

		C_DUAL vs DUAL			C_CUD vs CUD			C_SZ vs SZ					
Metab_ID	Name	log(FC)	-LOG(p)	V1	log(FC)	-LOG(p)	V1	log(FC)	-LOG(p)	V1	HMDB	PubChem	LipidMaps
Met_035	N-Isobutylhexacosanamide	1.02	5.50	1.67							Exogenous	Amide	https://www.lipidmaps.org/databases/lmsd/LMSP02010007?LMID=LMSP020
Met_100	Cer(d18:1/20:0)	1.08	4.96	1.64							Endogenous	Sphingolipid/Ceramide	
Met_094	Caproic acid	-1.53	3.32	1.39							Endogenous	Fatty Acyl/Fatty acid	https://lipidmaps.org/databases/lmsd/LMSP03020044?LMID=LMSP03020044
Met_110	Cer(d15:2(4E,6E)/20:0)	1.73	3.32	1.42							Exogenous	Sphingolipid/Ceramide	
Met_072	2-Geranylphenol	-1.14	3.31	1.43							Exogenous	Monoterpenoid	
Met_088	2,4,6,8,10-dodecapentaenal	-1.22	3.25	1.42							Endogenous	Fatty Acyl/Fatty Aldehyde	
Met_102	Cer(d18:1/16:0)	1.48	3.20	1.41							Endogenous	Sphingolipid/Ceramide	
Met_089	4-[(2R)-2-(Aminomethyl)-2-(hydroxymethyl)-5-oxo-1-pyrrolidinyl]-3-(3-pentanylamino)benzoic acid	1.18	2.73	1.29							0	0	
Met_107	Cer(d18:1/17:0)	1.52	2.64	1.27							Endogenous	Sphingolipid/Ceramide	
Met_052	32,35-anhydrobacteriohopaneterol	1.22	2.56	1.29							Exogenous - Exosome (phycotoxin)	Prenol Lipid/Hopanoid	
Met_022	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	-1.07	2.26	1.22							Endogenous	Glycerolphospholipid/ Glycerophosphocholines	
Met_066	N-arachidonoylethanolamine	1.15	2.14	1.16							Endogenous	Fatty acyl/ N-acyl ethanolamide	
Met_082	Oxaloterpin E	-1.40	2.13	1.19							Exogenous - Exosome (Bacteria)	Terpenoid	
Met_053	Luminmide B	-1.86	1.88	1.12							Exogenous - Exosome (Bacteria)	Cyclic peptide	
Met_073	Cer(m18:1(4E)/24:1(15Z))	1.45	1.61	0.99							Endogenous	Sphingolipid/Ceramide	
Met_112	Fukiic acid							-1.98	6.00	1.69	Exogenous	Phenylpropanoic acid	https://hmdb.ca/metabolites/HMDB0029496
Met_071	Trygliceride OPO							1.27	4.74	1.55	Endogenous	Glycerolipid/Triacylglycerol	
Met_090	11-oxo-undeca-5,8-dienoic acid							1.03	4.67	1.50	Exogenous	Fatty Acyl/Fatty Acid	
Met_121	2,4-dimethyl-5-vinylthiazole							-2.07	4.17	1.42	Exogenous	Thiazole	
Met_032	7-Dehydrodesmosterol							1.14	3.78	1.37	Endogenous	Sterol lipid/ Cholesterol and derivatives	
Met_060	1-Methylnicotinamide							-1.47	3.53	1.35	Endogenous	Nicotinamide	
Met_083	Calcimycin							-2.13	3.26	1.32	Exogenous - Exosome (Bacteria - Antibiotic)	Aminobenzoic acid.	
Met_111	PE(18:2(9Z,12Z)/0:0)							-3.07	3.14	1.29	Endogenous	Glycerolphospholipid/Glycerophosp hoethanolamine	
Met_047	PG(22:0/12:0)	-2.27	1.59	0.98				-2.11	3.10	1.25	Endogenous	Glycerophospholipids/Glycerophosp hoglycerols	

Met_065	N-(3-Hydroxy-9Z-octadecenoyl) glycine						2.97	3.03	1.31	Exogenous	Fatty acyl/N-acyl amine		
Met_004	Aripiprazole	8.62	2.68	1.35			8.80	2.95	1.28	Exogenous - Drug	N-arylpiperazine		
Met_031	Dehydroaripiprazole	5.66	2.70	1.34			5.51	2.93	1.27	Exogenous - Drug (Antipsychotic)	N-arylpiperazine		
Met_109	Histidylaspartic acid						-1.83	2.53	1.12	Exogenous	Dipeptide		
Met_017	PE(P-18:0/20:5(5Z,8Z,11Z,14Z,17Z))						-2.27	2.42	1.11	Endogenous	Glycerolphospholipid/ Glycerophosphoethanolamine	https://www.lipidmaps.org/data/LMSDRecord.php?LMID=LMGP02030001	
Met_092	12-Hydroxy-19-[(2Z)-4-hydroxy-3-methyl-2-buten-1-yl	-1.37	1.48	0.97			-1.61	2.38	1.13	0	0		
Met_069	PE(18:0/18:3(6Z,9Z,12Z))						-2.35	2.38	1.13	Endogenous	Glycerolphospholipid/Glycerophosp hoethanolamine	https://hmdb.ca/metabolites/HMDB0261461	
Met_018	medorinone						1.51	2.32	1.09	Exogenous - Drug (Cardiovascular Agent)	Naphthyridines		
Met_074	PE(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z))						-1.16	2.26	1.09	Endogenous	Glycerolphospholipid/Glycerophosp hoethanolamine		
Met_037	PE(18:1(9Z)/0:0)	-1.84	1.61	1.01			-2.52	1.90	1.00	Endogenous	Glycerolphospholipid/ Glycerophosphoethanolamine		
Met_038	Cer(t18:0/19:0(2OH))						1.00	1.78	0.95	Endogenous	Sphingolipid/Ceramide		
Met_028	Aminopentol	-1.42	1.57	0.99						Exogenous - Exposome (Micotoxin)	0		
Met_114	Temanogrel	-4.54	5.97	1.73	-4.62	14.31	2.44	-5.00	16.49	2.19	Exogenous	Benzamide	
Met_036	Tryptophan P1	-4.94	9.68	1.93	-4.32	13.21	2.36	-4.04	7.18	1.82	Exogenous - Exposome (Tobacco)	Pyridoindole.	
Met_040	Benzoylarginine nitroanilide	-3.67	4.79	1.62	-4.06	12.49	2.40	-4.05	13.79	2.13	Exogenous - Exposome	Aniline	
Met_079	Tropeolin	2.04	2.04	1.14	3.20	10.91	2.28	2.85	8.71	1.94	Exogenous - Food biomarker	Thiocyanate	
Met_029	Cotinine	5.67	4.94	1.69	4.57	8.73	2.13				Exogenous - Exposome (Tobacco)	Alkaloid	
Met_030	Nicotine	5.71	3.75	1.54	4.71	7.95	2.05				Exogenous - Exposome (Tobacco)	Alkaloid	
Met_115	9'-carboxy-gamma-tocotrienol				4.79	7.26	2.01				Endogenous	Monoterpenoid	
Met_034	2(3H)-Benzothiazolone				1.44	6.95	1.90	1.28	6.51	1.74	Exogenous - Exposome (Tobacco)	Benzothiazole	
Met_023	11-Nor-9-carboxy-delta9-THC				6.07	6.70	1.93				Exogenous - Drug (THC metabolite)	0	
Met_081	Docosanamide	-3.20	5.71	1.68	-3.04	5.60	1.79	-3.42	5.18	1.61	Endogenous	Fatty acyl/Primary amide	
Met_120	5-Hydroxy-1-(4-hydroxyphenyl)-3-decanone	-1.36	2.69	1.30	-1.16	4.50	1.60	-1.28	3.25	1.33	Exogenous	Fatty Acyl/Unsaturated fatty acid	
Met_077	Pelretin	-3.57	6.17	1.72	-3.13	4.46	1.60	-2.92	2.88	1.21	Exogenous - Exposome (Vitamin - Mineral)	0	
Met_093	Neryl acetate				-1.12	4.43	1.65	-1.57	5.68	1.72	Exogenous - Plant metabolite	Acetate ester	
Met_025	N-oleoyl L-serine				-1.25	3.97	1.43	-1.03	2.83	1.22	Endogenous	Fatty acyl/Fatty N-acyl amine	

Met_042	trans-2-Dodecenoylcarnitine				-1.15	3.70	1.40				Endogenous	Fatty Acyl/Acylcarnitine
Met_117	Protulactone A	-1.82	2.20	1.15	-1.56	3.70	1.43	-2.54	7.39	1.82	Exogenous	Polyketide
Met_020	N-palmitoyl serine				-1.12	3.13	1.28				Endogenous	Fatty acyl/N-acyl amine/Endocannabinoid-like
Met_116	4-vinylphenol sulfate				1.52	2.92	1.33				Exogenous	Sulfuric ester
Met_011	O-Decanoyl-L-carnitine	-1.41	2.20	1.18	-1.10	2.89	1.22	-1.20	3.12	1.26	Endogenous	Fatty acyl/Fatty acyl carnitines
Met_057	Medelamine A	-1.89	3.82	1.49	-1.13	2.64	1.24	-1.48	2.10	1.03	Exogenous - Exposome (Fungi)	Amine
Met_067	3,5-Tetradecadiencarnitine				-1.04	2.63	1.13	-1.16	3.44	1.33	Endogenous	Fatty Acyl/Acylcarnitine
Met_013	5-Methyl-1H-benzimidazole				1.11	1.80	1.05				Exogenous - Exposome	Imidazole
Met_024	O-octanoyl-R-carnitine							-1.68	4.11	1.39	Endogenous	Fatty acyl/Fatty acyl carnitines