

Online Supporting Information S1. The benchmark dataset **S** contains 4,002 samples, with 3,348 small molecules and 654 enzymes of yeast. These samples are classified into 11 metabolic pathway classes.

1. 592 samples in “Carbohydrate Metabolism”

(I) 394 small molecules

C00011	C00022	C00024	C00025	C00026	C00029	C00031	C00033
C00036	C00042	C00043	C00048	C00052	C00058	C00068	C00072
C00074	C00083	C00084	C00085	C00089	C00091	C00092	C00095
C00096	C00099	C00100	C00103	C00109	C00111	C00116	C00117
C00118	C00119	C00121	C00122	C00124	C00128	C00136	C00137
C00140	C00149	C00158	C00159	C00160	C00163	C00164	C00167
C00168	C00181	C00183	C00185	C00186	C00190	C00191	C00197
C00198	C00199	C00203	C00204	C00207	C00208	C00209	C00221
C00222	C00227	C00231	C00232	C00236	C00243	C00246	C00247
C00252	C00256	C00257	C00258	C00259	C00266	C00267	C00270
C00275	C00279	C00309	C00310	C00311	C00312	C00313	C00325
C00329	C00332	C00333	C00334	C00345	C00352	C00356	C00357
C00379	C00392	C00394	C00417	C00424	C00433	C00446	C00469
C00470	C00474	C00476	C00490	C00492	C00497	C00498	C00501
C00502	C00507	C00508	C00514	C00531	C00532	C00545	C00546
C00552	C00558	C00577	C00583	C00617	C00618	C00620	C00631
C00636	C00644	C00645	C00651	C00663	C00665	C00668	C00672
C00673	C00679	C00683	C00684	C00689	C00691	C00734	C00741
C00789	C00794	C00798	C00800	C00804	C00810	C00817	C00818
C00827	C00861	C00877	C00879	C00880	C00888	C00894	C00898
C00900	C00905	C00935	C00937	C00973	C00975	C00976	C00988
C00989	C01011	C01013	C01019	C01040	C01041	C01050	C01068
C01083	C01089	C01094	C01096	C01097	C01099	C01101	C01109
C01113	C01114	C01115	C01127	C01131	C01132	C01144	C01146
C01151	C01159	C01170	C01172	C01177	C01182	C01204	C01213
C01216	C01218	C01219	C01220	C01222	C01231	C01234	C01235
C01236	C01243	C01245	C01251	C01272	C01284	C01286	C01380
C01384	C01412	C01451	C01508	C01613	C01620	C01623	C01674
C01680	C01697	C01721	C01732	C01769	C01788	C01801	C01825
C01845	C01904	C01934	C01989	C01990	C02013	C02123	C02170
C02199	C02225	C02226	C02262	C02266	C02273	C02280	C02330
C02331	C02335	C02336	C02405	C02411	C02431	C02504	C02527
C02591	C02612	C02614	C02630	C02670	C02713	C02876	C02888
C02977	C02985	C02995	C03044	C03046	C03058	C03117	C03217
C03248	C03267	C03289	C03291	C03383	C03410	C03451	C03459
C03546	C03548	C03561	C03598	C03599	C03618	C03659	C03660
C03737	C03752	C03785	C03826	C03906	C03921	C03979	C03981
C04006	C04037	C04053	C04062	C04063	C04089	C04225	C04257

C04287 C04297 C04348 C04349 C04442 C04477 C04501 C04520
 C04546 C04563 C04573 C04575 C04579 C04593 C04631 C05125
 C05345 C05378 C05379 C05382 C05385 C05396 C05399 C05400
 C05401 C05402 C05404 C05411 C05412 C05422 C05668 C05731
 C05984 C05985 C05986 C05993 C05999 C06002 C06010 C06019
 C06023 C06027 C06028 C06029 C06030 C06032 C06033 C06118
 C06142 C06146 C06156 C06186 C06187 C06188 C06192 C06215
 C06216 C06217 C06218 C06219 C06240 C06241 C06311 C06376
 C06377 C06441 C06473 C06892 C06893 C11516 C11521 C11544
 C11555 C13952 C14899 C15923 C15925 C15926 C15930 C16153
 C16154 C16155 C16156 C16186 C16688 C16698 C17327 C17328
 C18026 C18324

(II) 198 enzymes

YAL038W	YAL054C	YAL060W	YAL061W	YBL015W
YBL068W	YBR001C	YBR006W	YBR018C	YBR019C
YBR020W	YBR023C	YBR038W	YBR084W	YBR117C
YBR126C	YBR145W	YBR196C	YBR218C	YBR221C
YBR299W	YCL009C	YCL040W	YCR005C	YCR012W
YCR036W	YDL021W	YDL037C	YDL055C	YDL066W
YDL078C	YDL080C	YDL103C	YDL131W	YDL168W
YDL174C	YDL182W	YDL246C	YDR001C	YDR009W
YDR050C	YDR074W	YDR148C	YDR173C	YDR178W
YDR208W	YDR248C	YDR261C	YDR272W	YDR287W
YEL011W	YEL058W	YEL070W	YER003C	YER065C
YER073W	YER099C	YER178W	YFL017C	YFL018C
YFL045C	YFR015C	YFR019W	YFR053C	YGL062W
YGL253W	YGL256W	YGR019W	YGR032W	YGR043C
YGR087C	YGR192C	YGR194C	YGR204W	YGR240C
YGR244C	YGR248W	YGR254W	YGR256W	YGR282C
YGR287C	YGR292W	YHL011C	YHL012W	YHR046C
YHR104W	YHR163W	YHR174W	YHR183W	YIL043C
YIL099W	YIL107C	YIL125W	YIL162W	YIL172C
YIR019C	YIR031C	YJL045W	YJL052W	YJL121C
YJL153C	YJL155C	YJL200C	YJL216C	YJL221C
YJR009C	YJR153W	YJR159W	YKL029C	YKL035W
YKL060C	YKL085W	YKL104C	YKL127W	YKL141W
YKL148C	YKL150W	YKL152C	YKL181W	YKR043C
YKR097W	YLL041C	YLR044C	YLR070C	YLR153C
YLR164W	YLR174W	YLR240W	YLR258W	YLR286C
YLR300W	YLR304C	YLR305C	YLR307W	YLR308W
YLR342W	YLR354C	YLR377C	YML004C	YML054C
YML100W	YML126C	YMR083W	YMR099C	YMR105C
YMR108W	YMR118C	YMR169C	YMR170C	YMR205C
YMR250W	YMR261C	YMR278W	YMR303C	YMR306W

YMR323W	YNL009W	YNL037C	YNL071W	YNL104C
YNL106C	YNL117W	YNL192W	YNL241C	YNL267W
YNR001C	YNR016C	YNR034W	YOL061W	YOL065C
YOL086C	YOL126C	YOL136C	YOL157C	YOR040W
YOR095C	YOR109W	YOR136W	YOR142W	YOR190W
YOR347C	YOR374W	YOR388C	YOR393W	YPL017C
YPL028W	YPL061W	YPL262W	YPL268W	YPR001W
YPR002W	YPR006C	YPR026W	YPR074C	YPR113W
YPR160W	YPR184W	YCR073W-A		

2. 297 samples in “Energy Metabolism”

(I) 151 small molecules

C00001	C00002	C00003	C00004	C00005	C00006	C00007	C00008
C00009	C00011	C00013	C00014	C00022	C00024	C00025	C00026
C00033	C00034	C00036	C00037	C00041	C00042	C00048	C00049
C00053	C00054	C00058	C00059	C00061	C00064	C00065	C00067
C00074	C00080	C00083	C00085	C00087	C00088	C00091	C00094
C00097	C00100	C00101	C00111	C00117	C00118	C00122	C00132
C00143	C00149	C00152	C00155	C00158	C00168	C00169	C00184
C00192	C00197	C00199	C00218	C00222	C00224	C00227	C00231
C00232	C00234	C00236	C00237	C00244	C00258	C00263	C00279
C00282	C00283	C00288	C00311	C00320	C00332	C00354	C00390
C00399	C00417	C00440	C00445	C00447	C00488	C00533	C00536
C00542	C00543	C00565	C00593	C00631	C00683	C00697	C00862
C00876	C00877	C00887	C00894	C00979	C00989	C01001	C01005
C01011	C01013	C01031	C01046	C01077	C01080	C01104	C01118
C01144	C01179	C01182	C01213	C01217	C01274	C01330	C01353
C01417	C01438	C01563	C01861	C02061	C02076	C02185	C02331
C03232	C03576	C03920	C04330	C04348	C04377	C04488	C04628
C04732	C04832	C05382	C05528	C05668	C06019	C06027	C06028
C11062	C11536	C11537	C11903	C11904	C14180	C18323	

(II) 146 enzymes

Q0045	Q0065	Q0070	Q0080	Q0085
Q0105	Q0110	Q0115	Q0120	Q0130
Q0250	Q0275	YAL012W	YAL038W	YAL054C
YAL062W	YBL045C	YBL099W	YBR011C	YBR039W
YBR117C	YBR127C	YBR263W	YCL050C	YCR012W
YDL004W	YDL021W	YDL067C	YDL078C	YDL085W
YDL168W	YDL171C	YDL185W	YDL215C	YDR019C
YDR050C	YDR111C	YDR178W	YDR256C	YDR298C
YDR321W	YDR376W	YDR377W	YDR529C	YEL024W
YEL027W	YEL051W	YER081W	YFL053W	YFR030W
YFR033C	YFR055W	YGL008C	YGL125W	YGL184C
YGL187C	YGL191W	YGR012W	YGR020C	YGR088W

YGR124W	YGR183C	YGR208W	YGR240C	YGR254W
YHR026W	YHR051W	YHR174W	YIL074C	YIL111W
YJL045W	YJL068C	YJL121C	YJL166W	YJR010W
YJR121W	YJR130C	YJR137C	YKL001C	YKL016C
YKL060C	YKL080W	YKL085W	YKL106W	YKL141W
YKL148C	YKL152C	YKL192C	YKR043C	YKR097W
YLL041C	YLL058W	YLR027C	YLR038C	YLR058C
YLR089C	YLR153C	YLR155C	YLR157C	YLR158C
YLR160C	YLR164W	YLR295C	YLR303W	YLR377C
YLR395C	YLR447C	YML070W	YML082W	YML120C
YMR054W	YMR118C	YMR145C	YMR205C	YMR256C
YMR267W	YMR323W	YNL052W	YNL277W	YOL064C
YOL126C	YOR065W	YOR095C	YOR184W	YOR270C
YOR332W	YOR347C	YOR375C	YOR388C	YOR393W
YPL023C	YPL036W	YPL078C	YPL234C	YPL271W
YPR020W	YPR035W	YPR036W	YPR074C	YPR145W
YPR167C	YPR191W	YHR001W-A	YHR039C-A	YML081C-A
YOL077W-A				

3. 483 samples in “Lipid Metabolism”

(I) 399 small molecules

C00010	C00024	C00029	C00037	C00065	C00083	C00084	C00093
C00100	C00111	C00114	C00116	C00136	C00154	C00164	C00184
C00187	C00189	C00197	C00207	C00219	C00245	C00249	C00258
C00280	C00307	C00319	C00332	C00346	C00356	C00410	C00412
C00427	C00448	C00468	C00479	C00489	C00510	C00513	C00517
C00523	C00527	C00535	C00570	C00577	C00583	C00584	C00588
C00599	C00639	C00670	C00674	C00695	C00696	C00712	C00735
C00751	C00762	C00823	C00836	C00877	C00909	C00951	C00969
C01054	C01089	C01120	C01124	C01144	C01164	C01176	C01189
C01210	C01226	C01227	C01233	C01301	C01312	C01530	C01561
C01571	C01595	C01673	C01694	C01724	C01747	C01753	C01780
C01789	C01794	C01802	C01832	C01902	C01921	C01943	C01944
C01953	C01996	C02041	C02050	C02140	C02141	C02165	C02166
C02198	C02249	C02373	C02457	C02528	C02537	C02538	C02593
C02679	C02934	C02990	C03035	C03205	C03242	C03428	C03547
C03561	C03577	C03594	C03595	C03640	C03681	C03772	C03845
C03852	C03872	C03917	C03990	C04042	C04056	C04295	C04373
C04483	C04518	C04525	C04554	C04555	C04577	C04672	C04676
C04717	C04722	C04742	C04780	C04785	C04805	C04822	C04853
C05103	C05107	C05108	C05109	C05122	C05138	C05139	C05140
C05141	C05259	C05261	C05264	C05267	C05269	C05270	C05272
C05274	C05275	C05284	C05285	C05290	C05291	C05293	C05294
C05295	C05296	C05297	C05298	C05299	C05300	C05301	C05302

C05337 C05356 C05401 C05437 C05439 C05440 C05441 C05442
 C05443 C05444 C05445 C05446 C05447 C05448 C05449 C05450
 C05451 C05452 C05453 C05454 C05455 C05460 C05465 C05466
 C05467 C05469 C05470 C05471 C05472 C05476 C05479 C05480
 C05481 C05482 C05484 C05485 C05488 C05490 C05497 C05498
 C05500 C05501 C05502 C05503 C05504 C05949 C05950 C05951
 C05952 C05953 C05954 C05956 C05957 C05958 C05959 C05960
 C05961 C05962 C05963 C05964 C05965 C05966 C05979 C05999
 C06083 C06124 C06309 C06310 C06314 C06341 C06423 C06424
 C06425 C06426 C06427 C06428 C06429 C06462 C06771 C06772
 C07289 C07354 C07880 C08281 C08316 C08320 C08323 C08357
 C08362 C08491 C08821 C08830 C11133 C11134 C11135 C11455
 C11508 C11512 C11521 C11522 C11523 C12144 C13482 C13550
 C13712 C13713 C13809 C14717 C14732 C14748 C14749 C14762
 C14765 C14766 C14767 C14772 C14773 C14774 C14775 C14776
 C14777 C14778 C14780 C14781 C14782 C14807 C14808 C14810
 C14811 C14812 C14813 C14814 C14815 C14822 C14823 C14824
 C14826 C14827 C14828 C14829 C14831 C14834 C14835 C15515
 C15517 C15518 C15519 C15520 C15610 C15613 C15776 C15777
 C15778 C15780 C15781 C15782 C15783 C15808 C15816 C15915
 C16162 C16300 C16308 C16309 C16310 C16311 C16316 C16317
 C16319 C16320 C16322 C16331 C16335 C16344 C16345 C16513
 C16522 C16525 C16526 C16527 C16528 C16529 C16530 C16532
 C17332 C17333 C17337 C17339 C17343 C17345 C17346 C17644
 C17647 C17649 C17650 C17654 C17657 C17658 C17660 C17661
 C17662 C17664 C17667 C17687 C17726 C17727 C17737 C18038
 C18040 C18041 C18042 C18043 C18044 C18045 C18075

(II) 84 enzymes

YBL011W YBR026C YBR029C YBR145W YBR244W
 YBR265W YCL004W YCR048W YDL022W YDL052C
 YDL168W YDR058C YDR062W YDR147W YDR294C
 YDR402C YER015W YER026C YER061C YER062C
 YER073W YFL053W YGL001C YGL012W YGL055W
 YGL205W YGL256W YGR007W YGR060W YGR157W
 YGR170W YGR175C YGR202C YHL003C YHL032C
 YHR007C YHR072W YHR104W YHR123W YHR190W
 YIL009W YIL049W YIL053W YIL124W YIL160C
 YIR037W YJR019C YKL008C YKL026C YKL182W
 YKR031C YKR067W YLR100W YLR133W YLR260W
 YLR299W YML008C YML070W YML126C YMR006C
 YMR008C YMR083W YMR246W YMR296C YMR303C
 YNL045W YNL130C YNL169C YNL280C YNR008W
 YNR016C YNR019W YOL011W YOL059W YOL086C
 YOR171C YOR175C YOR317W YOR374W YPL028W

YPL061W YPL206C YPL231W YPR113W

4. 240 samples in “Nucleotide Metabolism”

(I) 133 small molecules

C00002 C00008 C00011 C00014 C00015 C00020 C00029 C00035
 C00037 C00044 C00048 C00053 C00054 C00055 C00059 C00063
 C00064 C00075 C00081 C00086 C00099 C00104 C00105 C00106
 C00112 C00117 C00119 C00130 C00131 C00144 C00147 C00169
 C00178 C00206 C00212 C00214 C00224 C00239 C00242 C00262
 C00286 C00294 C00295 C00299 C00301 C00330 C00337 C00360
 C00361 C00362 C00363 C00364 C00365 C00366 C00380 C00383
 C00385 C00387 C00429 C00438 C00458 C00459 C00460 C00475
 C00499 C00526 C00559 C00575 C00603 C00620 C00655 C00672
 C00700 C00705 C00802 C00813 C00881 C00906 C00942 C01103
 C01168 C01228 C01260 C01261 C01345 C01346 C01367 C01368
 C01762 C02067 C02091 C02170 C02348 C02350 C02353 C02354
 C02355 C02376 C02642 C02718 C03090 C03373 C03483 C03794
 C03838 C03997 C04051 C04376 C04494 C04640 C04677 C04734
 C04751 C04823 C05100 C05145 C05239 C05512 C05513 C05515
 C05516 C05822 C05993 C06193 C06194 C06195 C06196 C06197
 C06198 C11821 C12248 C15607 C15667

(II) 107 enzymes

YAL038W YAR015W YBL039C YBL068W YBR111C
 YBR252W YBR278W YCL050C YCR014C YDL102W
 YDL140C YDL150W YDL238C YDR045C YDR121W
 YDR156W YDR226W YDR353W YDR408C YDR419W
 YDR441C YDR454C YDR530C YEL021W YEL055C
 YER005W YER070W YER099C YER170W YFL036W
 YGL063W YGL234W YGL248W YGR061C YGR180C
 YHL011C YHR106W YHR128W YHR144C YHR201C
 YHR216W YIL066C YIL139C YIR027C YIR029W
 YIR032C YJL005W YJL026W YJL130C YJL148W
 YJR010W YJR057W YJR063W YJR103W YJR105W
 YJR109C YKL001C YKL024C YKL067W YKL127W
 YKL144C YKL181W YKL216W YLR028C YLR209C
 YLR245C YLR359W YLR420W YLR432W YML022W
 YML035C YML056C YML106W YMR105C YMR120C
 YMR217W YMR271C YMR278W YMR300C YNL102W
 YNL113W YNL141W YNL151C YNL220W YNL248C
 YNL262W YNR003C YNR012W YOL061W YOL115W
 YOR074C YOR116C YOR128C YOR151C YOR207C
 YOR303W YOR330C YOR340C YOR341W YOR347C
 YOR360C YPL167C YPR010C YPR062W YPR110C
 YPR175W YPR190C

5. 647 samples in “Amino Acid Metabolism”

(I) 489 small molecules

C00011	C00014	C00019	C00021	C00022	C00024	C00025	C00026
C00036	C00037	C00041	C00042	C00047	C00048	C00049	C00051
C00059	C00062	C00064	C00065	C00068	C00073	C00074	C00077
C00078	C00079	C00082	C00083	C00084	C00086	C00091	C00094
C00097	C00100	C00101	C00108	C00109	C00114	C00119	C00122
C00123	C00134	C00135	C00141	C00143	C00146	C00148	C00152
C00155	C00156	C00164	C00166	C00168	C00169	C00170	C00179
C00180	C00183	C00188	C00197	C00213	C00223	C00230	C00232
C00233	C00251	C00254	C00258	C00263	C00279	C00283	C00296
C00300	C00315	C00320	C00322	C00323	C00327	C00328	C00331
C00332	C00334	C00352	C00355	C00356	C00388	C00398	C00402
C00406	C00407	C00408	C00409	C00423	C00430	C00431	C00433
C00436	C00437	C00438	C00439	C00441	C00449	C00450	C00463
C00483	C00487	C00489	C00491	C00493	C00506	C00512	C00527
C00530	C00533	C00544	C00546	C00547	C00555	C00576	C00581
C00582	C00596	C00601	C00606	C00624	C00628	C00630	C00632
C00637	C00642	C00643	C00666	C00671	C00680	C00683	C00719
C00739	C00740	C00750	C00755	C00763	C00780	C00785	C00788
C00791	C00793	C00805	C00811	C00822	C00826	C00860	C00877
C00884	C00940	C00944	C00954	C00955	C00956	C00957	C00978
C00979	C00986	C00990	C01005	C01010	C01026	C01028	C01035
C01036	C01042	C01043	C01044	C01045	C01060	C01061	C01077
C01100	C01102	C01110	C01118	C01137	C01142	C01144	C01149
C01152	C01157	C01161	C01165	C01179	C01180	C01181	C01186
C01198	C01207	C01213	C01234	C01250	C01251	C01252	C01259
C01262	C01267	C01269	C01302	C01575	C01586	C01598	C01672
C01682	C01693	C01717	C01772	C01817	C01829	C01850	C01877
C01888	C01929	C01962	C01987	C02043	C02137	C02161	C02167
C02170	C02172	C02218	C02220	C02226	C02265	C02291	C02298
C02305	C02362	C02442	C02465	C02470	C02504	C02505	C02514
C02515	C02565	C02612	C02631	C02637	C02647	C02693	C02700
C02714	C02727	C02739	C02741	C02763	C02765	C02775	C02835
C02937	C02938	C02939	C02946	C02989	C03063	C03069	C03077
C03078	C03082	C03087	C03089	C03090	C03145	C03166	C03175
C03194	C03227	C03230	C03231	C03232	C03239	C03273	C03277
C03283	C03284	C03287	C03296	C03340	C03344	C03345	C03375
C03406	C03415	C03440	C03453	C03460	C03506	C03508	C03519
C03539	C03564	C03589	C03656	C03672	C03680	C03722	C03758
C03765	C03771	C03793	C03794	C03824	C03871	C03912	C03955
C03972	C04002	C04020	C04043	C04044	C04045	C04052	C04076
C04092	C04133	C04137	C04148	C04185	C04186	C04188	C04236
C04272	C04281	C04282	C04302	C04368	C04390	C04405	C04409

C04411 C04421 C04462 C04479 C04498 C04582 C04642 C04666
 C04677 C04691 C04877 C04882 C04896 C04916 C05125 C05127
 C05130 C05135 C05161 C05235 C05332 C05338 C05519 C05527
 C05528 C05539 C05548 C05554 C05565 C05568 C05570 C05572
 C05575 C05576 C05577 C05578 C05579 C05580 C05581 C05582
 C05583 C05584 C05585 C05587 C05588 C05589 C05593 C05594
 C05598 C05600 C05604 C05607 C05620 C05629 C05634 C05635
 C05637 C05638 C05639 C05640 C05642 C05643 C05645 C05646
 C05651 C05653 C05658 C05659 C05660 C05662 C05663 C05823
 C05824 C05827 C05828 C05829 C05830 C05831 C05834 C05837
 C05852 C05853 C05931 C05932 C05933 C05936 C05939 C05942
 C05945 C05946 C05947 C06000 C06001 C06002 C06006 C06007
 C06010 C06032 C06044 C06046 C06047 C06048 C06181 C06199
 C06212 C06213 C06231 C06442 C06547 C06866 C07086 C07303
 C08276 C08300 C08301 C09306 C10447 C10497 C11457 C11481
 C11588 C12621 C12623 C12986 C12987 C12988 C12989 C15524
 C15532 C15606 C15650 C15651 C15699 C15700 C15767 C15980
 C16069 C16432 C16666 C16673 C16719 C16848 C16850 C17203
 C17268 C17935 C17938 C18048 C18172 C18174 C18202 C18325
 C18326

(II) 158 enzymes

YAL012W	YAL062W	YBL076C	YBL098W	YBR006W
YBR115C	YBR145W	YBR166C	YBR208C	YBR221C
YBR249C	YBR263W	YCL009C	YCL018W	YCL030C
YCL064C	YCR053W	YDL131W	YDL168W	YDL171C
YDL182W	YDL215C	YDR007W	YDR019C	YDR035W
YDR111C	YDR127W	YDR148C	YDR158W	YDR232W
YDR234W	YDR242W	YDR256C	YDR268W	YDR300C
YDR321W	YDR354W	YDR402C	YDR440W	YDR502C
YEL038W	YEL046C	YER023W	YER026C	YER043C
YER052C	YER055C	YER069W	YER073W	YER081W
YER086W	YER090W	YER091C	YER178W	YFL018C
YFR025C	YFR055W	YGL009C	YGL026C	YGL148W
YGL184C	YGL202W	YGL256W	YGR012W	YGR019W
YGR088W	YGR094W	YGR124W	YGR155W	YGR208W
YHR018C	YHR025W	YHR037W	YHR119W	YHR137W
YHR208W	YIL020C	YIL074C	YIL094C	YIL116W
YIL125W	YIL160C	YIR034C	YJL088W	YJL130C
YJL168C	YJR016C	YJR024C	YJR025C	YJR078W
YJR109C	YJR130C	YJR139C	YJR148W	YKL104C
YKL106W	YKL184W	YKL211C	YLL058W	YLR017W
YLR027C	YLR058C	YLR089C	YLR134W	YLR142W
YLR146C	YLR155C	YLR157C	YLR158C	YLR160C
YLR180W	YLR231C	YLR303W	YLR355C	YLR359W

YLR382C	YLR438W	YML082W	YML126C	YMR009W
YMR062C	YMR083W	YMR108W	YMR169C	YMR170C
YMR189W	YMR250W	YMR300C	YMR303C	YNL104C
YNL220W	YNL277W	YNL316C	YNR050C	YOL052C
YOL058W	YOL086C	YOL097C	YOL140W	YOR184W
YOR202W	YOR251C	YOR303W	YOR323C	YOR374W
YOR375C	YPL017C	YPL028W	YPL040C	YPL061W
YPL111W	YPL160W	YPR035W	YPR060C	YPR062W
YPR069C	YPR118W	YPR145W		

6. 200 samples in “Metabolism of Other Amino Acids”

(I) 156 small molecules

C00005	C00006	C00011	C00014	C00022	C00024	C00025	C00026
C00033	C00037	C00041	C00049	C00051	C00062	C00064	C00065
C00072	C00074	C00077	C00082	C00083	C00084	C00094	C00097
C00099	C00100	C00106	C00127	C00133	C00134	C00135	C00152
C00177	C00189	C00217	C00222	C00227	C00245	C00302	C00315
C00334	C00383	C00429	C00488	C00506	C00515	C00519	C00555
C00593	C00606	C00650	C00669	C00692	C00736	C00750	C00792
C00804	C00819	C00864	C00894	C00986	C00993	C01013	C01050
C01073	C01110	C01212	C01262	C01326	C01401	C01419	C01528
C01594	C01672	C01678	C01855	C01879	C01959	C02090	C02237
C02335	C02512	C02535	C02642	C02659	C02798	C03149	C03167
C03170	C03341	C03557	C03564	C03646	C03722	C03742	C03771
C03943	C04353	C05042	C05122	C05123	C05143	C05172	C05335
C05341	C05422	C05665	C05668	C05669	C05670	C05672	C05679
C05680	C05682	C05684	C05686	C05688	C05689	C05695	C05697
C05698	C05699	C05703	C05711	C05714	C05730	C05844	C06367
C06368	C06451	C06452	C06454	C06455	C06456	C06457	C06459
C06735	C08325	C14179	C16074	C16075	C16562	C16563	C16564
C16565	C16566	C16567	C17940	C17942	C17944	C17946	C17947
C17949	C17951	C17952	C17962				

(II) 44 enzymes

YBL064C	YBR244W	YBR263W	YDL066W	YDR242W
YDR321W	YDR453C	YER070W	YER073W	YGR007W
YGR019W	YGR180C	YGR202C	YGR256W	YHR123W
YHR183W	YIL010W	YIL066C	YIL145C	YIR037W
YJL026W	YJL101C	YKL026C	YKL184W	YKL215C
YLR058C	YLR109W	YLR146C	YLR155C	YLR157C
YLR158C	YLR160C	YLR174W	YLR299W	YML028W
YMR250W	YNL009W	YNL130C	YNL241C	YOL049W
YOR374W	YPL061W	YPL091W	YPR069C	

7. 65 samples in “Glycan Biosynthesis and Metabolism”

(I) 47 small molecules

C00009 C00033 C00043 C00053 C00054 C00096 C00105 C00110
 C00133 C00154 C00381 C00621 C00692 C00993 C01050 C01112
 C01187 C01212 C01246 C03862 C04121 C04478 C04574 C04631
 C04652 C04738 C04824 C04877 C04882 C04919 C04932 C05382
 C05892 C05897 C05898 C06022 C06024 C06025 C06026 C06251
 C06397 C06398 C07836 C07838 C11472 C17556 C17558

(II) 18 enzymes

YBL082C YBR070C YBR110W YBR229C YBR243C
 YGL022W YGL027C YGL047W YGL065C YGL156W
 YGR036C YJR131W YMR013C YMR281W YNR030W
 YPL175W YPL227C YPR183W

8. 437 samples in “Metabolism of Cofactors and Vitamins”

(I) 350 small molecules

C00001 C00003 C00006 C00007 C00010 C00016 C00018 C00022
 C00025 C00026 C00032 C00037 C00044 C00047 C00049 C00054
 C00061 C00068 C00082 C00097 C00099 C00101 C00106 C00111
 C00118 C00120 C00122 C00133 C00141 C00143 C00153 C00156
 C00163 C00183 C00188 C00194 C00199 C00217 C00223 C00232
 C00234 C00250 C00251 C00253 C00255 C00266 C00268 C00272
 C00279 C00314 C00341 C00376 C00378 C00399 C00415 C00429
 C00430 C00440 C00445 C00455 C00472 C00473 C00474 C00486
 C00500 C00504 C00522 C00530 C00534 C00541 C00544 C00568
 C00627 C00647 C00664 C00725 C00748 C00777 C00811 C00828
 C00831 C00847 C00853 C00857 C00864 C00882 C00885 C00899
 C00900 C00921 C00922 C00931 C00966 C00971 C00992 C01004
 C01020 C01024 C01037 C01051 C01056 C01059 C01063 C01079
 C01081 C01092 C01134 C01179 C01185 C01215 C01217 C01230
 C01268 C01270 C01279 C01297 C01300 C01304 C01352 C01384
 C01596 C01727 C01847 C01894 C01909 C01967 C02059 C02094
 C02110 C02139 C02191 C02295 C02463 C02469 C02477 C02483
 C02588 C02642 C02656 C02691 C02730 C02800 C02823 C02880
 C02892 C02918 C02930 C02949 C03028 C03043 C03056 C03114
 C03150 C03160 C03194 C03263 C03373 C03393 C03455 C03458
 C03479 C03492 C03516 C03541 C03652 C03657 C03672 C03684
 C03722 C03741 C03885 C04039 C04079 C04122 C04145 C04146
 C04226 C04244 C04294 C04327 C04332 C04352 C04454 C04536
 C04556 C04604 C04732 C04752 C04773 C04778 C04807 C04874
 C04895 C05200 C05306 C05307 C05313 C05380 C05427 C05552
 C05766 C05767 C05768 C05769 C05770 C05772 C05773 C05774
 C05775 C05777 C05778 C05786 C05787 C05789 C05790 C05791
 C05793 C05794 C05795 C05797 C05798 C05802 C05804 C05805
 C05807 C05809 C05810 C05811 C05812 C05813 C05814 C05815

C05817 C05818 C05840 C05841 C05842 C05843 C05847 C05848
 C05856 C05912 C05913 C05921 C05924 C05925 C05926 C05944
 C06051 C06052 C06054 C06055 C06056 C06178 C06319 C06320
 C06399 C06406 C06407 C06408 C06416 C06503 C06504 C06505
 C06506 C06507 C06508 C06509 C06510 C06986 C07335 C09332
 C10385 C10793 C11061 C11242 C11355 C11437 C11538 C11539
 C11540 C11542 C11543 C11545 C11630 C11638 C11829 C11830
 C11831 C11832 C11850 C11851 C12147 C13309 C13425 C14151
 C14152 C14818 C14819 C15492 C15493 C15523 C15547 C15556
 C15563 C15670 C15672 C15809 C15882 C15883 C15986 C15987
 C16150 C16151 C16159 C16238 C16242 C16243 C16244 C16390
 C16519 C16541 C16677 C16678 C16680 C16681 C16682 C16683
 C16999 C17018 C17401 C17432 C17551 C17554 C17561 C17562
 C17568 C17569 C17570 C18021 C18022 C18064 C18098 C18131
 C18133 C18134 C18154 C18155 C18157 C18239

(II) 87 enzymes

YAR071W YBL013W YBL033C YBR035C YBR084W
 YBR092C YBR093C YBR145W YBR153W YBR176W
 YBR213W YBR256C YBR263W YCL009C YCL017C
 YCR053W YDL024C YDL045C YDL141W YDL168W
 YDL205C YDR019C YDR044W YDR047W YDR196C
 YDR232W YDR236C YDR402C YDR408C YDR481C
 YDR487C YDR531W YEL029C YER014W YER183C
 YFR047C YGL037C YGL040C YGL125W YGL245W
 YGL256W YGR010W YGR204W YGR267C YGR286C
 YHR063C YHR074W YHR208W YHR215W YIL145C
 YJL046W YJR016C YJR148W YKR069W YKR080W
 YLR028C YLR058C YLR209C YLR239C YLR328W
 YLR355C YMR083W YMR108W YMR120C YMR303C
 YNL256W YNR027W YNR033W YNR057C YNR058W
 YOL033W YOL055C YOL086C YOL096C YOR074C
 YOR143C YOR176W YOR184W YOR196C YOR209C
 YOR236W YOR278W YPL023C YPL214C YPL258C
 YPR073C YPR127W

9. 525 samples in “Metabolism of Terpenoids and Polyketides”

(I) 507 small molecules

C00002 C00008 C00015 C00019 C00020 C00022 C00024 C00029
 C00033 C00061 C00082 C00083 C00100 C00103 C00118 C00129
 C00136 C00147 C00170 C00187 C00190 C00196 C00235 C00251
 C00332 C00341 C00353 C00356 C00371 C00400 C00418 C00448
 C00477 C00521 C00553 C00621 C00630 C00688 C00744 C00805
 C00842 C00843 C00859 C00885 C00964 C00979 C01033 C01107
 C01123 C01126 C01143 C01164 C01179 C01230 C01414 C01433

C01457	C01499	C01500	C01512	C01513	C01661	C01699	C01767
C01789	C01804	C01841	C01847	C01848	C01852	C01860	C01907
C01912	C01920	C01946	C02004	C02029	C02034	C02035	C02094
C02344	C02400	C02452	C02462	C02485	C02513	C02557	C02576
C02633	C02811	C03069	C03190	C03198	C03220	C03240	C03319
C03423	C03461	C03579	C03590	C04083	C04145	C04146	C04171
C04216	C04268	C04435	C04574	C04713	C05413	C05414	C05427
C05430	C05431	C05432	C05433	C05434	C05435	C05821	C05859
C06069	C06071	C06074	C06076	C06082	C06087	C06088	C06089
C06090	C06091	C06092	C06093	C06094	C06095	C06098	C06099
C06111	C06307	C06308	C06394	C06570	C06571	C06616	C06624
C06627	C06630	C06633	C06634	C06635	C06654	C06691	C06769
C06801	C07271	C07276	C07277	C07330	C07394	C07667	C08579
C08583	C08584	C08585	C08586	C08590	C08591	C08592	C08601
C08606	C08614	C08814	C09094	C09118	C09183	C09190	C09621
C09629	C09665	C09666	C09672	C09684	C09694	C09699	C09704
C09707	C09723	C09769	C09844	C09847	C09848	C09849	C09871
C09880	C09884	C09893	C11383	C11384	C11386	C11388	C11389
C11393	C11395	C11398	C11402	C11403	C11405	C11406	C11407
C11408	C11409	C11410	C11411	C11412	C11413	C11414	C11415
C11416	C11417	C11418	C11419	C11421	C11434	C11435	C11436
C11437	C11453	C11636	C11672	C11673	C11700	C11811	C11853
C11854	C11855	C11857	C11858	C11859	C11860	C11861	C11862
C11863	C11864	C11865	C11867	C11868	C11869	C11870	C11871
C11872	C11873	C11874	C11875	C11878	C11879	C11880	C11881
C11882	C11883	C11887	C11889	C11893	C11894	C11895	C11897
C11900	C11901	C11902	C11907	C11908	C11911	C11912	C11916
C11918	C11920	C11921	C11924	C11933	C11938	C11939	C11940
C11941	C11942	C11943	C11944	C11945	C11946	C11950	C11951
C11952	C11967	C11971	C11983	C11989	C11990	C11993	C11994
C11995	C11996	C11997	C12000	C12002	C12014	C12026	C12037
C12038	C12044	C12077	C12106	C12107	C12108	C12109	C12142
C12176	C12210	C12212	C12213	C12214	C12215	C12216	C12219
C12220	C12221	C12246	C12247	C12319	C12321	C12323	C12324
C12325	C12366	C12367	C12368	C12369	C12370	C12371	C12376
C12378	C12379	C12381	C12382	C12383	C12384	C12387	C12388
C12389	C12390	C12391	C12392	C12393	C12395	C12396	C12397
C12398	C12399	C12400	C12401	C12402	C12404	C12406	C12412
C12413	C12414	C12415	C12416	C12417	C12419	C12420	C12421
C12422	C12423	C12424	C12425	C12426	C12427	C12428	C12429
C12430	C12432	C12434	C12435	C12436	C12451	C13273	C13431
C13433	C13453	C13454	C13455	C13456	C14540	C14721	C14722
C15514	C15545	C15546	C15784	C15785	C15786	C15787	C15788
C15789	C15790	C15791	C15792	C15793	C15794	C15795	C15797

C15798 C15799 C15800 C15801 C15802 C15803 C15859 C15860
 C15870 C15874 C15877 C15878 C15881 C15885 C15886 C15888
 C15892 C15895 C15898 C15900 C15902 C15903 C15908 C15943
 C15965 C15966 C15967 C15968 C15969 C15970 C15971 C15981
 C16028 C16141 C16142 C16143 C16144 C16145 C16146 C16147
 C16148 C16251 C16269 C16270 C16276 C16280 C16282 C16284
 C16286 C16291 C16340 C16427 C16430 C16431 C16441 C16447
 C16448 C16449 C16461 C16462 C16464 C16470 C16493 C16494
 C16495 C16496 C16497 C16499 C16500 C16502 C16503 C16504
 C16521 C16523 C16826 C16829 C17277 C17432 C17621 C17622
 C17733 C17735 C17953 C17954 C18015 C18025 C18037 C18211
 C18221 C18222 C18223 C18224 C18225 C18226 C18227 C18228
 C18229 C18295 C18297

(II) 18 enzymes

YBR117C YER073W YIL160C YJL167W YLR450W
 YML075C YML126C YMR208W YMR220W YNR016C
 YNR043W YOR274W YOR374W YPL028W YPL061W
 YPL069C YPL117C YPR074C

10. 526 samples in “Biosynthesis of Other Secondary Metabolites”

(I) 509 small molecules

C00002 C00025 C00031 C00043 C00047 C00048 C00061 C00062
 C00073 C00078 C00079 C00082 C00092 C00097 C00103 C00108
 C00118 C00123 C00132 C00134 C00137 C00141 C00148 C00166
 C00183 C00223 C00233 C00253 C00254 C00315 C00323 C00355
 C00385 C00389 C00398 C00406 C00407 C00408 C00411 C00413
 C00423 C00450 C00463 C00482 C00483 C00509 C00540 C00590
 C00616 C00671 C00688 C00691 C00729 C00745 C00757 C00761
 C00783 C00786 C00811 C00814 C00822 C00842 C00852 C00858
 C00903 C00916 C00933 C00956 C00974 C01091 C01121 C01138
 C01179 C01180 C01197 C01214 C01221 C01263 C01265 C01283
 C01294 C01298 C01378 C01416 C01441 C01456 C01460 C01470
 C01477 C01479 C01494 C01514 C01516 C01527 C01533 C01562
 C01610 C01617 C01672 C01701 C01709 C01735 C01737 C01743
 C01745 C01746 C01752 C01759 C01761 C01762 C01772 C01795
 C01847 C01851 C01852 C02046 C02066 C02074 C02105 C02106
 C02134 C02151 C02153 C02325 C02495 C02621 C02627 C02646
 C02666 C02673 C02675 C02723 C02887 C02890 C02906 C02916
 C02920 C02937 C02947 C02954 C03005 C03112 C03219 C03239
 C03319 C03329 C03442 C03470 C03506 C03515 C03567 C03582
 C03648 C03719 C03758 C03765 C03882 C03951 C04006 C04043
 C04076 C04092 C04118 C04271 C04280 C04293 C04353 C04443
 C04444 C04608 C04673 C04767 C04831 C04858 C05080 C05158
 C05174 C05175 C05176 C05177 C05178 C05179 C05189 C05191

C05193 C05194 C05202 C05220 C05243 C05315 C05316 C05376
 C05556 C05557 C05587 C05604 C05607 C05608 C05610 C05619
 C05623 C05625 C05627 C05631 C05837 C05838 C05851 C05901
 C05903 C05904 C05905 C05906 C05907 C05908 C05909 C05911
 C06160 C06161 C06162 C06165 C06167 C06171 C06172 C06173
 C06174 C06175 C06176 C06177 C06178 C06179 C06180 C06181
 C06182 C06183 C06185 C06224 C06327 C06366 C06511 C06516
 C06520 C06521 C06524 C06533 C06561 C06562 C06563 C06564
 C06565 C06566 C06568 C06569 C06655 C06656 C06657 C06658
 C06659 C06660 C06661 C06662 C07026 C07031 C07032 C07130
 C07201 C07204 C07304 C07307 C07475 C07480 C07481 C07592
 C07593 C07756 C08401 C08409 C08412 C08417 C08426 C08526
 C08532 C08537 C08538 C08539 C08540 C08543 C08544 C08552
 C08557 C08565 C08578 C08604 C08620 C08639 C08641 C08650
 C08725 C09024 C09099 C09126 C09239 C09244 C09248 C09320
 C09328 C09330 C09337 C09390 C09421 C09581 C09614 C09727
 C09751 C09756 C09762 C09789 C09806 C09826 C09827 C10028
 C10044 C10098 C10107 C10126 C10171 C10173 C10192 C10200
 C10205 C10208 C10216 C10434 C10462 C10502 C10503 C10509
 C10516 C10520 C10521 C10522 C10538 C10632 C10738 C10773
 C10783 C10850 C10858 C10860 C10865 C10945 C11130 C11250
 C11351 C11620 C11632 C11633 C11634 C11635 C11641 C11643
 C11675 C11676 C11677 C11678 C11679 C11680 C11682 C11783
 C11807 C11808 C11809 C11810 C11812 C11813 C11814 C11816
 C11817 C11907 C12032 C12092 C12093 C12096 C12123 C12125
 C12127 C12128 C12134 C12136 C12137 C12138 C12139 C12140
 C12141 C12162 C12173 C12203 C12204 C12205 C12206 C12208
 C12249 C12312 C12440 C12449 C12452 C12453 C12454 C12455
 C12456 C12457 C12458 C12468 C12473 C12474 C12476 C12477
 C12480 C12626 C12631 C12633 C12634 C12640 C12643 C12644
 C12646 C12647 C13747 C14314 C14536 C15509 C15525 C15530
 C15567 C15612 C15666 C15769 C15770 C15772 C16075 C16187
 C16190 C16191 C16192 C16195 C16197 C16222 C16223 C16225
 C16226 C16228 C16229 C16230 C16232 C16299 C16303 C16306
 C16315 C16352 C16353 C16355 C16356 C16357 C16358 C16359
 C16360 C16361 C16362 C16363 C16364 C16365 C16366 C16404
 C16406 C16416 C16417 C16418 C16419 C16422 C16700 C16709
 C16710 C16712 C17209 C17213 C17217 C17221 C17235 C17239
 C17245 C17246 C17250 C17254 C17580 C17581 C17582 C17585
 C17591 C17592 C17742 C17743 C17746 C17749 C17750 C17753
 C17754 C17755 C17756 C17757 C18004

(II) 17 enzymes

YCL040W YDR287W YDR402C YFR053C YGL202W
 YGL253W YHR046C YHR137W YHR208W YIL116W

YJL153C YJR148W YKL106W YKL127W YLR027C
YMR105C YMR278W

11. 730 samples in “Xenobiotics Biodegradation and Metabolism”

(I) 709 small molecules

C00011 C00022 C00024 C00036 C00042 C00048 C00058 C00067
C00084 C00086 C00090 C00091 C00108 C00122 C00146 C00156
C00160 C00163 C00164 C00180 C00186 C00196 C00209 C00222
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C02271 C02274 C02357 C02359 C02364 C02370 C02371 C02372
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C07111	C07113	C07114	C07118	C07163	C07185	C07189	C07208
C07209	C07211	C07212	C07213	C07214	C07215	C07216	C07446
C07447	C07490	C07492	C07493	C07495	C07496	C07501	C07535
C07557	C07572	C07585	C07643	C07644	C07645	C07646	C07647
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C07731	C07732	C07888	C08012	C08060	C08061	C08063	C08733
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C11149	C11150	C11173	C11249	C11272	C11348	C11376	C11422
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C14097	C14098	C14099	C14101	C14103	C14110	C14111	C14113
C14114	C14115	C14116	C14117	C14120	C14143	C14144	C14145
C14147	C14220	C14298	C14315	C14335	C14401	C14418	C14419
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C14783	C14785	C14786	C14787	C14788	C14789	C14790	C14839
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C14864	C14866	C14867	C14868	C14869	C14870	C14871	C14872
C14873	C14875	C14876	C14877	C16074	C16075	C16181	C16182
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C16207	C16208	C16209	C16211	C16212	C16213	C16215	C16234
C16235	C16246	C16247	C16248	C16262	C16266	C16267	C16268
C16272	C16273	C16281	C16283	C16348	C16391	C16392	C16393
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(II) 21 enzymes

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