescine), sugar acids, and hydroxy acids were decreased, thus pointing to a non-cancerous metabolome phenotype.

**Table S2, A.** ChemRICH statistical analysis on Zn-treated vs Zn-untreated rat esophagus metabolites

Cluster name	Cluster size	p-values	FDR	Key comp	Altered me	Increased	Decreased	Increased r	Altered Ratio
purinones	3	0.000033	0.00094	uric acid	3	2	1	0.7	1
hydroxy acids	4	<b>0.00012</b>	<b>0.0018</b>	3-phenyllac	<b>2</b>	0	<b>2</b>	0	0.5
hexoses	4	<b>0.0015</b>	<b>0.014</b>	glucose	<b>3</b>	<b>3</b>	0	1	0.8
pyrimidine nucleosides	4	0.0048	0.034	thymidine	3	1	2	0.3	0.8
sugar acids	6	<b>0.019</b>	0.11	glyceric acid	<b>2</b>	0	<b>2</b>	0	0.3
cholestanes	4	0.042	0.2	beta-sitoste	2	1	1	0.5	0.5

**Table S2, B.** ChemRICH analysis compounds\*

\*Compounds that are significantly (p value < 0.05) increased (red) or decreased (blue) are highlighted in their respective clusters.- Hexoses, sugar acids, hydroxy acids, and biogen

Compound.Name	InChiKeys	Pubchem.ID	SMILES	pvalue	foldchange	CID	ClusterNum	xlogp	ClusterLabel	TreeLabels	FDR
pyruvic acid	LCTONWCAN	1060	CC(=O)C(=O)O	0.044	0.88	1060	50	-0.426	pyruvates		1
citric acid	KRKNYBCHX	311	C(C(=O)O)C(C(=O)O)C(=O)O	0.93	0.99	311	49	-2.247	citrates		1
succinic acid	KDYFGRWQC	1110	C(CC(=O)O)C(=O)O	0.014	0.54	1110	47	-0.71	dicarboxylic acids		1
fumaric acid	VZCYOOQTP	444972	C=C/C(=O)O	0.98	0.99	444972	53	-0.416	dicarboxylic acids		1
malic acid	BJEPYKJPYRN	525	C(C(C(=O)O)C(=O)O)C(=O)O	0.53	0.9	525	1	-1.474	dicarboxylic acids		1
xylulose	LQXVFWRQN	439205	C1[C@@H]([C@@H](O)[C@H](O)[C@@H](O)CO)O	0.18	0.53	439205	25	-1.497	pentoses	a	1
xylose	SRBFZHDQG	135191	C1[C@H]([C@@H](O)[C@H](O)[C@@H](O)CO)O	0.15	0.75	135191	8	-1.454	pentoses		1
xylonic acid isomer	QXKAIJAYHK	10264	C(C(C(C(=O)O)C(=O)O)C(=O)O)C(=O)O	0.0039	0.65	10264	19	-3.067	gum arabic		0.67
xanthine	LRFVTYWQO	1188	C1=NC2=C(N1)C(=O)N(C(=O)N2)C	0.024	1.8	1188	11	-0.654	purinones	b	1
valine	KZSNJWFQE	6287	CC(C)[C@@H](N)C(=O)O	0.31	1.2	6287	13	-2.169	amino acids, branched-ch		1
uridine-5'-monophosphate	DJJCFXVJDGT	6030	C1=CN(C(=O)NC1=O)COP(=O)([O-])[O-]	0.055	0.47	6030	12	-3.775	uracil nucleotides		1
uridine	DRTQHQJPM	6029	C1=CN(C(=O)NC1=O)N	0.012	2.2	6029	12	-2.117	pyrimidine nucleosides		1
uric acid	LEHOTFFKMJ	1175	C12=C(NC(=O)NC1=O)N(C)N2	0.0089	0.51	1175	11	-1.191	purinones	b	1
urea	XSQUKJJFZC	1176	C(=O)N(N)C(=O)O	0.92	1	1176	0	-1.686	organic chemicals		1
uracil	ISAKRJDGNU	1174	C1=CNC(=O)NC1=O	1	1	1174	28	-0.875	pyrimidinones		1
UDP-N-acetylglucosamine	LFTYTUAZOP	445675	CC(=O)N[C@@H]1[C@@H](O[C@@H]2[C@H](O)[C@@H](CO)O[C@H]2O)C[C@H](O)[C@@H](O)[C@H]1O	0.64	0.93	445675	42	-5.903	uridine diphosphate suga		1
UDP-glucuronic acid	HDYANYHVC	17473	C1=CN(C(=O)NC1=O)COP(=O)([O-])[O-]	0.31	0.76	17473	42	-5.955	uridine diphosphate suga		1
tyrosine	OUYCCASQ	6057	C1=CC(=CC=C1)C(N)C(=O)O	0.49	0.9	6057	31	-2.711	amino acids, aromatic		1
tryptophan	QIVBCDIJIAJF	6305	C1=CC=C2C(=C1)C(=CN2)C	0.26	0.83	6305	15	-2.023	amino acids, aromatic		1
trans-4-hydroxyproline	PMMYEEVYN	5810	C1[C@H](CN)C(=O)N[C@@H]1C(=O)O	0.071	0.49	5810	16	-0.786	amino acids, cyclic		1
tocopherol gamma-	QUEDXNHFT	92729	CC1=C(C=C2C=C(C=C(C=C2)O)O)O	0.022	1.5	92729	52	10.514	tocopherols		1
tocopherol alpha-	NCYCYXNIZ	638015	CC1=C(C(CCC)C=C(C=C1)O)O	0.92	0.99	638015	5	6.335	retinoids		1
thymine	RWQNBRODI	1135	CC1=CNC(=O)NC1=O	0.011	0.18	1135	28	-0.694	pyrimidinones		1
thymidine	IQFYKMKVC	5789	CC1=CN(C(=O)NC1=O)N	0.001	0.57	5789	12	-1.335	pyrimidine nucleosides		0.18
threonine	AYFVYJQAPC	6288	C[C@H]([C@@H](O)[C@H](O)CO)N	0.47	1.1	6288	17	-3.496	amino acids		1
threonic acid	JPIJQSOTBSS	5460407	C([C@@H]([C@@H](O)[C@H](O)CO)O)C(=O)O	0.044	0.68	5460407	1	-2.395	butyrates		1
taurine	XOAAWQZAT	1123	C(CS(=O)(=O)N)C(=O)O	0.52	1.1	1123	35	-1.678	alkanesulfonic acids		1
sulfuric acid	QAOWNCQO	1118	OS(=O)(=O)O	0.29	1.3	1118	14	-1.764	sulfuric acids		1
sucrose	CZMRCDWA	5988	C([C@@H]1[C@H]([C@@H]([C@H]([C@@H]1O)O)O)O)O	0.93	1	5988	40	-3.277	disaccharides		1
stearic acid	QIQXTHQIDY	5281	CCCCCCCC	0.91	0.99	5281	2	8.708	Saturated FA		1



squalene	YYGNTYWPH 638072	CC(=CCC/C(=	0.99	1	638072	5	11.482	polyenes		1
spermidine	ATHGHQPGF 1102	C(CCNCCCN)I	0.65	1.1	1102	34	-0.654	putrescine		1
sorbitol	FBPFZTCFMR 5780	C([C@H])([C@	0.96	0.99	5780	7	-3.896	sugar alcohols		1
sinigrin	PHZOWSSBX 6911854	C=CC/C(=N\C	0.54	0.91	6911854	4	-1.84	glucosinolates	c	1
serine	MTCFGRXMJ 5951	C([C@@H])(C	0.56	0.96	5951	17	-3.956	amino acids		1
<b>*saccharic acid</b>	DSLZVSRJTYR 33037	[C@H]([C@@	<b>0.016</b>	<b>0.55</b>	33037	10	-3.582	<b>sugar acids</b>		1
ribulose-5-phosphate	FNZLKVNUW 439184	C([C@H])([C@	0.79	0.94	439184	10	-4.396	ribulosephosphates		1
ribose-5-phosphate	KTVPXOYAKL 439167	C([C@@H]1[	0.064	1.4	439167	23	-3.112	hexosephosphates		1
ribose	HMFHBZSHG 5779	C([C@@H]1[	0.61	1.2	5779	25	-1.454	pentoses	a	1
ribonic acid	QXKAIJAYHKI 5460677	C([C@H])([C@	0.0032	1.9	5460677	19	-3.067	gum arabic		0.55
ribitol	HEBKCHPVOI 827	C(C(C(C(CO)C	0.63	0.94	827	7	-3.224	sugar alcohols		1
raffinose	MUPFEKGTN 439242	C([C@@H]1[	0.28	0.57	439242	4	-4.814	trisaccharides	c	1
pyrophosphate	XPPKVPWEQ 1023	OP(=O)(O)OP	0.18	0.76	1023	14	-3.476	diphosphonates		1
<b>*putrescine</b>	KIDHWZJUCF 1045	C(CCN)CN	<b>0.022</b>	<b>0.25</b>	1045	34	-0.626	<b>biogenic polyamines</b>		1
p-tolyl glucuronide	JPAUCQAJHL 154035	CC1=CC=C(C=C	0.007	0.43	154035	52	0.189	resols		1
pseudo-uridine	PTJWIQPHW 15047	C1=C(C(=O)N	0.0021	0.45	15047	12	-2.477	pyrimidine nucleosides		0.37
proline	ONIBWKKTO 145742	C1C[C@H](N	0.58	1.1	145742	16	-0.185	amino acids, cyclic		1
pimelic acid	WLJVNTCWH 385	C(CCC(=O)O)	0.27	0.42	385	26	0.575	dicarboxylic acids		1
phytosphingosine	AERBNYCJB 122121	CCCCCCCCC	0.16	0.76	122121	51	5.027			1
phosphogluconic acid	BIRSGZKFKXL 91493	C([C@H])([C@	0.3	1.2	91493	10	-4.968	gluconates		1
phosphoethanolamine	SUHOOTKUP 1015	C(COP(=O)(O	0.47	0.9	1015	35	-2.504	amino alcohols		1
phosphoenolpyruvate	DTBNBXWJW 58114173	C=C(C(=O)O)I	0.075	1.4	58114173	53	-1.296	hydroxy acids		1
phosphate	NBIIXVUZAF 1004	OP(=O)(O)O	0.9	0.98	1004	14	-2.247	polymers		1
<b>*phenylpyruvate</b>	BTNMPGBKD	C1=CC=C(C=C	<b>0.019</b>	<b>0.45</b>	cid_54	43	0.907	<b>hydroxy acids</b>		1
phenylalanine	COLNVLHVI 6140	C1=CC=C(C=C	0.3	0.83	6140	31	-1.575	amino acids, aromatic		1
pelargonic acid	FBUKVWPVB 8158	CCCCCCCCC(	0.57	0.9	8158	2	3.587	Saturated FA		1
parabanic acid	FZLIKDUSUDI 67126	C1(=O)C(=O)I	0.55	1.1	67126	18	-0.58	hydantoin		1
pantothenic acid	GHOKWGTU; 6613	CC(C)(CO)[C@	0.65	0.93	6613	54	-1.343	beta-alanine		1
palmitoleic acid	SECPZKHBEN 445638	CCCCC/C=C	0.14	0.73	445638	3	7.054	UnSaturated FA		1
palmitic acid	IPCSVZSSVZV 985	CCCCCCCCC	0.69	0.97	985	2	7.57	Saturated FA		1
oxoproline	ODHCTXKNV 7405	C1CC(=O)N[C	0.018	0.86	7405	16	-0.827	amino acids, cyclic		1
ornithine	AHLPHDHHV 6262	C(C[C@@H])(	0.66	0.93	6262	29	-3.307	amino acids, basic		1
O-phosphoserine	BZQFBWGGL 57689797	C([C@@H])(C	0.7	1	57689797	17	-5.185	plasmalogens		1
oleic acid	ZQPPMHVWI 445639	CCCCCCC/C	0.53	0.87	445639	3	8.192	UnSaturated FA		1
octadecylglycerol	OGBUMNBN 3681	CCCCCCCCC	0.038	0.56	3681	20	7.955	glyceryl ethers	d	1
noradrenaline	SFLSHLXELF 439260	C1=CC(=C(C=	0.5	1.7	439260	31	-0.714	catecholamines		1
nicotinic acid	PVNIIMVLHY 938	C1=CC(=CN=I	0.39	1.3	938	46	-0.508	nicotinic acids		1
nicotinamide	DFPAKSUCGF 936	C1=CC(=CN=I	0.37	1.2	936	46	-1.236	nicotinic acids		1
N-acetylmannosamine	OVNRDRQMI 439281	CC(=O)N[C@	0.12	1.3	439281	54	-1.488	hexosamines		1
N-acetylaspartic acid	OTCCIMWXF 65065	CC(=O)N[C@	0.14	0.47	65065	32	-1.265	amino acids, acidic		1
myristic acid	TUNFSRHWC 11005	CCCCCCCCC	0.8	0.97	11005	2	6.432	Saturated FA		1
myo-inositol	CDAISMWEC 892	C1(C(C(C(C(C	0.018	1.6	892	30	-1.458	sugar alcohols		1
methionine sulfoxide	QEFRNWWL; 158980	CS(=O)CC[C@	0.54	0.93	158980	27	-3.882	amino acids, sulfur		1
methionine	FFEARJCKVFF 6137	CSCC[C@@H	0.43	1.1	6137	27	-1.853	amino acids, sulfur		1
methanolphosphate	CAAULPUQFI 13130	COP(=O)(O)C	0.81	1	13130	14	-1.728	organophosphates		1

<b>*mannose</b>	WQZGKKKJJI 18950	C([C@@H]1[	0.044	1.3	18950	8	-1.697	<b>hexoses</b>		1
maltotriose	FGDTMLNYI 439586	C([C@@H]1[	0.36	0.58	439586	4	-5.629	trisaccharides	c	1
maltose	GUBGYTABK 439186	C([C@@H]1[	0.79	0.93	439186	4	-3.663	disaccharides	c	1
maleimide	PEHTFAAVS 10935	C1=CC(=O)N	0.9	1	10935	18	-0.676	maleimides		1
lyxitol	HEBKCHPVOI 439255	C([C@@H](C	0.28	1.3	439255	7	-3.224	sugar alcohols		1
lysine	KDXKERNBSI 5962	C(CCN)C[C@	0.49	0.85	5962	44	-2.949	amino acids, basic		1
linoleic acid	OYHQOLUKZ 5280450	CCCCC/C=C\	0.91	0.97	5280450	3	7.865	UnSaturated FA		1
leucine	ROHFNLRQFI 6106	CC(C)C[C@@	0.68	0.94	6106	38	-1.389	amino acids, branched-ch		1
lauric acid	POULHZVOKI 3893	CCCCCCCCC	0.86	1	3893	2	5.294	Saturated FA		1
lanosterol	CAHGCLMLT 246983	C[C@H](CCC	0.034	0.48	246983	5	10.21	cholestanes		1
lactic acid	JVTAAEKZFI 612	CC(C(=O)O)O	0.1	0.72	612	41	-0.591	hydroxy acids		1
isothreonine acid	JPIJQSOTBSS 151152	C([C@H]([C@	0.18	0.8	151152	1	-2.395	butyrates		1
isomaltose	DLRVVLDZNN 439193	C([C@@H]1[	0.038	2.4	439193	4	-3.234	disaccharides	c	1
isoleucine	AGPKZVBTJJ 6306	CC[C@H](C)[	0.49	0.9	6306	38	-1.6	amino acids, branched-ch		1
inositol-4-monophosphate	INAPMGXU 440043	[C@H]1([C@	0.73	1.1	440043	30	-3.545	inositol phosphates		1
inosine 5'-monophosphate	GRSZFWQUA 8582	C1=NC2=C(CI	0.1	0.29	8582	9	-3.605	purine nucleosides		1
inosine	UGQMRVRM 6021	C1=NC2=C(CI	0.0042	2.4	6021	9	-1.947	purine nucleosides		0.71
indole-3-lactate	XGILAAAMKEC 92904	C1=CC=C2C(=	0.004	0.27	92904	15	0.21	amino acids, aromatic		0.68
hypoxanthine	FDGQSTZJBF 790	C1=NC2=C(N	0.032	2	790	11	0.556	purinones	b	1
histidine	HNDVDQJCI 6274	C1=C(NC=N1	0.88	0.96	6274	9	-3.429	amino acids, cyclic		1
hexadecylglycerol	OOWQBDFW 72733	CCCCCCCCC	0.017	0.35	72733	20	6.817	glyceryl ethers	d	1
heptadecanoic acid	KEMQGTRYU 10465	CCCCCCCCC	0.66	0.96	10465	2	8.139	Saturated FA		1
guanosine	NYHBQMYG 6802	C1=NC2=C(N	0.0022	3.6	6802	9	-2.272	purine nucleosides		0.38
glycine	DHMQDGOQ 750	C(C(=O)O)N	0.46	1.1	750	33	-3.35	amino acids		1
glycerol-alpha-phosphate	AWUCVROL 754	C(C(COP(=O)	0.016	0.66	754	21	-3.109	glycerophosphates		1
glycerol	PEDCQBHIV 753	C(C(CO)O)O	0.65	1	753	45	-1.788	sugar alcohols		1
<b>*glyceric acid</b>	RBNPOMFGC 752	C(C(C(=O)O)C	0.0043	0.33	752	1	-1.723	<b>sugar acids</b>		0.72
glutathione	RWSXRVCMC 124886	C(CC(=O)N)C	0.12	1.5	124886	48	-4.23	oligopeptides		1
glutamine	ZDXPYRJPND 5961	C(CC(=O)N)[C	0.92	1	5961	29	-4.077	amino acids, basic		1
glutamic acid	WHUUTDBJX 33032	C(CC(=O)O)[C	0.081	0.8	33032	29	-3.349	amino acids, acidic		1
glucuronic acid	AEMOLEFTQ 94715	[C@H]1([C	0.47	0.89	94715	6	-1.54	glucuronates		1
glucose-6-phosphate	NBSCHQHZL 5958	C([C@@H]1[	0.17	0.19	5958	22	-3.355	hexosephosphates	e	1
glucose-1-phosphate	HXXFSFRBO 65533	C([C@@H]1[	0.4	0.83	65533	22	-3.355	hexosephosphates	e	1
<b>*glucose</b>	WQZGKKKJJI 64689	C([C@@H]1[	0.019	3.4	64689	8	-1.697	<b>hexoses</b>		1
gluconic acid lactone	PHOQVHQST 7027	C([C@@H]1[	0.087	0.47	7027	6	-1.203	gluconates		1
gluconic acid	RGHNJXZEO 6857417	C([C@@H]([C	0.082	0.34	6857417	10	-3.739	gluconates		1
gamma-aminobutyric acid	BTCSSZJGUN 119	C(CC(=O)O)C	0.46	1.1	119	33	-0.668	aminobutyrate		1
galacturonic acid	AEMOLEFTQ 441476	[C@H]1([C	0.4	1.2	441476	6	-1.54	hexuronic acids		1
galactose-6-phosphate	NBSCHQHZL 439404	C([C@@H]1[	0.25	0.35	439404	22	-3.355	hexosephosphates	e	1
galactinol	VCWMRQDB 11727586	C([C@@H]1[	0.41	2	11727586	4	-3.424	disaccharides	c	1
fucose	SHZGCJCMOI 439650	C[C@@H]1[C	0.2	1.3	439650	8	-0.994	hexoses		1
fructose-6-phosphate	BGWGXPA 440641	C([C@@H]1[	0.15	0.22	440641	23	-3.398	hexosephosphates		1
fructose-1-phosphate	RHKKBWRN 439394	C([C@@H]1[	0.2	1.2	439394	23	-3.398	hexosephosphates		1
<b>*fructose</b>	RFSUNEUAIZ 439709	C([C@@H]1[	0.011	1.7	439709	25	-1.74	<b>hexoses</b>	a	1
ethanolamine	HZAXFHJVJLS 700	C(CO)N	0.77	0.96	700	35	-1.275	amino alcohols		1





3,6-anhydro-D-galactose	WZYRMLAW 16069996	C1[C@H]([C@H]1O)O	0.73	1.1 16069996	6	-1.449 methylgalactosides	1
2-monoolein	UPWGQKDV 5319879	CCCCCCCC/C	0.46	0.77 5319879	36	7.132 glycerides	1
2-ketoisocaproic acid	BKAJNAXTPS 70	CC(C)CC(=O)O	0.041	0.66 70	50	0.904 keto acids	1
2-hydroxyglutaric acid	HWXBTNAVF 43	C(CC(=O)O)C	0.012	0.5 43	19	-1.116 dicarboxylic acids	1
2-hydroxybutanoic acid	AFENDNXGA 440864	CC[C@H](C(=O)O)O	0.37	1.2 440864	41	-0.233 hydroxybutyrates	1
2-aminobutyric acid	QWCKQJZIFL 6657	CCC(C(=O)O)N	0.014	0.54 6657	13	-2.466 aminobutyrate	1
2,3-dihydroxybutanoic acid	LOUGYXZSUF 250402	CC(C(C(=O)O)O)O	0.13	0.81 250402	1	-1.263 sugar acids	1
1-monostearin	VBICKXHEKH 24699	CCCCCCCCC	0.34	0.88 24699	37	7.648 glycerides	1
1-monopalmitin	QHZLMUACJ 14900	CCCCCCCCC	0.095	0.74 14900	37	6.51 glycerides	1
1-monoolein	RZRNAYUHW 5283468	CCCCCCCC/C	0.19	0.45 5283468	36	7.132 glycerides	1
1-kestose	VAWYEUIPHI 440080	C([C@@H]1[C@H]([C@@H]([C@H](O1)CO)O)O)O	0.35	0.58 440080	40	-4.857 trisaccharides	1