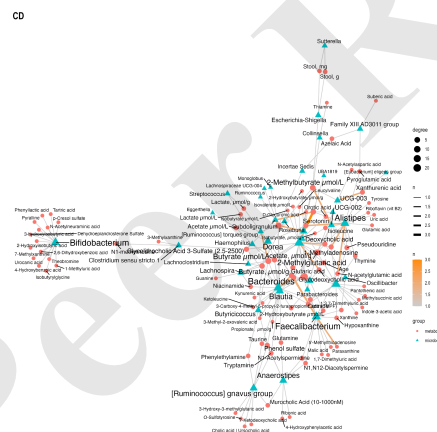


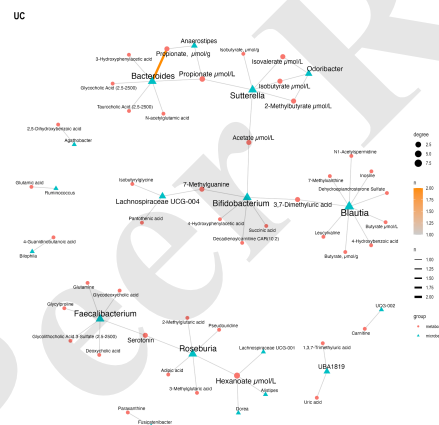
Healthy



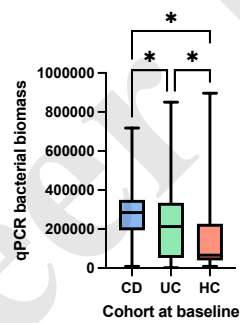
Suppl. Fig 2



Suppl. Fig 3



Suppl. Fig 5



Supplementary Appendices:

Appendices:

1. Additional details regarding metataxonomic analysis:

1a. V1-2 primer sequences.

Primer name	Primer sequence	Primer ratio
28F-YM (Forward primer)	GAGTTTGATYMTGGCTCAG	4
28F-Borrellia (Forward primer)	GAGTTTGATCCTGGCTTAG	1
28FChloroflex (Forward primer)	GAATTTGATCTTGGTTCAG	1
28F-Bifdo (Forward primer)	GGGTTTCGATTCTGGCTCAG	1
388R (Reverse primer)	TGCTGCCTCCCGTAGGAGT	

1b. Reads generated by metataxonomics:

During processing of sequencing data, we removed samples with < 7757 reads to remove poor quality reads / samples; however, we included two samples with <10K reads due to the relatively low sample numbers of the unique cohort. We were satisfied that the remaining data is of very good quality, as reflected by the first quantile being 25K read depth.

2. ¹H NMR setup.

Urine and fecal water extracts were analyzed using a Bruker 600 MHz AVANCE III NMR spectrometer. The 1D ¹H NMR spectra were acquired using a standard one-dimensional pulse sequence, with saturation of the water resonance (noesygppr1d pulse program) during both the relaxation delay (RD = 4s) and mixing time (tm = 10 ms). A standard one-dimensional NOESY pulse sequence was acquired using a pulse width of approximately 13 μs. During this time, a water pre-saturation pulse was applied to suppress the water signal. The two magnetic field z-gradients implemented were applied for 1 ms, the receiver gain was set to 90.5 and acquisition time (ACQ) to 2.73s for all experiments. Each spectrum was acquired using 4 dummy scans, 32 scans, 64 K data points and a spectral

window of 20 ppm. Prior to Fourier Transformation, each free induction decay was multiplied by an exponential function corresponding to a line broadening of 0.3 Hz. For serum, following the recording of the 1D NOESY-presat, one-dimensional CPMG with water saturation was acquired using the Carr–Purcell–Meiboom–Gill pulse sequence (cpmgpr1d). The acquisition parameters are set up in the same way as the 1D NOESY-presat, with the addition of the spin-echo delay (Delta1/Delta2) that is set at 0.3 ms and the implementation of 128 loops for T2 filter (L4).

2D 1H – 1H J-resolved experiment was also acquired for each sample to detect the J-couplings in the second dimension using the pulse program with suppression of the water resonance during the relaxation delay (jresgpprqf). The acquisition parameters used for this experiment were as follows: 16 dummy scans and 2 scans, 8K points with spectral window of 16.7 ppm for f2 and 40 increments with a spectral window of 78 Hz for f1, incremented delay of 3µs, RD of 2 s and ACQ of 0.41 s. The receiver gain was set to 90.5. A sine-bell apodization function was applied on both dimensions, followed by Fourier transformation, tilting by 45°, and summarization along f1.

The NMR spectra of urine and FW samples were acquired at 300 K, and those for serum were acquired at 310 K.

3. α diversity comparisons of HCs compared to IBD cohorts.

α diversity vs HC	Estimated STD	Error	FDR P value
Shannon vs UC	-4.4417	43.6334	0.860681
Shannon vs CD	20.5496	25.2009	0.463707
InvSimp vs UC	-3.3224	4.8611	0.49689
InvSimp vs CD	-3.6301	5.3755	0.50203
Chao1 vs UC	-4.4417	25.2009	0.860681
Chao1 vs CD	20.5496	27.8676	0.463707
Faith's PD vs UC	-2.6429	3.6969	0.4774
Faith's PD vs CD	0.1447	4.0881	0.9719

Abbreviations of Table: InvSimp =Inverse Simpson. STD = Standard deviation. FDR = false discovery rate

47 4. OPLS-DA statistics for ¹H NMR data

OPLS-DA comparison	R ² X (cum)	R ² Y (cum)	Q ² (cum)	CV-ANOVA P value.
Fecal HC vs CD	0.168	0.453	0.263	0.00355
Fecal HC vs UC	0.391	0.466	0.257	0.00341
Fecal CD vs UC	0.242	0.181	-0.0016	1
Serum HC vs CD	0.157	0.869	0.415	0.0008
Serum HC vs UC	0.112	0.42	0.142	0.0199
Serum CD vs UC	0.295	0.8	0.224	0.0279
Urine HC vs CD	0.185	0.836	0.437	0.0006
Urine HC vs UC	0.148	0.743	0.153	0.0806
Urine CD vs UC	0.159	0.907	0.0806	0.5937

48

49 5. Global LC-MS analyses using RP +ve and -ve modes for feces and RP -ve mode
50 for urine:

51 (Highlighted in yellow if higher in HC compared to IBD subtypes. Highlighted in
52 magenta if higher in CD compared to UC and HCs. Highlighted in blue if highest in CD
53 more than HCs and higher in HCs more than UC. Highlighted in green if lower in HCs
54 compared to IBD subtypes. Highlighted in cyan if higher in HC compared to UC.
55 Highlighted in red if lower in UC compared to CD and HC. Highlighted in grey if higher
56 in CD compared to HC)

Metabolite	Biofluid	q value (ANOVA)	Comparison
Azelaic Acid	Feces	0.008943	HC > CD; HC > UC
1,3,7-Trimethyluric acid	Feces	0.008943	HC > CD; HC > UC
Serotonin	Feces	0.0056889	HC > CD; HC > UC
1-Methyladenosine	Feces	0.0056889	HC > CD; HC > UC
N-alpha-acetyl-L-lysine	Feces	0.010159	HC > CD; HC > UC
Suberic acid	Feces	0.0111	HC > CD; HC > UC
3-Methylglutaric acid	Feces	0.011196	HC > CD; HC > UC
Adipic acid	Feces	0.011196	HC > CD; HC > UC
3,5-Dihydroxybenzoic acid	Feces	0.015839	HC > CD; HC > UC
N-acetylglutamic acid	Feces	0.017343	HC > CD; HC > UC
2-Methylglutaric acid	Feces	0.021755	HC > CD; HC > UC
3HP3HP	Urine	0.055758	HC > CD; HC > UC

Glutamic acid	Feces	0.06438	HC > CD; HC > UC
N-Isovaleroylglycine	Feces	0.073789	HC > CD; HC > UC
4-Hydroxybenzoic acid	Feces	0.073789	HC > CD; HC > UC
D-Glucuronic acid	Feces	0.015834	CD > HC; CD > UC
Glycylproline	Feces	0.017343	CD > HC; CD > UC
Malic acid	Feces	0.021755	CD > HC; CD > UC
Adenosine 3',5'-cyclic monophosphate	Urine	0.063054	CD > HC; CD > UC
5-hydroxyindole sulphate	Urine	0.081918	CD > HC; CD > UC
Xanthurenic acid	Feces	0.088469	CD > HC; CD > UC
Glycoursodeoxycholic acid	Feces	0.073789	CD > HC; HC > UC
Guanine	Feces	0.088469	CD > UC; HC > UC
Riboflavin (vit B2)	Feces	0.088469	CD > UC; HC > UC
Na-acetyl-L-arginine	Urine	0.055758	CD > UC; HC > UC
Isobutyrylglycine	Urine	0.063054	CD > UC; HC > UC
2,5-Dihydroxybenzoic acid	Urine	0.063054	CD > UC; HC > UC
Hypoxanthine	Urine	0.089285	CD > UC; HC > UC
Xanthine	Urine	0.089285	CD > UC; HC > UC
Dehydroepiandrosterone Sulphate	Feces	0.024999	CD > HC; UC > HC
Suberic acid	Urine	0.04848	CD > HC; UC > HC
23-Norcholic acid	Urine	0.04848	CD > HC; UC > HC
Azelaic Acid	Urine	0.04848	CD > HC; UC > HC
Dopamine 3-O-sulphate	Urine	0.063054	CD > HC; UC > HC
Glutamine	Feces	0.085147	CD > HC; UC > HC
Hypoxanthine	Feces	0.085147	CD > HC; UC > HC
Tryptophan	Feces	0.088469	CD > HC; UC > HC
1,7-Dimethyluric acid	Feces	0.096193	HC > UC
3-Hydroxyhippuric acid	Urine	0.063054	HC > UC
Succinylaminoimidazole carboxamide riboside	Urine	0.063054	CD > HC

57

58

	A	B	C	D	E	F	G	H
1	cpdName	feature	rt	rt_minutes	mz	mzMin	mzMax	rtMin
2	RPOS-001	Xanthurenic acid	RPOS-001.1	167.88	2.798	206.04533	206.0422393	206.0484207
3	RPOS-002	Urocanic acid	RPOS-002.1	57.54	0.959	139.05075	139.0486642	139.0528358
4	RPOS-003	Uric acid	RPOS-003.1	67.5	1.125	169.03617	169.0336345	169.0387055
5	RPOS-004	Trigonelline	RPOS-004.1	37.26	0.621	138.0555	138.0534292	138.0575708
6	RPOS-005	Theobromine	RPOS-005.1	145.14	2.419	181.07255	181.0698339	181.0752661
7	RPOS-006	S-Adenosylhom	RPOS-006.1	84.24	1.404	385.12941	385.1236331	385.1351869
8	RPOS-007	Pyridoxine	RPOS-007.1	75.96	1.266	170.08172	170.0791688	170.0842712
9	RPOS-008	Pseudouridine	RPOS-008.1	56.94	0.949	245.07736	245.0736838	245.0810362
10	RPOS-009	L-prolyl-L-proli	RPOS-009.1	85.98	1.433	213.12392	213.1207231	213.1271169
11	RPOS-010	Propionylcarniti	RPOS-010.1	98.28	1.638	218.13923	218.1359579	218.1425021
12	RPOS-011	Proline betaine	RPOS-011.1	41.04	0.684	144.10245	144.1002885	144.1046115
13	RPOS-012	Prolylhydroxypr	RPOS-012.1	46.08	0.768	229.11883	229.1153932	229.1222668
14	RPOS-013	Pipecolic acid	RPOS-013.1	54.36	0.906	130.0868	130.0848487	130.0887513
15	RPOS-014	Phenylacetylglut	RPOS-014.1	217.14	3.619	265.11883	265.1148532	265.1228068
16	RPOS-015	Pantothenic acid	RPOS-015.1	141.06	2.351	220.1185	220.1151982	220.1218018
17	RPOS-016	L-Acetylcarnitin	RPOS-016.1	58.56	0.976	204.12358	204.1205181	204.1266419
18	RPOS-017	N6-Methyladenos	RPOS-017.1	123.6	2.06	282.12023	282.1159982	282.1244618
19	RPOS-018	1-Methyladenos	RPOS-018.1	75.3	1.255	282.12023	282.1159982	282.1244618
20	RPOS-019	Symmetric dim	RPOS-019.1	38.4	0.64	172.1086	172.1060184	172.1111816
21	RPOS-020	Niacinamide	RPOS-020.1	67.14	1.119	123.05584	123.0539942	123.0576858
22	RPOS-021	N6-Acetyl-L-lys	RPOS-021.1	55.08	0.918	189.12392	189.1210831	189.1267569
23	RPOS-022	Guanidinossuccin	RPOS-022.1	35.1	0.585	176.06713	176.064489	176.0697771
24	RPOS-023	N-Acetylasparag	RPOS-023.1	46.32	0.772	175.07188	175.0692539	175.0745061
25	RPOS-024	N-Acetylneuram	RPOS-024.1	36.6	0.61	310.11381	310.1091583	310.1184617
26	RPOS-025	N-a-Acetyl-L-ar	RPOS-025.1	54.96	0.916	217.13007	217.126813	217.133327
27	RPOS-026	N2,N2-Dimethyl	RPOS-026.1	143.22	2.387	312.13079	312.126108	312.135472
28	RPOS-027	2-Furoylglycine	RPOS-027.1	141.66	2.361	170.04533	170.0427793	170.0478807
29	RPOS-028	1,1-Dimethylbig	RPOS-028.1	40.2	0.67	130.10927	130.1073184	130.1112216
30	RPOS-029	Tryptophan	RPOS-029.1	165.06	2.751	188.07115	188.0683289	188.0739711
31	RPOS-030	Lysine	RPOS-030.1	28.08	0.468	147.11335	147.1111433	147.1155567
32	RPOS-031	Kynurenine	RPOS-031.1	121.02	2.017	209.09262	209.0894836	209.0957564
33	RPOS-032	Histidine	RPOS-032.1	31.62	0.527	156.0773	156.0749588	156.0796412
34	RPOS-033	Riboflavin (vit B	RPOS-033.1	231.36	3.856	377.14611	377.1404528	377.1517672
35	RPOS-036	Hypoxanthine	RPOS-036.1	72.66	1.211	137.04634	137.0442843	137.0483957
36	RPOS-037	Hippuric acid	RPOS-037.1	215.04	3.584	180.06607	180.063369	180.0687771
37	RPOS-038	Glycylproline	RPOS-038.1	52.56	0.876	173.09262	173.0900236	173.0952164
38	RPOS-039	Glutamine	RPOS-039.1	32.34	0.539	147.07697	147.0747638	147.0791762
39	RPOS-040	Aminoadipic acid	RPOS-040.1	37.68	0.628	162.07663	162.0741989	162.0790611
40	RPOS-041	Creatine	RPOS-041.1	36.48	0.608	132.0773	132.0753188	132.0792812
41	RPOS-042	Citric acid	RPOS-042.1	65.7	1.095	215.01677	215.0135447	215.0199953
42	RPOS-044	Caffeine	RPOS-044.1	208.92	3.482	195.0882	195.0852737	195.0911263
43	RPOS-045	Isobutyrylcarniti	RPOS-045.1	144.42	2.407	232.15488	232.1513977	232.1583623
44	RPOS-046	Atenolol	RPOS-046.1	147.6	2.46	267.17087	267.1668624	267.1748776
45	RPOS-047	Symmetric 1-Asy	RPOS-047.1	37.8	0.63	203.1502523	203.147205	203.1532996
46	RPOS-048	N-acetylglutami	RPOS-048.1	81.6	1.36	190.07155	190.0686989	190.0744011
47	RPOS-049	Acetaminophen	RPOS-049.1	116.88	1.948	328.10324	328.0983185	328.1081615
48	RPOS-050	Acetaminophen	RPOS-050.1	154.5	2.575	152.07115	152.0688689	152.0734311
49	RPOS-051	7-Methylguanin	RPOS-051.1	75.66	1.261	166.07288	166.0703889	166.0753711
50	RPOS-052	Pyroglutamic ac	RPOS-052.1	76.38	1.273	130.05042	130.0484692	130.0523708
51	RPOS-053	5'-Methylthioad	RPOS-053.1	165.3	2.755	298.0968365	298.0923651	298.101308
52	RPOS-054	5-Methylcytosin	RPOS-054.1	39.36	0.656	126.06674	126.064849	126.068631
53	RPOS-055	4-Pyridoxic acid	RPOS-055.1	103.26	1.721	184.06098	184.0582191	184.0637409
54	RPOS-056	Imidazoleacetic	RPOS-056.1	36.18	0.603	127.05075	127.0488442	127.0526558
55	RPOS-057	Kynurenic acid	RPOS-057.1	185.52	3.092	190.05042	190.0475692	190.0532708
56	RPOS-058	4-Guanidinobut	RPOS-058.1	52.44	0.874	146.09295	146.0907586	146.0951414
57	RPOS-059	1-Methylpiperid	RPOS-059.1	55.86	0.931	144.10245	144.1002885	144.1046115
58	RPOS-061	Paraxanthine	RPOS-061.1	166.26	2.771	181.07255	181.0698339	181.0752661
59	RPOS-062	1-Methyluric ac	RPOS-062.1	109.98	1.833	183.05182	183.0490742	183.0545658
60	RPOS-063	N4-Acetylcytidi	RPOS-063.1	130.8	2.18	286.10391	286.0996184	286.1082016
61	RPOS-064	Doxycycline	RPOS-064.1	331.8	5.53	445.16109	445.1544126	445.1677674
62	RPOS-065	Homocitrulline	RPOS-065.1	39	0.65	190.11917	190.1163182	190.1220218
63	RPOS-066	Neopterin	RPOS-066.1	55.8	0.93	254.08893	254.0851187	254.0927413
64	RPOS-067	Cortisone	RPOS-067.1	417.6	6.96	361.2015	361.196082	361.206918
65	RPOS-068	Disaccharides	RPOS-068.1	40.8	0.68	365.10598	365.1005034	365.1114566
66	RPOS-069	Indole-3-acetic a	RPOS-069.1	335.4	5.59	176.07115	176.0685089	176.0737911
67	RPOS-070	Tryptamine	RPOS-070.1	182.4	3.04	144.08132	144.0791588	144.0834812
68	RPOS-072	a-glycerophosph	RPOS-072.1	33.6	0.56	258.11065	258.1067783	258.1145217
69	RPOS-073	N-Acetylaspart	RPOS-073.1	87.6	1.46	305.09849	305.0939135	305.1030665
70	RPOS-074	Theophylline	RPOS-074.1	165.6	2.76	181.07255	181.0698339	181.0752661

	A	B	C	D	E	F	G	H
71	RPOS-075	18-Hydroxycort	RPOS-075.1	337.8	5.63	379.21206	379.2063718	379.2177482
72	RPOS-076	Betaine	RPOS-076.1	33.6	0.56	118.0868	118.0850287	118.0885713
73	RPOS-077	Quinolinic acid	RPOS-077.1	61.8	1.03	168.02968	168.0271596	168.0322004
74	RPOS-078	5-Hydroxyindol	RPOS-078.1	195.6	3.26	192.06607	192.063189	192.068951
75	RPOS-079	Adenosine 3',5'	RPOS-079.1	99	1.65	330.06035	330.0553991	330.0653009
76	RPOS-080	Carnitine	RPOS-080.1	32.4	0.54	162.11302	162.1105883	162.1154517
77	RPOS-081	N6,N6,N6-Trim	RPOS-081.1	27.6	0.46	189.1603	189.1574626	189.1631374
78	RPOS-082	Serotonin	RPOS-082.1	105.6	1.76	160.07624	160.0738389	160.0786411
79	RPOS-083	Argininosuccini	RPOS-083.1	31.8	0.53	291.13046	291.126093	291.134827
80	RPOS-084	3-Hydroxykynu	RPOS-084.1	81.6	1.36	225.08753	225.0841537	225.0909063
81	RPOS-085	5-Hydroxy-L-tr	RPOS-085.1	106.8	1.78	221.09262	221.0893036	221.0959364
82	RPOS-086	Imidazolelactic	RPOS-086.1	36.6	0.61	157.06132	157.0589641	157.0636759
83	RPOS-087	Tyrosine	RPOS-087.1	84	1.4	182.08172	182.0789888	182.0844512
84	RPOS-088	Tyramine	RPOS-088.1	87.6	1.46	121.06534	121.063524	121.067156
85	RPOS-089	Dopamine	RPOS-089.1	69	1.15	137.06025	137.0581941	137.0623059
86	RPOS-090	Butyrylcarnitine	RPOS-090.1	149.76	2.496	232.15488	232.1513977	232.1583623
87	RPOS-091	N-methyl-L-pro	RPOS-091.1	40.8	0.68	130.0868	130.0848487	130.0887513
88	RPOS-092	Saccharopine	RPOS-092.1	33.6	0.56	277.13996	277.1358029	277.1441171
89	RPOS-093	Thymine	RPOS-093.1	98.4	1.64	127.05075	127.0488442	127.0526558
90	RPOS-094	Guanine	RPOS-094.1	55.2	0.92	152.05723	152.0549491	152.0595109
91	RPOS-095	Adenosine	RPOS-095.1	96.6	1.61	268.10458	268.1005584	268.1086016
92	RPOS-096	3-Methylxanthir	RPOS-096.1	117.6	1.96	167.0569	167.0543941	167.0594059
93	RPOS-097	3-Methoxytyros	RPOS-097.1	106.2	1.77	212.09228	212.0890986	212.0954614
94	RPOS-098	7-Methylguan	RPOS-098.1	123	2.05	298.11514	298.1106683	298.1196117
95	RPOS-099	Quinaldic acid	RPOS-099.1	194.4	3.24	174.0555	174.0528892	174.0581108
96	RPOS-0100	Tiglylcarnitine	RPOS-0100.1	181.8	3.03	244.15488	244.1512177	244.1585423
97	RPOS-0101	Hexanoylcarniti	RPOS-0101.1	272.4	4.54	260.18618	260.1822772	260.1900828
98	RPOS-0102	Decanoylcarniti	RPOS-0102.1	484.2	8.07	316.24878	316.2440363	316.2535237
99	RPOS-0103	Lauroylcarnitine	RPOS-0103.1	565.2	9.42	344.28008	344.2749158	344.2852442
100	RPOS-0104	Tetradecanoylca	RPOS-0104.1	636.6	10.61	372.31138	372.3057953	372.3169647
101	RPOS-0105	Hexadecenoylca	RPOS-0105.1	643.2	10.72	398.32703	398.3210551	398.3330049
102	RPOS-0106	Palmitoylcarniti	RPOS-0106.1	648	10.8	400.34268	400.3366749	400.3486851
103	RPOS-0107	Stearoylcarnitine	RPOS-0107.1	652.8	10.88	428.37398	428.3675544	428.3804056
104	RPOS-0108	O-Sulfotyrosine	RPOS-0108.1	89.4	1.49	262.03853	262.0345994	262.0424606
105	RPOS-0109	Pyralline	RPOS-0109.1	148.8	2.48	237.12392	237.1203631	237.1274769
106	RPOS-0110	7-Methylxanthir	RPOS-0110.1	108.6	1.81	167.0569	167.0543941	167.0594059
107	RPOS-0111	Leucine	RPOS-0111.1	88.2	1.47	132.10245	132.1004685	132.1044315
108	RPOS-0112	Isoleucine	RPOS-0112.1	84	1.4	132.10245	132.1004685	132.1044315
109	RPOS-0113	AICA-riboside	RPOS-0113.1	78	1.3	259.10424	259.1003534	259.1081266
110	RPOS-0114	S-Adenosylmeth	RPOS-0114.1	34.8	0.58	399.14506	399.1390728	399.1510472
111	RPOS-0115	Succinylaminoir	RPOS-0115.1	99.6	1.66	375.1152	375.1095733	375.1208267
112	RPOS-0116	N1-methylinosi	RPOS-0116.1	120	2	151.06199	151.0597241	151.0642559
113	RPOS-0117	Succinyladenosi	RPOS-0117.1	138.6	2.31	384.11554	384.1097783	384.1213017
114	RPOS-0118	3-Hydroxyanthr	RPOS-0118.1	151.8	2.53	136.03985	136.0378094	136.0418906
115	RPOS-0119	N-Acetyltyrosin	RPOS-0119.1	178.2	2.97	224.09228	224.0889186	224.0956414
116	RPOS-0120	Tryptophan beta	RPOS-0120.1	192	3.2	188.07115	188.0683289	188.0739711
117	RPOS-0121	Leucylleucine	RPOS-0121.1	219.6	3.66	245.18652	245.1828422	245.1901978
118	RPOS-0122	Phenylalanyltry	RPOS-0122.1	282	4.7	352.16612	352.1608375	352.1714025
119	RPOS-0123	Leucylvaline	RPOS-0123.1	157.2	2.62	231.17087	231.1674024	231.1743376
120	RPOS-0124	N1,N12-Diacety	RPOS-0124.1	37.8	0.63	287.2447	287.2403913	287.2490087
121	RPOS-0125	N-Acetylisoputr	RPOS-0125.1	55.8	0.93	203.13957	203.1365229	203.1426171
122	RPOS-0126	N-Acetylisoputr	RPOS-0126.1	156	2.6	185.129	185.1262231	185.1317769
123	RPOS-0127	N-alpha-Acetyl	RPOS-0127.1	41.4	0.69	189.12392	189.1210831	189.1267569
124	RPOS-0128	N-Methylpyridi	RPOS-0128.1	36	0.6	94.06567	94.06425901	94.06708099
125	RPOS-0129	Quinine	RPOS-0129.1	227.4	3.79	325.1916	325.1867221	325.1964779
126	RPOS-0130	Imidazolepropic	RPOS-0130.1	48.6	0.81	141.0664	141.064284	141.068516
127	RPOS-0131	Phenylethylamin	RPOS-0131.1	142.8	2.38	105.07043	105.0688539	105.0720061
128	RPOS-0132	Cotinine	RPOS-0132.1	85.2	1.42	177.10279	177.1001335	177.1054465
129	RPOS-0133	Cotinine N-oxid	RPOS-0133.1	111	1.85	193.0977	193.0948035	193.1005965
130	RPOS-0134	Norcotinine	RPOS-0134.1	61.8	1.03	163.08714	163.0846937	163.0895863
131	RPOS-0135	Nicotine	RPOS-0135.1	72	1.2	163.12352	163.1210731	163.1259669
132	RPOS-0136	Nornicotine	RPOS-0136.1	56.4	0.94	149.10787	149.1056334	149.1101066
133	RNEG-001	1,3,7-Trimethyl	RNEG-001.1	176.94	2.949	209.06747	209.064334	209.070606
134	RNEG-002	1,7-Dimethyluri	RNEG-002.1	154.14	2.569	195.05182	195.0488942	195.0547458
135	RNEG-003	2,6-Dihydroxyb	RNEG-003.1	225.6	3.76	153.01878	153.0164847	153.0210753
136	RNEG-004	2-Hydroxy-2-m	RNEG-004.1	146.88	2.448	117.05517	117.0534142	117.0569258
137	RNEG-005	Salicyluric acid	RNEG-005.1	263.28	4.388	194.04533	194.0424193	194.0482407
138	RNEG-006	3,5-Dihydroxyb	RNEG-006.1	141	2.35	153.01878	153.0164847	153.0210753
139	RNEG-007	3-Methylglutaric	RNEG-007.1	159.72	2.662	145.05008	145.0479042	145.0522558
140	RNEG-008	Adipic acid	RNEG-008.1	155.46	2.591	145.05008	145.0479042	145.0522558

	A	B	C	D	E	F	G	H
141	RNEG-009	Azelaic Acid	RNEG-009.1	328.86	5.481	187.09703	187.0942235	187.0998365
142	RNEG-010	Cholic acid	RNEG-010.1	584.94	9.749	407.27975	407.2736408	407.2858592
143	RNEG-011	Indolelactic acid	RNEG-011.1	291.84	4.864	204.06607	204.063009	204.069131
144	RNEG-012	4-Hydroxyphenyl	RNEG-012.1	168.72	2.812	181.05008	181.0473642	181.0527958
145	RNEG-013	2,5-Dihydroxybenzoic	RNEG-013.1	189.66	3.161	153.01878	153.0164847	153.0210753
146	RNEG-014	Guanosine	RNEG-014.1	85.5	1.425	282.08384	282.0796087	282.0880713
147	RNEG-015	Histidine	RNEG-015.1	30.9	0.515	154.06165	154.0593391	154.0639609
148	RNEG-016	Hypoxanthine	RNEG-016.1	71.94	1.199	135.03069	135.0286645	135.0327155
149	RNEG-017	Ibuprofen Acyl	RNEG-017.1	517.38	8.623	381.15494	381.1492227	381.1606573
150	RNEG-018	Indoxyl sulfate	RNEG-018.1	203.7	3.395	212.00175	211.99857	212.00493
151	RNEG-019	Inosine	RNEG-019.1	96.66	1.611	267.07294	267.0689339	267.0769461
152	RNEG-020	Tyrosine	RNEG-020.1	82.5	1.375	180.06607	180.063369	180.068771
153	RNEG-021	Methylsuccinic acid	RNEG-021.1	131.16	2.186	131.03443	131.0324645	131.0363955
154	RNEG-022	N-Acetylglutamine	RNEG-022.1	58.68	0.978	187.07188	187.0690739	187.0746861
155	RNEG-023	Acetaminophen	RNEG-023.1	115.02	1.917	326.08759	326.0826987	326.0924813
156	RNEG-024	Pantothenic acid	RNEG-024.1	138.84	2.314	218.10285	218.0995785	218.1061215
157	RNEG-025	Acetaminophen	RNEG-025.1	135.6	2.26	230.01232	230.0088698	230.0157702
158	RNEG-026	p-Cresol sulfate	RNEG-026.1	252	4.2	187.0065	187.0036949	187.0093051
159	RNEG-027	Dehydroepiandrosterone	RNEG-027.1	475.2	7.92	367.15792	367.1524126	367.1634274
160	RNEG-028	Salicylic acid	RNEG-028.1	328.86	5.481	137.02387	137.0218146	137.0259254
161	RNEG-029	Succinic acid	RNEG-029.1	82.2	1.37	117.01878	117.0170247	117.0205353
162	RNEG-030	Theophylline	RNEG-030.1	165.36	2.756	179.0569	179.0542141	179.0595859
163	RNEG-031	1,2,3-Propanetriol	RNEG-031.1	82.8	1.38	175.02426	175.0216346	175.0268854
164	RNEG-032	Uric acid	RNEG-032.1	67.08	1.118	167.02051	167.0180047	167.0230153
165	RNEG-033	Uridine	RNEG-033.1	82.92	1.382	243.06171	243.0580641	243.0653559
166	RNEG-034	D-Gluconic acid	RNEG-034.1	34.8	0.58	195.05048	195.0475542	195.0534058
167	RNEG-035	D-Glucuronic acid	RNEG-035.1	32.4	0.54	193.03483	193.0319345	193.0377255
168	RNEG-036	Aspartic acid	RNEG-036.1	31.8	0.53	132.02968	132.0276996	132.0316604
169	RNEG-037	3-(3-hydroxyphenyl)propanoic acid	RNEG-037.1	174	2.9	181.05008	181.0473642	181.0527958
170	RNEG-038	3,7-Dimethyluracil	RNEG-038.1	116.4	1.94	195.05182	195.0488942	195.0547458
171	RNEG-039	Malic acid	RNEG-039.1	45.12	0.752	133.0137	133.0117048	133.0156952
172	RNEG-040	Glutamic acid	RNEG-040.1	32.4	0.54	146.04533	146.0431393	146.0475207
173	RNEG-041	3-Hydroxyhippuric acid	RNEG-041.1	164	2.733	194.04533	194.0424193	194.0482407
174	RNEG-042	N-acetylglutamine	RNEG-042.1	80.76	1.346	188.0559	188.0530792	188.0587208
175	RNEG-043	Phenylalanine	RNEG-043.1	123	2.05	164.07115	164.0686889	164.0736111
176	RNEG-044	Glutaric acid	RNEG-044.1	111.6	1.86	131.03443	131.0324645	131.0363955
177	RNEG-045	N-Acetylneuraminic acid	RNEG-045.1	37.2	0.62	308.09816	308.0935385	308.1027815
178	RNEG-046	Taurine	RNEG-046.1	31.8	0.53	124.00684	124.0049799	124.0087001
179	RNEG-047	Quinic acid	RNEG-047.1	39	0.65	191.0561135	191.0532477	191.0589794
180	RNEG-048	Xanthine	RNEG-048.1	78.6	1.31	151.0256	151.0233346	151.0278654
181	RNEG-049	4-Hydroxyhippuric acid	RNEG-049.1	147	2.45	194.04533	194.0424193	194.0482407
182	RNEG-050	Tartric acid	RNEG-050.1	37.2	0.62	149.00861	149.0063749	149.0108451
183	RNEG-051	Pyroglutamic acid	RNEG-051.1	75	1.25	128.03477	128.0328495	128.0366905
184	RNEG-052	Xanthosine	RNEG-052.1	109.8	1.83	283.06786	283.063614	283.072106
185	RNEG-054	N-Acetylaspargine	RNEG-054.1	60	1	174.04025	174.0376394	174.0428606
186	RNEG-055	Adenosine 3',5'-bisphosphate	RNEG-055.1	97.2	1.62	328.0447	328.0397793	328.0496207
187	RNEG-056	N-acetyl-L-carnitine	RNEG-056.1	55.2	0.92	267.10933	267.1053234	267.1133366
188	RNEG-057	Riboflavin	RNEG-057.1	229.2	3.82	375.13046	375.124833	375.136087
189	RNEG-058	D-Glucaric acid	RNEG-058.1	34.2	0.57	209.02974	209.0266046	209.0328754
190	RNEG-059	Pimelic acid	RNEG-059.1	207.6	3.46	159.06573	159.063344	159.068116
191	RNEG-060	Suberic acid	RNEG-060.1	267.6	4.46	173.08138	173.0787838	173.0839762
192	RNEG-061	Sucrose	RNEG-061.1	40.8	0.68	341.10839	341.1032734	341.1135066
193	RNEG-062	p-Hydroxymandelic acid	RNEG-062.1	94.2	1.57	167.03443	167.0319245	167.0369355
194	RNEG-063	Homovanillic acid	RNEG-063.1	228	3.8	181.05008	181.0473642	181.0527958
195	RNEG-064	Vanillylmandelic acid	RNEG-064.1	118.2	1.97	197.045	197.0420443	197.0479557
196	RNEG-065	Phenylactic acid	RNEG-065.1	270.6	4.51	165.05517	165.0526942	165.0576458
197	RNEG-066	2-Hydroxyisobutyric acid	RNEG-066.1	97.2	1.62	103.03952	103.0379744	103.0410656
198	RNEG-067	Sorbitol	RNEG-067.1	34.2	0.57	181.07121	181.0684939	181.0739261
199	RNEG-068	Indoxyl glucuronide	RNEG-068.1	203.4	3.39	308.07703	308.0724088	308.0816512
200	RNEG-069	Na-acetyl-L-arginine	RNEG-069.1	54.6	0.91	215.11442	215.1111933	215.1176467
201	RNEG-070	Citric acid	RNEG-070.1	67.5	1.125	191.01918	191.0163147	191.0220453
202	RNEG-071	Isocitric acid	RNEG-071.1	46.2	0.77	191.01918	191.0163147	191.0220453
203	RNEG-072	Pregnanediol-3-one	RNEG-072.1	553.8	9.23	495.29579	495.2883606	495.3032194
204	RNEG-073	Gallic acid	RNEG-073.1	103.32	1.722	169.0137	169.0111648	169.0162352
205	RNEG-074	Phenylacetylglutamine	RNEG-074.1	240.6	4.01	192.06607	192.063189	192.068951
206	RNEG-075	4-Hydroxyphenyl	RNEG-075.1	204.6	3.41	151.03952	151.0372544	151.0417856
207	RNEG-076	2-Hydroxyphenyl	RNEG-076.1	246.6	4.11	151.03952	151.0372544	151.0417856
208	RNEG-077	3-Hydroxyphenyl	RNEG-077.1	224.4	3.74	219.02694	219.0236546	219.0302254
209	RNEG-078	4-Hydroxybenzoic acid	RNEG-078.1	189.6	3.16	137.02387	137.0218146	137.0259254
210	RNEG-079	Citraconic acid	RNEG-079.1	103.8	1.73	129.01878	129.0168447	129.0207153

	A	B	C	D	E	F	G	H
211	RNEG-080	Cis-aconitic acid	RNEG-080.1	78	1.3	173.00861	173.0060149	173.0112051
212	RNEG-082	4-Hydroxycinnamic acid	RNEG-082.1	261	4.35	163.03952	163.0370744	163.0419656
213	RNEG-083	m-Coumaric acid	RNEG-083.1	293	4.883	163.03952	163.0370744	163.0419656
214	RNEG-084	Succinylamino acid	RNEG-084.1	99	1.65	373.09955	373.0939535	373.1051465
215	RNEG-085	Isobutyrylglycine	RNEG-085.1	124.2	2.07	144.06607	144.063909	144.068231
216	RNEG-086	Succinyladenosine	RNEG-086.1	138.6	2.31	382.09989	382.0941585	382.1056215
217	RNEG-087	5-hydroxyindole	RNEG-087.1	168.6	2.81	212.00175	211.99857	212.00493
218	RNEG-088	Tiglylglycine	RNEG-088.1	175.2	2.92	156.06607	156.063729	156.068411
219	RNEG-089	N-Acetyltyrosine	RNEG-089.1	178.2	2.97	222.07663	222.0732989	222.0799611
220	RNEG-090	N-Acetyliso-leucine	RNEG-090.1	241.8	4.03	172.09737	172.0947885	172.0999515
221	RNEG-091	N-Acetyltryptophan	RNEG-091.1	297.6	4.96	245.09262	245.0889436	245.0962964
222	RNEG-092	Ketoleucine	RNEG-092.1	211.2	3.52	129.05517	129.0532342	129.0571058
223	RNEG-093	3-Methyl-2-oxo-4-pyridinecarboxylic acid	RNEG-093.1	193.2	3.22	129.05517	129.0532342	129.0571058
224	RNEG-094	3-Hydroxy-3-methyl-2-oxo-4-pyridinecarboxylic acid	RNEG-094.1	93	1.55	161.045	161.0425843	161.0474157
225	RNEG-095	Dopamine 4-O-sulfate	RNEG-095.1	89.4	1.49	232.02797	232.0244896	232.0314504
226	RNEG-096	Dopamine 3-O-sulfate	RNEG-096.1	93.6	1.56	232.02797	232.0244896	232.0314504
227	RNEG-097	Ribonic acid	RNEG-097.1	36	0.6	165.03991	165.0374344	165.0423856
228	RNEG-098	L-Ascorbic acid	RNEG-098.1	42.6	0.71	254.98108	254.9772553	254.9849047
229	RNEG-099	Orotic acid	RNEG-099.1	48.6	0.81	155.00928	155.0069549	155.0116051
230	RNEG-100	Acesulfame	RNEG-100.1	114	1.9	161.9861	161.9836702	161.9885298
231	RNEG-101	Sumiki's acid	RNEG-101.1	126	2.1	141.01878	141.0166647	141.0208953
232	RNEG-102	Saccharin	RNEG-102.1	162	2.7	181.99119	181.9884601	181.9939199
233	RNEG-103	Phenol sulfate	RNEG-103.1	180.6	3.01	172.99085	172.9882551	172.9934449
234	RNEG-104	N-Isovaleroylglycine	RNEG-104.1	184.2	3.07	158.08172	158.0793488	158.0840912
235	RNEG-105	N-Acetylphenylalanine	RNEG-105.1	279.6	4.66	206.08172	206.0786288	206.0848112
236	RNEG-106	4-Ethylphenylsulfate	RNEG-106.1	343.8	5.73	201.02215	201.0191347	201.0251653
237	RNEG-107	Thymol Sulfate	RNEG-107.1	442.2	7.37	229.05346	229.0500242	229.0568958
238	RNEG-108	Dehydroisoandrosterone	RNEG-108.1	445.8	7.43	463.23319	463.2262415	463.2401385
239	RNEG-109	Pregnenolone sulfate	RNEG-109.1	588.6	9.81	396.19705	396.191107	396.202993
240	RNEG-110	2-Methylglutaryl-CoA	RNEG-110.1	168	2.8	145.05008	145.0479042	145.0522558
241	RNEG-111	3-Methoxytyrosine	RNEG-111.1	106.2	1.77	210.07663	210.0734789	210.0797811
242	RNEG-112	7-Methylguanosine	RNEG-112.1	123	2.05	296.09949	296.0950485	296.1039315
243	RNEG-113	3-Carboxy-4-methylphenylsulfate	RNEG-113.1	486	8.1	239.09195	239.0883636	239.0955364
244	RNEG-114	Pyrraline	RNEG-114.1	124.5	2.49	253.11883	253.1150332	253.1226268
245	RNEG-115	O-Sulfotyrosine	RNEG-115.1	90	1.5	260.02288	260.0189797	260.0267803
246	RNEG-116	Glycodeoxycholic acid	RNEG-116.1	606.6	10.11	448.3063	448.2995754	448.3130246
247	RNEG-117	23-Norcholic acid	RNEG-117.1	514.8	8.58	393.2641	393.258201	393.269999
248	RNEG-118	7-Ketodeoxycholic acid	RNEG-118.1	519	8.65	405.2641	405.258021	405.270179
249	RNEG-119	Deoxycholic acid	RNEG-119.1	654	10.9	391.28483	391.2789607	391.2906993
250	RNEG-120	Glycoursodeoxycholic acid	RNEG-120.1	447.6	7.46	528.26311	528.2551861	528.2710339
251	RNEG-121	Glycodeoxycholic acid	RNEG-121.1	536.4	8.94	528.26311	528.2551861	528.2710339
252	RNEG-122	Glycochenodeoxycholic acid	RNEG-122.1	525.6	8.76	528.26311	528.2551861	528.2710339
253	RNEG-123	Taurolithocholic acid	RNEG-123.1	535.8	8.93	280.6215	280.6172907	280.6257093
254	RNEG-124	Glycolithocholic acid	RNEG-124.1	609	10.15	512.2682	512.260516	512.275884
255	RNEG-125	Glycoursodeoxycholic acid	RNEG-125.1	504	8.4	448.3063	448.2995754	448.3130246
256	RNEG-126	Glycocholic acid	RNEG-126.1	504	8.4	464.30121	464.2942455	464.3081745
257	RNEG-127	3-hydroxyisobutyrate	RNEG-127.1	95.4	1.59	103.03952	103.0379744	103.0410656
258	RNEG-128	2-hydroxy-3-methylglutaryl-CoA	RNEG-128.1	164.4	2.74	117.05517	117.0534142	117.0569258
259	RNEG-129	3-hydroxyisovaleryl-CoA	RNEG-129.1	126	2.1	117.05517	117.0534142	117.0569258

	I	J	K	L	M	N	O	P
1	rtMax	Monoisotopic	chemicalFormula	KEGGID	chemspiderID	PubChemID	ChEBIID	InChI
2	152.88	182.88	205.0375077	C02470	5497	5699	10072	InChI=1S/C10H
3	42.54	72.54	138.0429274	C00785	643824	1178	30817	InChI=1S/C6H6
4	52.5	82.5	168.02834	C00366	1142	1175	17775	InChI=1S/C5H4
5	22.26	52.26	137.0476785	C01004	5369	5570	18123	InChI=1S/C7H7
6	130.14	160.14	180.0647255	C07480	5236	5429	28946	InChI=1S/C7H8
7	69.24	99.24	384.1215885	C00021	388301	439155	16680	InChI=1S/C14F
8	60.96	90.96	169.0738932	C00314	1025	1054	16709	InChI=1S/C8H1
9	41.94	71.94	244.0695361	C02067	14319	15047	17802	InChI=1S/C9H1
10	70.98	100.98	212.1160924	NA	9797341	11622593	73646	InChI=1S/C10F
11	83.28	113.28	217.1314081	C03017	96904	107738	53210	InChI=1S/C10H
12	26.04	56.04	143.0946287	C10172	103115	115244	35280	InChI=1S/C7H1
13	31.08	61.08	228.1111007	NA	10077215	11902893	74767	InChI=1S/C10H
14	39.36	69.36	129.0789786	C00408	826	849	17964	InChI=1S/C6H1
15	202.14	232.14	264.1111007	C04148	83292	92258	17884	InChI=1S/C13F
16	126.06	156.06	219.1106727	C00864	963	6613	46905	InChI=1S/C9H1
17	43.56	73.56	203.115758	C02571	5406074	7045767	57589	InChI=1S/C9H1
18	108.6	138.6	281.112404	NA	92307	102175	21891	InChI=1S/C11H
19	60.3	90.3	281.112404	C02494	23256663	27476	16020	InChI=1S/C11H
20	23.4	53.4	202.14298	NA	147942	169148	25682	InChI=1S/C8H1
21	52.14	82.14	122.0480128	C00153	911	936	17154	InChI=1S/C6H6
22	40.08	70.08	188.1160924	C02727	83801	92832	17752	InChI=1S/C8H1
23	20.1	50.1	175.0593058	C03139	388951	439918	17072	InChI=1S/C5H9
24	31.32	61.32	174.0640568	NA	90090	99715	139582	InChI=1S/C6H1
25	21.6	51.6	309.1059812	C00270	388337	439197	17012	InChI=1S/C11H
26	39.96	69.96	216.1222404	NA	92866	67427	40521	InChI=1S/C8H1
27	128.22	158.22	311.1229687	NA	83878	92919	19289	InChI=1S/C12H
28	126.66	156.66	169.0375077	NA	20549	21863	82912	InChI=1S/C7H7
29	25.2	55.2	129.1014454	C07151	3949	4091	6801	InChI=1S/C4H1
30	150.06	180.06	204.0898776	C00078	6066	6305	16828	InChI=1S/C11H
31	13.08	43.08	146.1055277	C00047	5747	5962	18019	InChI=1S/C6H1
32	106.02	136.02	208.0847923	C00328	141580	161166	16946	InChI=1S/C10H
33	16.62	46.62	155.0694765	C00135	6038	6274	15971	InChI=1S/C6H9
34	216.36	246.36	376.1382844	C00255	431981	493570	17015	InChI=1S/C17H
35	57.66	87.66	136.0385108	C00262	361584	790	17368	InChI=1S/C5H4
36	200.04	230.04	179.0582432	C01586	451	464	18089	InChI=1S/C9H9
37	37.56	67.56	172.0847923	NA	2282246	79101	70744	InChI=1S/C7H1
38	17.34	47.34	146.0691422	C00064	718	5961	18050	InChI=1S/C5H1
39	22.68	52.68	161.0688078	C00956	456	469	37024	InChI=1S/C6H1
40	21.48	51.48	131.0694765	C00300	566	586	16919	InChI=1S/C4H9
41	50.7	80.7	192.0270026	C00158	305	311	30769	InChI=1S/C6H8
42	193.92	223.92	194.0803756	C07481	2424	2519	27732	InChI=1S/C8H1
43	129.42	159.42	231.1470582	C02301	147286	168379	84838	InChI=1S/C11H
44	132.6	162.6	266.1630426	NA	2162	2249	2904	InChI=1S/C14F
45	22.8	52.8	202.1429758	NA C03626	147942 110375	169148 12383	25682 17929	InChI=1S/C8H1
46	66.6	96.6	189.0637225	C00624	64077	70914	17533	InChI=1S/C7H1
47	101.88	131.88	327.0954165	NA	75744	83944	32636	InChI=1S/C14F
48	139.5	169.5	151.0633285	C06804	1906	1983	46195	InChI=1S/C8H9
49	60.66	90.66	165.0650599	C02242	10883	11361	28664	InChI=1S/C6H7
50	61.38	91.38	129.0425931	C01879	485	7405	18183	InChI=1S/C5H7
51	150.3	180.3	297.0895601	C00170	16739738	149	17509	InChI=1S/C11H
52	24.36	54.36	125.0589119	C02376	58551	65040	27551	InChI=1S/C5H7
53	88.26	118.26	183.0531578	C00847	6467	6723	17405	InChI=1S/C8H9
54	21.18	51.18	126.0429274	C02835	86856	96215	16974	InChI=1S/C5H6
55	170.52	200.52	189.0425931	C01717	3712	3845	18344	InChI=1S/C10H
56	37.44	67.44	145.0851266	C01035	486	500	15728	InChI=1S/C5H1
57	40.86	70.86	143.0946287	NA	368258	415939	NA	InChI=1S/C7H1
58	151.26	181.26	180.0647255	C13747	4525	4687	25858	InChI=1S/C7H8
59	94.98	124.98	182.04399	C16359	62926	69726	68441	InChI=1S/C6H6
60	115.8	145.8	285.0960852	NA	96702	107461	70989	InChI=1S/C11H
61	316.8	346.8	444.1532657	C06973	10469369	54671203	50845	InChI=1S/C22H
62	24	54	189.1113414	C02427	58582	65072	17443	InChI=1S/C7H1
63	40.8	70.8	253.0811039	C05926	NA	135398721	NA	InChI=1S/C9H1
64	402.6	432.6	360.193674	C00762	193441	222786	16962	InChI=1S/C21H
65	25.8	55.8	342.1162115	C00089	5768	5988	17992	InChI=1S/C12H
66	320.4	350.4	175.0633285	C00954	780	802	16411	InChI=1S/C10H
67	167.4	197.4	160.1000484	C00398	1118	1150	16765	InChI=1S/C10H
68	18.6	48.6	257.102824	C00670	10760	657272	135063	InChI=1S/C8H2
69	72.6	102.6	304.0906655	C12270	164080	5255	73688	InChI=1S/C11H
70	150.6	180.6	180.0647255	C07130	2068	2153	28177	InChI=1S/C7H8

	I	J	K	L	M	N	O	P
71	322.8	352.8	378.2042387	NA	24840620	44263343	89455	InChI=1S/C21H
72	18.6	48.6	117.0789786	C00719	242	248	17750	InChI=1S/C5H1
73	46.8	76.8	167.0218577	C03722	1037	1066	16675	InChI=1S/C7H5
74	180.6	210.6	191.0582432	C05635	1760	1826	27823	InChI=1S/C10H
75	84	114	329.0525198	C00575	5851	6076	17489	InChI=1S/C10H
76	17.4	47.4	161.1051933	C00318	10455	10917	16347	InChI=1S/C7H1
77	12.6	42.6	188.1524779	C03793	389120	440120	165870	InChI=1S/C9H2
78	90.6	120.6	176.094963	C00780	5013	5202	28790	InChI=1S/C10H
79	16.8	46.8	290.1226343	C03406	16059	16950	184023	InChI=1S/C10H
80	66.6	96.6	224.0797069	C03227	87	89	17380	InChI=1S/C10H
81	91.8	121.8	220.0847923	C00643	388413	439280	17780	InChI=1S/C11H
82	21.6	51.6	156.0534921	NA	404046	459122	70808	InChI=1S/C6H8
83	69	99	181.0738932	C00082	5833	6057	17895	InChI=1S/C9H1
84	72.6	102.6	137.084064	C00483	5408	3766	15760	InChI=1S/C8H1
85	54	84	153.0789786	C03758	661	681	18243	InChI=1S/C8H1
86	134.76	164.76	231.1470582	C02862	388877	213144	21949	InChI=1S/C11H
87	25.8	55.8	129.0789786	NA	558617	643474	90344	InChI=1S/C6H1
88	18.6	48.6	276.1321364	C00449	141086	160556	16927	InChI=1S/C11H
89	83.4	113.4	126.0429274	C00178	1103	1135	17821	InChI=1S/C5H6
90	40.2	70.2	151.04941	C00242	744	764	16235	InChI=1S/C5H5
91	81.6	111.6	267.09675	C00212	54923	60961	16335	InChI=1S/C10H
92	102.6	132.6	166.04908	C16357	63805	70639	62207	InChI=1S/C6H6
93	91.2	121.2	211.08446	NA	1607	1670	172453	InChI=1S/C10H
94	108	138	298.11514	NA	393054	135445750	20794	InChI=1S/C11H
95	179.4	209.4	173.04768	C06325	6857	7124	18386	InChI=1S/C10H
96	166.8	196.8	243.14706	C02301	34999729	91825636	85520	InChI=1S/C12H
97	257.4	287.4	259.17836	C02301	2497478	3246938	84834	InChI=1S/C13H
98	469.2	499.2	315.24096	C02301	8420677	11953821	68830	InChI=1S/C17H
99	550.2	580.2	343.27226	C02301	147288	168381	77086	InChI=1S/C19H
100	621.6	651.6	371.30356	C02301	30776567	53477791	84634	InChI=1S/C21H
101	628.2	658.2	397.31921	C02301	NA	NA	75659	NA
102	633	663	399.33486	C02990	10128117	11953816	17490	InChI=1S/C23H
103	637.8	667.8	427.36616	C02301	113603366	52922056	84644	InChI=1S/C25H
104	74.4	104.4	261.03071	NA	448617	514186	46215	InChI=1S/C9H1
105	133.8	163.8	254.12666	NA	19980286	14274616	NA	InChI=1S/C12H
106	93.6	123.6	166.04908	C16353	61660	68374	48991	InChI=1S/C6H6
107	73.2	103.2	131.09463	C00123	5880	6106	15603	InChI=1S/C6H1
108	69	99	131.09463	C00407	6067	6306	17191	InChI=1S/C6H1
109	63	93	258.09642	NA	16560	17513	28498	InChI=1S/C9H1
110	19.8	49.8	399.14506	C00019	1049	34756	15414	InChI=1S/C15H
111	84.6	114.6	374.10738	NA	4159901	54478644	NA	InChI=1S/C13H
112	105	135	282.09642	NA	58605	65095	19065	InChI=1S/C11H
113	123.6	153.6	383.10771	NA	17216022	20849086	71169	InChI=1S/C14H
114	136.8	166.8	153.04259	C00632	84	86	15793	InChI=1S/C7H7
115	163.2	193.2	223.08446	NA	61606	68310	21563	InChI=1S/C11H
116	177	207	246.13683	C09213	390633	442106	5832	InChI=1S/C14H
117	204.6	234.6	244.17869	C11332	69263	94244	73531	InChI=1S/C12H
118	267	297	351.15829	NA	118886	134906	74751	InChI=1S/C20H
119	142.2	172.2	230.16304	NA	312585	352038	NA	InChI=1S/C11H
120	22.8	52.8	286.23688	C03413	117134	132680	28101	InChI=1S/C14H
121	40.8	70.8	202.13174	NA	74849628	131802901	NA	InChI=1S/C9H1
122	141	171	184.12118	NA	114601	129397	133185	InChI=1S/C9H1
123	26.4	56.4	188.11609	C12989	167134	92907	35704	InChI=1S/C8H1
124	21	51	94.06567	C02724	13008	13597	15761	InChI=1S/C6H8
125	212.4	242.4	324.18378	C06526	84989	3034034	15854	InChI=1S/C20H
126	33.6	63.6	140.05858	C20522	63798	70630	73087	InChI=1S/C6H8
127	127.8	157.8	121.08915	C05332	13856352	1001	18397	InChI=1S/C8H1
128	70.2	100.2	176.09496	NA	395	408	182609	InChI=1S/C10H
129	96	126	192.08988	NA	7991264	9815514	89087	InChI=1S/C10H
130	46.8	76.8	162.07931	NA	400	413	89406	InChI=1S/C9H1
131	57	87	162.1157	C00745	80863	89594	17688	InChI=1S/C10H
132	41.4	71.4	148.10005	C06524	82588	412	NA	InChI=1S/C9H1
133	161.94	191.94	210.0752902	C16361	71754	79437	691622	InChI=1S/C8H1
134	139.14	169.14	196.0596401	C16356	82720	91611	68449	InChI=1S/C7H8
135	210.6	240.6	154.0266087	C21298	8974	9338	68465	InChI=1S/C7H6
136	131.88	161.88	118.0629942	NA	86129	95433	68454	InChI=1S/C5H1
137	248.28	278.28	195.0531578	C07588	9835	10253	9008	InChI=1S/C9H9
138	126	156	154.0266087	NA	7146	7424	39912	InChI=1S/C7H6
139	144.72	174.72	146.0579088	NA	11781	12284	68566	InChI=1S/C6H1
140	140.46	170.46	146.0579088	C06104	191	196	30832	InChI=1S/C6H1

	I	J	K	L	M	N	O	P
141	313.86	343.86	188.104859	C08261	2179	2266	48131	InChI=1S/C9H1
142	569.94	599.94	408.2875744	C00695 C1764	4573890 10908	221493 12234	16359 81240	InChI=1S/C24H
143	276.84	306.84	205.0738932	C02043	83867	92904	NA	InChI=1S/C11H
144	153.72	183.72	182.0579088	C03672	10807549	9378	17385	InChI=1S/C9H1
145	174.66	204.66	154.0266087	C00628	3350	3469	17189	InChI=1S/C7H6
146	70.5	100.5	283.0916686	C00387	6544	135398635	16750	InChI=1S/C10H
147	15.9	45.9	155.0694765	C00135	6038	6274	15971	InChI=1S/C6H9
148	56.94	86.94	136.0385108	C00262	768	135398638	17368	InChI=1S/C5H4
149	502.38	532.38	382.1627678	NA	143793	163959	NA	InChI=1S/C19H
150	188.7	218.7	213.0095784	NA	9840	10258	43355	InChI=1S/C8H7
151	81.66	111.66	268.0807695	C00294	5799	135398641	17596	InChI=1S/C10H
152	67.5	97.5	181.0738932	C00082	5833	6057	17895	InChI=1S/C9H1
153	116.16	146.16	132.0422587	NA	9922	10349	91316	InChI=1S/C5H8
154	43.68	73.68	188.0797069	NA	19076037	182230	21553	InChI=1S/C7H1
155	100.02	130.02	327.0954165	NA	75744	83944	32636	InChI=1S/C14H
156	123.84	153.84	219.1106727	C00864	963	6613	46905	InChI=1S/C9H1
157	120.6	150.6	231.0201431	NA	75741	83939	32635	InChI=1S/C8H9
158	237	267	188.0143294	NA	3806481	4615423	82914	InChI=1S/C7H8
159	460.2	490.2	368.1657447	C04555	12074	12594	16814	InChI=1S/C19H
160	313.86	343.86	138.0316941	C00805	331	338	16914	InChI=1S/C7H6
161	67.2	97.2	118.0266087	C00042	140973	1110	15741	InChI=1S/C4H6
162	150.36	180.36	180.0647255	C07130	2068	2153	28177	InChI=1S/C7H8
163	67.8	97.8	176.032088	C19806	14220	14925	45969	InChI=1S/C6H8
164	52.08	82.08	168.02834	C00366	1142	1175	17775	InChI=1S/C5H4
165	67.92	97.92	244.0695361	C00299	5807	6029	16704	InChI=1S/C9H1
166	19.8	49.8	196.0583027	C00257	10240	10690	33198	InChI=1S/C6H1
167	17.4	47.4	194.0426527	C00191	392615	444791	42717	InChI=1S/C6H1
168	16.8	46.8	133.0375077	C00049	5745	5960	17053	InChI=1S/C4H7
169	159	189	182.05791	NA	93013	102959	86369	InChI=1S/C9H1
170	101.4	131.4	196.0596401	C16360	74994	83126	68531	InChI=1S/C7H8
171	30.12	60.12	134.0215233	C03668	193317	222656	30797	InChI=1S/C4H6
172	17.4	47.4	147.0531578	C00217	21814	23327	15966	InChI=1S/C5H9
173	149	179	195.0531578	NA	396603	450268	70824	InChI=1S/C9H9
174	65.76	95.76	189.0637225	C00624	64077	70914	17533	InChI=1S/C7H1
175	108	138	165.0789786	C00079	5910	6140	17295	InChI=1S/C9H1
176	96.6	126.6	132.0422587	C00489	723	743	17859	InChI=1S/C5H8
177	22.2	52.2	309.10598	C19910	392810	445063	45744	InChI=1S/C11H
178	16.8	46.8	125.0146641	C00245	1091	1123	15891	InChI=1S/C2H7
179	24	54	192.06339	C00296	10246715	6508	17521	InChI=1S/C7H1
180	63.6	93.6	152.03343	C00385	1151	1188	17712	InChI=1S/C5H4
181	132	162	195.0531578	NA	133104	151012	71018	InChI=1S/C9H9
182	22.2	52.2	150.0164379	C0089	392277	444305	15671	InChI=1S/C4H6
183	60	90	129.0425931	C01879	7127	7405	18183	InChI=1S/C5H7
184	94.8	124.8	284.07568	C01762	58484	64959	18107	InChI=1S/C10H
185	45	75	175.0480724	C0104	58576	65065	21547	InChI=1S/C6H9
186	82.2	112.2	329.05252	C00575	5851	6076	17489	InChI=1S/C10H
187	40.2	70.2	268.117155	NA	8396518	10221026	172509	InChI=1S/C11H
188	214.2	244.2	376.1382844	C00255	431981	493570	17015	InChI=1S/C17H
189	19.2	49.2	210.0375673	C0081 C00879	30577 2301286	33037 303758	16002 30852	InChI=1S/C6H1
190	192.6	222.6	160.07356	C02656	376	385	30531	InChI=1S/C7H1
191	252.6	282.6	174.08921	C08278	10025	10457	9300	InChI=1S/C8H1
192	25.8	55.8	342.1162115	C00089	5768	5988	17992	InChI=1S/C12H
193	79.2	109.2	168.0422587	C11527	321	328	16388	InChI=1S/C8H8
194	213	243	182.0579088	C05582	1675	1738	545959	InChI=1S/C9H1
195	103.2	133.2	198.0528234	C05584	1207	1245	NA	InChI=1S/C9H1
196	255.6	285.6	166.0629942	C00994	3715	3848	25998	InChI=1S/C9H1
197	82.2	112.2	104.0473441	NA	11181	11671	50129	InChI=1S/C4H8
198	19.2	49.2	182.0790382	C00794 C00392 C01697	5780 6251 11	17924 16899		InChI=1S/C6H1
199	188.4	218.4	309.0848518	NA	2015556	2733785	145223	InChI=1S/C14H
200	39.6	69.6	216.1222404	NA	60752	67427	40521	InChI=1S/C8H1
201	52.5	82.5	192.0270026	C00158	305	311	30769	InChI=1S/C6H8
202	31.2	61.2	192.0270026	C00311	1161	1198	30887	InChI=1S/C6H8
203	538.8	568.8	496.3036184	NA	110346	123796	88765	InChI=1S/C27H
204	88.32	118.32	170.0215233	C01424	361	370	30778	InChI=1S/C7H6
205	225.6	255.6	193.0738932	C05598	61452	68144	27480	InChI=1S/C10H
206	189.6	219.6	152.0473441	C00642	124	127	18101	InChI=1S/C8H8
207	231.6	261.6	152.0473441	C05852	11476	11970	28478	InChI=1S/C8H8
208	209.4	239.4	152.0473441	C05593	11624	12122	17445	InChI=1S/C8H8
209	174.6	204.6	138.0316941	C00156	132	135	30763	InChI=1S/C7H6
210	88.8	118.8	130.0266087	C02226	553689	643798	17626	InChI=1S/C5H6

	I	J	K	L	M	N	O	P
211	63	93	174.0164379	C00417	558863	643757	32805	InChI=1S/C6H6
212	246	276	164.0473441	C00811	553148	637542	32374	InChI=1S/C9H8
213	278	308	164.0473441	C12621	553147	637541	32357	InChI=1S/C9H8
214	84	114	374.10738	NA	4159901	54478644	NA	InChI=1S/C13H
215	109.2	139.2	145.07389	NA	9030891	10855600	70979	InChI=1S/C6H1
216	123.6	153.6	383.10771	NA	17216022	20849086	71169	InChI=1S/C14H
217	153.6	183.6	213.00958	NA	NA	152531758	NA	InChI=1S/C8H7
218	160.2	190.2	157.07389	NA	4945715	6441567	73018	InChI=1S/C7H1
219	163.2	193.2	223.08446	C01657	61606	68310	21563	InChI=1S/C11H
220	226.8	256.8	173.10519	NA	5397969	7036275	21555	InChI=1S/C8H1
221	282.6	312.6	246.10044	NA	1925	700653	74640	InChI=1S/C13H
222	196.2	226.2	130.06299	C00233	69	70	48430	InChI=1S/C6H1
223	178.2	208.2	130.06299	C00671	388419	439286	15614	InChI=1S/C6H1
224	78	108	162.05282	C03761	1600	1662	16831	InChI=1S/C6H1
225	74.4	104.4	233.03579	C13691	110461	123932	34729	InChI=1S/C8H1
226	78.6	108.6	233.03579	C13690	108936	122136	37946	InChI=1S/C8H1
227	21	51	166.04774	C01685	4574162	5460677	21077	InChI=1S/C5H1
228	27.6	57.6	255.9889	NA	77998	54676864	167715	InChI=1S/C6H8
229	33.6	63.6	156.01711	C00295	942	967	16742	InChI=1S/C5H4
230	99	129	162.99393	NA	33607	36573	83501	InChI=1S/C4H5
231	111	141	142.02661	C20448	72827	80642	89118	InChI=1S/C6H6
232	147	177	182.99901	C12283	4959	5143	32111	InChI=1S/C7H5
233	165.6	195.6	173.99868	C02180	4601	74426	27905	InChI=1S/C6H6
234	169.2	199.2	159.08954	NA	475516	546304	70984	InChI=1S/C7H1
235	264.6	294.6	207.08954	C03519	67404	74839	16259	InChI=1S/C11H
236	328.8	358.8	202.02998	NA	34448630	20822574	82932	InChI=1S/C8H1
237	427.2	457.2	230.06128	NA	10709958	12456386	82911	InChI=1S/C10H
238	430.8	460.8	464.24102	NA	413525	53480448	NA	InChI=1S/C25H
239	573.6	603.6	396.19705	NA	94802	105074	NA	InChI=1S/C21H
240	153	183	146.05791	NA	11549	12046	68567	InChI=1S/C6H1
241	91.2	121.2	211.08446	NA	1607	1670	172453	InChI=1S/C10H
242	108	138	298.11514	NA	393054	135445750	20794	InChI=1S/C11H
243	471	501	240.09977	NA	110498	123979	41254	InChI=1S/C12H
244	109.5	139.5	254.12666	NA	19980286	14274616	NA	InChI=1S/C12H
245	75	105	261.03071	NA	448617	514186	46215	InChI=1S/C9H1
246	591.6	621.6	449.31412	C05464	17215983	22833539	NA	InChI=1S/C26H
247	499.8	529.8	394.27192	NA	139637	158738	168310	InChI=1S/C23H
248	504	534	406.27192	NA	163659	188292	16390	InChI=1S/C24H
249	639	669	392.29266	C04483	193196	222528	28834	InChI=1S/C24H
250	432.6	462.6	529.27094	NA	19973535	21116917	89129	InChI=1S/C26H
251	521.4	551.4	529.27094	NA	58827480	101602538	133678	InChI=1S/C26H
252	510.6	540.6	529.27094	NA	19991236	21125002	72733	InChI=1S/C26H
253	520.8	550.8	563.25866	C03642	389078	440071	17864	InChI=1S/C26H
254	594	624	513.27602	C11301	65188	72222	9347	InChI=1S/C26H
255	489	519	449.31412	NA	19973534	12310288	89929	InChI=1S/C26H
256	489	519	465.30904	C01921	9734	10140	17687	InChI=1S/C26H
257	80.4	110.4	104.04734	C06001	389707	440873	37373	InChI=1S/C4H8
258	149.4	179.4	118.06299	NA	90190	99823	60645	InChI=1S/C5H1
259	111	141	118.06299	NA	62571	69362	37084	InChI=1S/C5H1

	Q	R
1	InChIKey	MSIAnnotation
2	FBZONXHGGF	1
3	LOIYMIARKY	1
4	LEHOTFFKMJ	1
5	WWNNZCOKK	1
6	YAPQBXQYLJ	1
7	ZJUKTBDSGO	1
8	LXNHXLXTXN	1
9	PTJWIQPHWP	1
10	RWCOTTLHDJ	1
11	UFAHZIUFPNS	1
12	CMUNUTVVO	1
13	ONPXCLZMBS	1
14	HXEACLLIILL	1
15	JFLIEFSWGNQ	1
16	GHOKWGTUZ	1
17	RDHQFKQIGN	1
18	VQAYFKKCN	1
19	GFYLSDSUCH	1
20	HVPFXCBJHIL	1
21	DFPAKSUCGF	1
22	DTERQYGMU	1
23	VVHOUVWJCO	1
24	HXFOXFJUNF	1
25	SQVRNKJHWF	1
26	SNEIUMQYRC	1
27	RSPURTUNRH	1
28	KSPQDMRTZZ	1
29	XZWYZXLIPX	1
30	QIVBCDIJAJP	1
31	KDXKERNSEI	1
32	YGPSJZOEDV	1
33	HNDVDQJICG	1
34	AUNGANRZJE	1
35	FDGQSTZJBFJ	1
36	QIAFMBKCNZ	1
37	KZNQNBZMBZ	1
38	ZDXPYRJPND	1
39	OYIFNHCXNC	1
40	CVSVTCORWI	1
41	KRKNYBCHXY	1
42	RYYVLZVUVI	1
43	LRCNOZRCYE	1
44	METKIMKYRF	1
45	HVPFXCBJHIL	1
46	RFMMMVDNI	1
47	IPROLSVTVHL	1
48	RZVAJINKPM	1
49	FZWGECJQAC	1
50	ODHCTXKNW	1
51	WUUGFSXJNC	1
52	LRSASMSXMS	1
53	HXACOUQIXZ	1
54	PRJKNHOMHF	1
55	HCZHHEIFKR	1
56	TUHVEAJXIM	1
57	BPSLZWSRHT	1
58	QUNWUDVFR	1
59	QFDRTOONIS	1
60	NIDVTARKFB	1
61	JBWJCJUYHH	1
62	XIGSAGMEBX	1
63	BMQYVXCPA	1
64	MFYSYFVPBJ	1
65	CZMRCDWAG	1
66	SEOVTRFCIG	1
67	APIJDQYYAC	1
68	SUHOQUVVVI	1
69	OPVPGKGADY	1
70	ZFXYFBGIUFE	1

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71	HESFZGWRDU	1
72	KWIUHFFTVR	1
73	GJAWHXHKY	1
74	DUUGKQCEG	1
75	IVOMOUWHD	1
76	PHIQHXFUZV	1
77	MXNRLFUSFK	1
78	QZAYGJVTTN	1
79	KDZOASGQNC	1
80	VCKPUUFAIG	1
81	LDCYZAJDBX	1
82	JTYMXXCJQK	1
83	OUYCCCASQS	1
84	DZGWFCGJZK	1
85	VYFYTLLBU	1
86	QWYFHHGCZ	1
87	CWLQUGTUX	1
88	ZDGJAHTZVH	1
89	RWQNBRDOK	1
90	UYTPUDQBN	1
91	OIRDTQYFTA	1
92	GMSNIKWWO	1
93	PFDUUKDQEF	1
94	OGHAROSJZR	1
95	LOAUVZALPP	1
96	WURBQCVBQ	1
97	VVPRQWTYSN	1
98	LZOSYCMHQ	1
99	FUJLYHJROO	1
100	PSHXNVGSVN	1
101	NA	1
102	XOMRRQXKH	1
103	FNPHNLNTJN	1
104	CIQHWLTYGN	1
105	VTYFITADLSV	1
106	PFWLFWPASU	1
107	ROHFNLRQFU	1
108	AGPKZVBTJJN	1
109	RTRQQBHATC	1
110	MEFKEPWME	1
111	XNKLTQHYNI	1
112	WJNGQIYEQL	1
113	VKGZCEJTCK	1
114	WJXSWCUQA	1
115	CAHKINHBCV	1
116	AOHCBEAZXF	1
117	LCPYQJIKPJD	1
118	JMCOUWKXL	1
119	MDSUKZSLOA	1
120	NPDTUDWGJN	1
121	YGIAGXACEX	1
122	OAUYENAPBF	1
123	VEYYWZRYIY	1
124	PQBAWAQIRZ	1
125	LOUPRKONTZ	1
126	ZCKYOWGFR	1
127	BHHGXPLMPV	1
128	UIKROCXWU	1
129	CIPULDKLIIV	1
130	FXFANIORDK	1
131	SNICXCGAKA	1
132	2N2/c1-3-8(7-10	1
133	BYXCFUMGEI	1
134	NOFNCLGCUJ	1
135	AKEUNCKRJA	1
136	MBIQENSCDN	1
137	ONJSZLXSECC	1
138	UYEMGAFJOZ	1
139	XJMMNTGIMI	1
140	WNLRTBVMV	1

	Q	R
141	BDJRBEYXGG	1
142	BHQCQFFYZ	1
143	XGILAAAMKEQ	1
144	JVGVDSSUAV	1
145	WXTMDXOMI	1
146	NYHBQMYGN	1
147	HNDVDQJGIG	1
148	FDGQSTZJBFJ	1
149	ABOLXXZAJLA	1
150	BXFFHSIDQOI	1
151	UGQMRVRMY	1
152	OUYCCCASQS	1
153	WXUAQHNMI	1
154	KSMRODHGG	1
155	IPROLSVTVHA	1
156	GHOKWGTUZ	1
157	IGTYILLPRJO	1
158	WGNACKZGUS	1
159	CZWCKYRVO	1
160	YGSDEFSMJL	1
161	KDYFGRWQO	1
162	ZFXYFBGIUFI	1
163	KQTHICEAUM	1
164	LEHOTFFKMJ	1
165	DRTQHJPVMC	1
166	RGHNJXZEOK	1
167	AEMOLEFTQE	1
168	CKLJMWZTIZ	1
169	KHTAGVZHYU	1
170	HMLZLHKHNI	1
171	BJEPYKJPYRN	1
172	WHUUTDBJXJ	1
173	XDOFWFNMY	1
174	RFMMMVDNI	1
175	COLNVLDHVI	1
176	JFCQEDHGNN	1
177	SQVRNKJHWK	1
178	XOAAWQZAT	1
179	AAWZDTNXL	1
180	LRFVTYWOQI	1
181	ZMHLUFWWV	1
182	FEWJPZIEWO	1
183	ODHCTXKNW	1
184	UBORTCNDUI	1
185	OTCCIMWXFI	1
186	IVOMOUWHD	1
187	BKAYIFDRRZ	1
188	AUNGANRZJF	1
189	DSLZVSRJTYF	1
190	WLJVNTCWHI	1
191	TYFQFVWCEI	1
192	CZMRCDWAG	1
193	YHXHKYRQL	1
194	QRMZSPFSDQ	1
195	CGQCWMIAEI	1
196	VOXXWSYKY	1
197	BWLBGMIXKS	1
198	4O6/c7-1-3(9)5	1
199	KUYNOZVWC	1
200	SNEIUMQYRC	1
201	KRKNYBCHX	1
202	ODBLHEXUDA	1
203	ZFFFJLDTCLJ	1
204	LNTHITQWFM	1
205	UTYVDVLMY	1
206	XQXPVVBIME	1
207	CCVYRRGZDE	1
208	FVMDYYGIDE	1
209	FJKROLUGYX	1
210	HNEGQIOMVE	1

	Q	R
211	GTZCVFVGUC	1
212	NGSWKAQJJW	1
213	KKSDGJDHHZ	1
214	XNKLTQHYNI	1
215	DCICDMMXFI	1
216	VKGZCEJTCK	1
217	YJRFFCVUYD	1
218	WRUSVQOKJI	1
219	CAHKINHBCV	1
220	JDTWZSUNGH	1
221	DZTHIGRZJP	1
222	BKAJNAXTPS	1
223	JVQYSWDUAC	1
224	NPOAOTPXW	1
225	DEKNNWJXAC	1
226	NZKRYJGNYP	1
227	QXKAJJAYHK	1
228	XDBMXUKHM	1
229	PXQPEWDEAF	1
230	YGCFIWIQZP	1
231	PCSKKIURR	1
232	CVHZOJKTDC	1
233	CTYRPMGLI	1
234	ZRQXMKMBB	1
235	CBQJSKKFN	1
236	DWZGLEPNCI	1
237	NODSEPOUFZ	1
238	GLONBVCUAY	1
239	DIJBBIOWGC	1
240	AQYCMVICBN	1
241	PFDUUKDQEH	1
242	OGHAROSJZR	1
243	WMCQWXZM	1
244	VTYFITADLS	1
245	CIQHWLTYGN	1
246	WVULKSPCQY	1
247	SHUYNJFEXPI	1
248	RHCPKKNRW	1
249	KXGVEGMKQ	1
250	DKXXSIJHWW	1
251	QJZCNFGUZP	1
252	DKXXSIJHWW	1
253	HSNPMXROZI	1
254	FHXBAFXQVZ	1
255	GHCZAUBVM	1
256	RFDAIACWW	1
257	DBXBTMSZEC	1
258	NGEWQZIDQI	1
259	003/c1-5(2,8)3-	1

LEGEND for Figures:

Figure 1: A. PCoA of α diversity measurements HC vs UC vs CD (Ellipses representing 95% CI). Alpha diversity measurements HC vs UC vs CD utilising B. Shannon Index, C. Inverse Simpson Index, D. Chao 1 Index, E. Faith's PD. (Median signified by middle horizontal line, 25% and 75% confidence intervals (CI) by box ends and range signified by vertical line extents)

Figure 2: Median bacterial phyla count (qPCR data), HC vs CD vs UC for A. *Bacteroidetes* (ANOVA $P < 0.001$, CD vs HC $q < 0.001$, UC vs HC $q < 0.001$, CD vs UC $q < 0.001$). B. *Proteobacteria* (ANOVA $P = 0.01$, CD vs HC $q = 0.0075$, UC vs HC $q = 0.043$, CD vs UC $q = 0.16$). C. *Firmicutes* (ANOVA $P = 0.001$, CD vs HC $q < 0.001$, UC vs HC $q = 0.011$, CD vs UC $q = 0.17$).

Figure 3: Univariate analyses of $^1\text{H-NMR}$ data from inception cohort – A: **Serum GlycA** (ANOVA $P < 0.001$, CD vs HC $q < 0.001$, UC vs HC $q = 0.019$, CD vs UC $q = 0.048$). B: **Serum GlycB** (ANOVA $P < 0.001$, CD vs HC $q < 0.001$, UC vs HC $q = 0.0017$, CD vs UC $q = 0.10$). C: **Serum Pyruvate** (ANOVA $P = 0.0079$, CD vs HC $q = 0.028$, UC vs HC $q = 0.0072$, CD vs UC $q = 0.64$). D: **Fecal Nicotinate** (ANOVA $P = 0.0047$, CD vs HC $q = 0.0032$, UC vs HC $q = 0.071$, CD vs UC $q = 0.083$). E: **Urine Hippurate** (ANOVA $P < 0.001$, CD vs HC $q = 0.0027$, UC vs HC $q < 0.001$, CD vs UC $q = 0.74$).

Figure 4: Univariate analyses of serum tryptophan metabolites, inception cohort A. **5-HIAA** (ANOVA $P < 0.001$, CD vs HC $q = 0.0057$, UC vs HC $q < 0.001$, CD vs UC $q = 0.35$). B. **Xanthurenic acid** (ANOVA $P = 0.0018$, CD vs HC $q = 0.0018$, UC vs HC $q = 0.20$, CD vs UC $q = 0.013$). C. **Picolinic acid** (ANOVA $P = 0.0055$, CD vs HC $q = 0.0092$, UC vs HC $q = 0.56$, CD vs UC $q = 0.0092$). D. **Neopterin** (ANOVA $P = 0.018$, CD vs HC $q = 0.19$, UC vs HC $q = 0.015$, CD vs UC $q = 0.19$). E. **Kynurenic acid** (ANOVA $P = 0.018$, CD vs HC $q = 0.015$, UC vs HC $q = 0.17$, CD vs UC $q = 0.10$). F. **3-HAA** (ANOVA $P = 0.034$, CD vs HC $q = 0.031$, UC vs HC $q = 0.24$, CD vs UC $q = 0.12$). G. **Quinolinic acid** (ANOVA $P = 0.039$, CD vs HC $q = 0.23$, UC vs HC $q = 0.034$, CD vs UC $q = 0.23$).

Figure 5: Univariate analyses of serum SCFAs, inception cohort A. **Butyrate** (ANOVA $P < 0.001$, CD vs HC $q < 0.001$, UC vs HC $q < 0.001$, CD vs UC $q = 0.58$). B. **Lactate** (ANOVA $P = 0.0049$, CD vs HC $q = 0.11$, UC vs HC $q = 0.0034$, CD vs UC $q = 0.11$). C. **Isobutyrate** (ANOVA $P = 0.029$, CD vs HC $q = 0.054$, UC vs HC $q = 0.032$, CD vs UC $q = 0.80$). D. **2-Methylbutyrate** (ANOVA $P = 0.012$, CD vs HC $q = 0.24$, UC vs HC $q = 0.011$, CD vs UC $q = 0.13$). E. **Isovalerate** (ANOVA $P = 0.029$, CD vs HC $q = 0.054$, UC vs HC $q = 0.032$, CD vs UC $q = 0.80$).

Figure 6: Univariate analyses of serum BAs inception cohort. A. **Glycochendeoxycholic acid** (ANOVA $P = 0.0065$, CD vs HC $q = 0.014$, UC vs HC $q = 0.0081$, CD vs UC $q = 0.89$). B. **5-Cholenic Acid-3-beta-ol** (ANOVA $P = 0.0071$, CD vs HC $q = 0.011$, UC vs HC $q = 0.010$, CD vs UC $q = 0.98$). C. **Glycochenodeoxycholic Acid 3-Sulfate** (ANOVA $P = 0.059$, CD vs HC $q = 0.078$, UC vs HC $q = 0.072$, CD vs UC $q = 0.90$). D. **Glycocholic Acid** (ANOVA $P = 0.0072$, CD vs HC $q = 0.19$, UC vs

HC $q=0.0062$, CD vs UC $q=0.13$). **E. Murocholic Acid** (ANOVA $P=0.0082$, CD vs HC $q=0.45$, UC vs HC $q=0.070$, CD vs UC $q=0.0099$). **F. Taurocholic Acid** (ANOVA $P=0.017$, CD vs HC $q=0.58$, UC vs HC $q=0.029$, CD vs UC $q=0.059$).

Figure 7: A: Distribution of correlation values across disease and health states B: Venn-diagram of strong positive ($r \geq 0.5$) associations across cohorts. C: Number of strong positive associations per genera and state D: Genera with the most variable strong positive associations across states E: KEGG Pathway enrichment of strong positive associations across states F: Associations strongly positively correlated with health and negatively correlated with ulcerative colitis and/or Crohn's disease.

Supplementary Figure 1: Microbe-metabolite correlations for healthy controls.

Supplementary Figure 2: Microbe-metabolite correlations for CD patients.

Supplementary Figure 3: Microbe-metabolite correlations for UC patients.

Supplementary Figure 4: Shared anti-correlating microbe-metabolite pairs shown on scatterplots, CD and UC, respectively. Enrichment analysis of the associations to the top left quadrant (positively associated with health, negative with UC/CD, highlighted in blue).

Supplementary Figure 5: Median bacterial biomass (qPCR data), HC vs CD vs UC (ANOVA $P<0.001$, CD vs HC $q<0.001$, UC vs HC $q<0.001$, CD vs UC $q<0.001$). Median values: CD=284833, UC=212687, HC=227063