

#	Substrate	Product	Condition	Replicate	Final rate	Fitting moc	Comment
1	Aco	Pyr	control	1			nd
2	Aco	Pyr	control	2			nd
3	Aco	Pyr	control	3			nd
4	Aco	Ssa	control	1			nd
5	Aco	Ssa	control	2			nd
6	Aco	Ssa	control	3			nd
7	Aco	Suc	control	1			no reliable decrease
8	Aco	Suc	control	2			no reliable decrease
9	Aco	Suc	control	3			no reliable decrease
10	Akg	Akg	control	1	0.029738	linform	
11	Akg	Akg	control	2	0.04689	linform	
12	Akg	Akg	control	3	0.013107	linform	
13	Akg	Mal	control	1	-0.00096	linform	
14	Akg	Mal	control	2	0.000426	linform	
15	Akg	Mal	control	3	3.33E-05	linform	
16	Akg	Pyr	control	1	0.001645	linform	
17	Akg	Pyr	control	2	-0.00096	linform	
18	Akg	Pyr	control	3	-0.00072	linform	
19	Akg	Suc	control	1	0.004688	linform	
20	Akg	Suc	control	2	0.00456	linform	
21	Akg	Suc	control	3	0.003864	linform	
22	Cit	Cit	control	1	0.028822	linform	low qual
23	Cit	Cit	control	2	-0.00706	linform	low qual
24	Cit	Cit	control	3	0.01378	linform	low qual
25	Cit	Pyr	control	1	-0.00031	linform	low qual
26	Cit	Pyr	control	2	0.000419	linform	low qual
27	Cit	Pyr	control	3	0.001868	linform	low qual
28	Cit	Suc	control	1	0.000888	linform	
29	Cit	Suc	control	2	0.000625	linform	
30	Cit	Suc	control	3	0.000565	linform	
31	Fum	Fum	control	1	0.035833	linform	
32	Fum	Fum	control	2	0.020377	linform	
33	Fum	Fum	control	3	0.032688	linform	
34	Fum	Pyr	control	1	-0.00141	linform	
35	Fum	Pyr	control	2	0.000866	linform	
36	Fum	Pyr	control	3	0.000273	linform	
37	Fum	Suc	control	1	0.003595	linform	
38	Fum	Suc	control	2	0.000524	linform	
39	Fum	Suc	control	3	0.000354	linform	
40	Iso	Aco	control	1	8.89E-05	linform	unreliable
41	Iso	Aco	control	2	0.00063	linform	unreliable
42	Iso	Aco	control	3	0.000711	linform	unreliable
43	Iso	Akg	control	1			nd
44	Iso	Akg	control	2			nd
45	Iso	Akg	control	3			nd
46	Iso	Cit	control	1	-0.0076	nlform	

47	Iso	Cit	control	2	-0.00451	nlform	
48	Iso	Cit	control	3	-0.00721	nlform	
49	Iso	Pyr	control	1			nd
50	Iso	Pyr	control	2			nd
51	Iso	Pyr	control	3			nd
52	Iso	Ssa	control	1			nd
53	Iso	Ssa	control	2			nd
54	Iso	Ssa	control	3			nd
55	Iso	Suc	control	1			nd
56	Iso	Suc	control	2			nd
57	Iso	Suc	control	3			nd
58	Mal	Mal	control	1	-0.0094	linform	
59	Mal	Mal	control	2	0.052024	linform	
60	Mal	Mal	control	3	0.000455	linform	
61	Mal	Pyr	control	1	-0.00119	linform	
62	Mal	Pyr	control	2	0.000724	linform	
63	Mal	Pyr	control	3	-0.00116	linform	
64	Mal	Suc	control	1	-0.00045	linform	
65	Mal	Suc	control	2	0.000804	linform	
66	Mal	Suc	control	3	0.00109	linform	
67	Suc	Aco	control	1	0.00669	exdc	
68	Suc	Aco	control	2	0.002608	exdc	
69	Suc	Aco	control	3	0.001964	exdc	
70	Suc	Pyr	control	1	7.48E-05	linform	
71	Suc	Pyr	control	2	0.0009	linform	
72	Suc	Pyr	control	3	-0.00038	linform	
73	Suc	Suc	control	1			nd
74	Suc	Suc	control	1			nd
75	Suc	Suc	control	2			nd
76	Suc	Suc	control	2			nd
77	Suc	Suc	control	3			nd
78	Suc	Suc	control	3			nd
79	Aco	Pyr	peroxydisu	1	0.005553	linform	
80	Aco	Pyr	peroxydisu	2	0.005477	linform	
81	Aco	Pyr	peroxydisu	3	0.008421	linform	
82	Aco	Ssa	peroxydisu	1	6.95E-07	linform	low quality
83	Aco	Ssa	peroxydisu	2	2.97E-07	linform	low quality
84	Aco	Ssa	peroxydisu	3	3.97E-07	linform	low quality
85	Aco	Suc	peroxydisu	1	-0.01485	linform	
86	Aco	Suc	peroxydisu	2	-0.03033	linform	
87	Aco	Suc	peroxydisu	3	-0.01879	linform	
88	Akg	Akg	peroxydisu	1	-0.1755	linform	
89	Akg	Akg	peroxydisu	2	-0.2187	linform	
90	Akg	Akg	peroxydisu	3	-0.1748	linform	
91	Akg	Mal	peroxydisu	1	0.009416	linform	
92	Akg	Mal	peroxydisu	2	0.007637	linform	
93	Akg	Mal	peroxydisu	3	0.007265	linform	

94	Akg	Pyr	peroxydisu	1	0.044902	nlform	
95	Akg	Pyr	peroxydisu	2	0.0501	nlform	
96	Akg	Pyr	peroxydisu	3	0.048099	nlform	
97	Akg	Suc	peroxydisu	1	0.438108	nlform	
98	Akg	Suc	peroxydisu	2	0.494169	nlform	
99	Akg	Suc	peroxydisu	3	0.438063	nlform	
100	Cit	Cit	peroxydisu	1	0.011897	linform	low qual
101	Cit	Cit	peroxydisu	2	-0.00107	linform	low qual
102	Cit	Cit	peroxydisu	3	0.002211	linform	low qual
103	Cit	Pyr	peroxydisu	1	0.001279	linform	low qual
104	Cit	Pyr	peroxydisu	2	0.002819	linform	low qual
105	Cit	Pyr	peroxydisu	3	0.002948	linform	low qual
106	Cit	Suc	peroxydisu	1	0.00182	linform	
107	Cit	Suc	peroxydisu	2	0.001464	linform	
108	Cit	Suc	peroxydisu	3	-0.00095	linform	
109	Fum	Fum	peroxydisu	1	-1.50185	nlform	
110	Fum	Fum	peroxydisu	2	-1.41881	nlform	
111	Fum	Fum	peroxydisu	3	-1.44352	nlform	
112	Fum	Pyr	peroxydisu	1	0.009846	linform	
113	Fum	Pyr	peroxydisu	2	0.013241	linform	
114	Fum	Pyr	peroxydisu	3	0.00952	linform	
115	Fum	Suc	peroxydisu	1	0.01011	nlform	
116	Fum	Suc	peroxydisu	2	0.004004	nlform	
117	Fum	Suc	peroxydisu	3	0.002536	nlform	
118	Iso	Aco	peroxydisu	1	-3.00E-05	linform	unreliable
119	Iso	Aco	peroxydisu	2	-4.87E-06	linform	unreliable
120	Iso	Aco	peroxydisu	3	-3.52E-05	linform	unreliable
121	Iso	Akg	peroxydisu	1	0.007321	linform	
122	Iso	Akg	peroxydisu	2	0.007642	linform	
123	Iso	Akg	peroxydisu	3	0.006636	linform	
124	Iso	Cit	peroxydisu	1	-0.07131	nlform	
125	Iso	Cit	peroxydisu	2	-0.06936	nlform	
126	Iso	Cit	peroxydisu	3	-0.06279	nlform	
127	Iso	Pyr	peroxydisu	1	0.009748	linform	
128	Iso	Pyr	peroxydisu	2	0.013362	linform	
129	Iso	Pyr	peroxydisu	3	0.00979	linform	
130	Iso	Ssa	peroxydisu	1	2.68E-05	linform	
131	Iso	Ssa	peroxydisu	2	7.13E-05	linform	
132	Iso	Ssa	peroxydisu	3	2.24E-05	linform	
133	Iso	Suc	peroxydisu	1	0.084718	nlform	
134	Iso	Suc	peroxydisu	2	0.0831	nlform	
135	Iso	Suc	peroxydisu	3	0.05253	nlform	
136	Mal	Mal	peroxydisu	1	-0.18451	linform	
137	Mal	Mal	peroxydisu	2	-0.24198	linform	
138	Mal	Mal	peroxydisu	3	-0.16712	linform	
139	Mal	Pyr	peroxydisu	1	0.262853	linform	
140	Mal	Pyr	peroxydisu	2	0.380588	linform	

141	Mal	Pyr	peroxydisu	3	0.377526	linform	
142	Mal	Suc	peroxydisu	1	0.002589	linform	
143	Mal	Suc	peroxydisu	2	0.001653	linform	
144	Mal	Suc	peroxydisu	3	0.003283	linform	
145	Suc	Aco	peroxydisu	1	0.017124	exdc	
146	Suc	Aco	peroxydisu	2	0.021769	exdc	
147	Suc	Aco	peroxydisu	3	0.01611	exdc	
148	Suc	Pyr	peroxydisu	1	0.047347	linform	
149	Suc	Pyr	peroxydisu	2	0.048926	linform	
150	Suc	Pyr	peroxydisu	3	0.046438	linform	
151	Suc	Suc	peroxydisu	1	2.51E-06	linform	
152	Suc	Suc	peroxydisu	1	0.002248	linform	
153	Suc	Suc	peroxydisu	2	4.46E-06	linform	
154	Suc	Suc	peroxydisu	2	0.00272	linform	
155	Suc	Suc	peroxydisu	3	2.06E-06	linform	
156	Suc	Suc	peroxydisu	3	0.001812	linform	
157	Aco	Pyr	peroxydisu	1	0.003598	linform	
158	Aco	Pyr	peroxydisu	2	0.003216	linform	
159	Aco	Pyr	peroxydisu	3	0.003244	linform	
160	Aco	Ssa	peroxydisu	1			nd
161	Aco	Ssa	peroxydisu	2			nd
162	Aco	Ssa	peroxydisu	3			nd
163	Aco	Suc	peroxydisu	1			no reliable decrease
164	Aco	Suc	peroxydisu	2			no reliable decrease
165	Aco	Suc	peroxydisu	3			no reliable decrease
166	Akg	Akg	peroxydisu	1	0.055254	linform	
167	Akg	Akg	peroxydisu	2	0.076368	linform	
168	Akg	Akg	peroxydisu	3	0.052658	linform	
169	Akg	Mal	peroxydisu	1	-0.00126	linform	
170	Akg	Mal	peroxydisu	2	0.000487	linform	
171	Akg	Mal	peroxydisu	3	-0.00048	linform	
172	Akg	Pyr	peroxydisu	1	-0.00116	linform	
173	Akg	Pyr	peroxydisu	2	0.000869	linform	
174	Akg	Pyr	peroxydisu	3	0.001748	linform	
175	Akg	Suc	peroxydisu	1	0.03015	linform	
176	Akg	Suc	peroxydisu	2	0.007146	linform	
177	Akg	Suc	peroxydisu	3	0.028147	linform	
178	Cit	Cit	peroxydisu	1	0.024614	linform	low qual
179	Cit	Cit	peroxydisu	2	-2.49E-05	linform	low qual
180	Cit	Cit	peroxydisu	3	0.004818	linform	low qual
181	Cit	Pyr	peroxydisu	1	0.00231	linform	low qual
182	Cit	Pyr	peroxydisu	2	0.00241	linform	low qual
183	Cit	Pyr	peroxydisu	3	0.001769	linform	low qual
184	Cit	Suc	peroxydisu	1	-0.00026	linform	
185	Cit	Suc	peroxydisu	2	-0.00014	linform	
186	Cit	Suc	peroxydisu	3	0.000095	linform	
187	Fum	Fum	peroxydisu	1	-1.96032	nlform	

188	Fum	Fum	peroxydisu	2	-1.77137	nlform	
189	Fum	Fum	peroxydisu	3	-1.93382	nlform	
190	Fum	Pyr	peroxydisu	1	-0.0008	linform	
191	Fum	Pyr	peroxydisu	2	-0.00573	linform	
192	Fum	Pyr	peroxydisu	3	0.001874	linform	
193	Fum	Suc	peroxydisu	1	-0.00142	linform	
194	Fum	Suc	peroxydisu	2	0.000899	linform	
195	Fum	Suc	peroxydisu	3	0.000366	linform	
196	Iso	Aco	peroxydisu	1	0.000267	linform	unreliable
197	Iso	Aco	peroxydisu	2	0.000232	linform	unreliable
198	Iso	Aco	peroxydisu	3	0.000374	linform	unreliable
199	Iso	Akg	peroxydisu	1			nd
200	Iso	Akg	peroxydisu	2			nd
201	Iso	Akg	peroxydisu	3			nd
202	Iso	Cit	peroxydisu	1	-0.04942	nlform	
203	Iso	Cit	peroxydisu	2	-0.04104	nlform	
204	Iso	Cit	peroxydisu	3	-0.03599	nlform	
205	Iso	Pyr	peroxydisu	1	0.000226	linform	
206	Iso	Pyr	peroxydisu	2	0.00053	linform	
207	Iso	Pyr	peroxydisu	3	0.002076	linform	
208	Iso	Ssa	peroxydisu	1	2.71E-05	linform	
209	Iso	Ssa	peroxydisu	2	2.27E-05	linform	
210	Iso	Ssa	peroxydisu	3	2.15E-05	linform	
211	Iso	Suc	peroxydisu	1	0.006307	nlform	
212	Iso	Suc	peroxydisu	2	0.007355	nlform	
213	Iso	Suc	peroxydisu	3	0.002788	nlform	
214	Mal	Mal	peroxydisu	1	0.118417	linform	
215	Mal	Mal	peroxydisu	2	0.044913	linform	
216	Mal	Mal	peroxydisu	3	0.103536	linform	
217	Mal	Pyr	peroxydisu	1	0.003446	linform	
218	Mal	Pyr	peroxydisu	2	0.002643	linform	
219	Mal	Pyr	peroxydisu	3	0.003582	linform	
220	Mal	Suc	peroxydisu	1	0.000311	linform	
221	Mal	Suc	peroxydisu	2	-1.20E-05	linform	
222	Mal	Suc	peroxydisu	3	-9.86E-05	linform	
223	Suc	Aco	peroxydisu	1			nd
224	Suc	Aco	peroxydisu	2			nd
225	Suc	Aco	peroxydisu	3			nd
226	Suc	Pyr	peroxydisu	1	0.005104	linform	
227	Suc	Pyr	peroxydisu	2	0.004016	linform	
228	Suc	Pyr	peroxydisu	3	0.003442	linform	
229	Suc	Suc	peroxydisu	1	6.55E-06	linform	
230	Suc	Suc	peroxydisu	1	0.000276	linform	
231	Suc	Suc	peroxydisu	2	7.85E-06	linform	
232	Suc	Suc	peroxydisu	2	0.000434	linform	
233	Suc	Suc	peroxydisu	3	3.95E-06	linform	
234	Suc	Suc	peroxydisu	3	0.000195	linform	

235	Aco	Pyr	peroxydisu	1	0.00837	linform	
236	Aco	Pyr	peroxydisu	2	0.006079	linform	
237	Aco	Pyr	peroxydisu	3	0.008468	linform	
238	Aco	Ssa	peroxydisu	1	1.19E-06	linform	low quality
239	Aco	Ssa	peroxydisu	2	6.26E-07	linform	low quality
240	Aco	Ssa	peroxydisu	3	2.28E-07	linform	low quality
241	Aco	Suc	peroxydisu	1			no reliable decrease
242	Aco	Suc	peroxydisu	2			no reliable decrease
243	Aco	Suc	peroxydisu	3			no reliable decrease
244	Akg	Akg	peroxydisu	1	-0.07265	linform	
245	Akg	Akg	peroxydisu	2	-0.04245	linform	
246	Akg	Akg	peroxydisu	3	-0.10556	linform	
247	Akg	Mal	peroxydisu	1	0.006096	linform	
248	Akg	Mal	peroxydisu	2	0.00384	linform	
249	Akg	Mal	peroxydisu	3	0.001755	linform	
250	Akg	Pyr	peroxydisu	1	0.058946	nlform	
251	Akg	Pyr	peroxydisu	2	0.058238	nlform	
252	Akg	Pyr	peroxydisu	3	0.044174	nlform	
253	Akg	Suc	peroxydisu	1	0.387414	nlform	
254	Akg	Suc	peroxydisu	2	0.404046	nlform	
255	Akg	Suc	peroxydisu	3	0.318542	nlform	
256	Cit	Cit	peroxydisu	1	0.054369	linform	low qual
257	Cit	Cit	peroxydisu	2	0.001441	linform	low qual
258	Cit	Cit	peroxydisu	3	0.004039	linform	low qual
259	Cit	Pyr	peroxydisu	1	0.00018	linform	low qual
260	Cit	Pyr	peroxydisu	2	0.002926	linform	low qual
261	Cit	Pyr	peroxydisu	3	0.003554	linform	low qual
262	Cit	Suc	peroxydisu	1	0.000846	linform	
263	Cit	Suc	peroxydisu	2	0.001036	linform	
264	Cit	Suc	peroxydisu	3	0.000681	linform	
265	Fum	Fum	peroxydisu	1	-0.92355	nlform	
266	Fum	Fum	peroxydisu	2	-0.92612	nlform	
267	Fum	Fum	peroxydisu	3	-0.81325	nlform	
268	Fum	Pyr	peroxydisu	1	0.00242	linform	
269	Fum	Pyr	peroxydisu	2	0.00325	linform	
270	Fum	Pyr	peroxydisu	3	0.003598	linform	
271	Fum	Suc	peroxydisu	1	0.000702	linform	
272	Fum	Suc	peroxydisu	2	0.002509	linform	
273	Fum	Suc	peroxydisu	3	0.001886	linform	
274	Iso	Aco	peroxydisu	1	0.000222	linform	unreliable
275	Iso	Aco	peroxydisu	2	0.000173	linform	unreliable
276	Iso	Aco	peroxydisu	3	0.000107	linform	unreliable
277	Iso	Akg	peroxydisu	1	0.003992	linform	
278	Iso	Akg	peroxydisu	2	0.003424	linform	
279	Iso	Akg	peroxydisu	3	0.004034	linform	
280	Iso	Cit	peroxydisu	1	-0.05737	nlform	
281	Iso	Cit	peroxydisu	2	-0.06204	nlform	

282	Iso	Cit	peroxydisu	3	-0.0563	nlform	
283	Iso	Pyr	peroxydisu	1	0.00667	linform	
284	Iso	Pyr	peroxydisu	2	0.006648	linform	
285	Iso	Pyr	peroxydisu	3	0.006423	linform	
286	Iso	Ssa	peroxydisu	1	3.09E-05	linform	
287	Iso	Ssa	peroxydisu	2	3.88E-05	linform	
288	Iso	Ssa	peroxydisu	3	2.46E-05	linform	
289	Iso	Suc	peroxydisu	1	0.041464	nlform	
290	Iso	Suc	peroxydisu	2	0.087802	nlform	
291	Iso	Suc	peroxydisu	3	0.036189	nlform	
292	Mal	Mal	peroxydisu	1	-0.03914	linform	
293	Mal	Mal	peroxydisu	2	-0.04933	linform	
294	Mal	Mal	peroxydisu	3	-0.02194	linform	
295	Mal	Pyr	peroxydisu	1	0.095974	linform	
296	Mal	Pyr	peroxydisu	2	0.124043	linform	
297	Mal	Pyr	peroxydisu	3	0.099042	linform	
298	Mal	Suc	peroxydisu	1	0.001563	linform	
299	Mal	Suc	peroxydisu	2	0.003768	linform	
300	Mal	Suc	peroxydisu	3	0.000798	linform	
301	Suc	Aco	peroxydisu	1			nd
302	Suc	Aco	peroxydisu	2	0.005055	exdc	
303	Suc	Aco	peroxydisu	3	0.007866	exdc	
304	Suc	Pyr	peroxydisu	1	0.017116	linform	
305	Suc	Pyr	peroxydisu	2	0.018588	linform	
306	Suc	Pyr	peroxydisu	3	0.019223	linform	
307	Suc	Suc	peroxydisu	1	8.71E-06	linform	
308	Suc	Suc	peroxydisu	1	0.002091	linform	
309	Suc	Suc	peroxydisu	2	8.78E-06	linform	
310	Suc	Suc	peroxydisu	2	0.002198	linform	
311	Suc	Suc	peroxydisu	3	2.77E-06	linform	
312	Suc	Suc	peroxydisu	3	0.001372	linform	
313	Aco	Pyr	hydrogen ç	1			nd
314	Aco	Pyr	hydrogen ç	2			nd
315	Aco	Pyr	hydrogen ç	3			nd
316	Aco	Ssa	hydrogen ç	1			nd
317	Aco	Ssa	hydrogen ç	2			nd
318	Aco	Ssa	hydrogen ç	3			nd
319	Aco	Suc	hydrogen ç	1			no reliable decrease
320	Aco	Suc	hydrogen ç	2			no reliable decrease
321	Aco	Suc	hydrogen ç	3			no reliable decrease
322	Akg	Akg	hydrogen ç	1	-0.00203	linform	
323	Akg	Akg	hydrogen ç	2	0.000702	linform	
324	Akg	Akg	hydrogen ç	3	0.004521	linform	
325	Akg	Mal	hydrogen ç	1	-0.00043	linform	
326	Akg	Mal	hydrogen ç	2	-0.00094	linform	
327	Akg	Mal	hydrogen ç	3	0.001937	linform	
328	Akg	Pyr	hydrogen ç	1	-0.00115	linform	

329	Akg	Pyr	hydrogen ç	2	-0.00081	linform	
330	Akg	Pyr	hydrogen ç	3	0.001688	linform	
331	Akg	Suc	hydrogen ç	1	0.093769	linform	
332	Akg	Suc	hydrogen ç	2	0.205736	linform	
333	Akg	Suc	hydrogen ç	3	0.214886	linform	
334	Cit	Cit	hydrogen ç	1	0.065146	linform	low qual
335	Cit	Cit	hydrogen ç	2	0.001098	linform	low qual
336	Cit	Cit	hydrogen ç	3	0.003153	linform	low qual
337	Cit	Pyr	hydrogen ç	1	-0.00128	linform	low qual
338	Cit	Pyr	hydrogen ç	2	-0.00158	linform	low qual
339	Cit	Pyr	hydrogen ç	3	-0.00112	linform	low qual
340	Cit	Suc	hydrogen ç	1	6.14E-06	linform	
341	Cit	Suc	hydrogen ç	2	0.000284	linform	
342	Cit	Suc	hydrogen ç	3	0.000223	linform	
343	Fum	Fum	hydrogen ç	1	0.54686	linform	
344	Fum	Fum	hydrogen ç	2	0.131686	linform	
345	Fum	Fum	hydrogen ç	3	-0.01191	linform	
346	Fum	Pyr	hydrogen ç	1	0.002109	linform	
347	Fum	Pyr	hydrogen ç	2	0.001035	linform	
348	Fum	Pyr	hydrogen ç	3	-0.00071	linform	
349	Fum	Suc	hydrogen ç	1	0.002566	linform	
350	Fum	Suc	hydrogen ç	2	0.002287	linform	
351	Fum	Suc	hydrogen ç	3	0.001005	linform	
352	Iso	Aco	hydrogen ç	1	6.55E-05	linform	unreliable
353	Iso	Aco	hydrogen ç	2	8.62E-05	linform	unreliable
354	Iso	Aco	hydrogen ç	3	8.68E-05	linform	unreliable
355	Iso	Akg	hydrogen ç	1			nd
356	Iso	Akg	hydrogen ç	2			nd
357	Iso	Akg	hydrogen ç	3			nd
358	Iso	Cit	hydrogen ç	1	-0.02081	nlform	
359	Iso	Cit	hydrogen ç	2	-0.00242	nlform	
360	Iso	Cit	hydrogen ç	3	-0.00727	nlform	
361	Iso	Pyr	hydrogen ç	1			nd
362	Iso	Pyr	hydrogen ç	2			nd
363	Iso	Pyr	hydrogen ç	3			nd
364	Iso	Ssa	hydrogen ç	1			nd
365	Iso	Ssa	hydrogen ç	2			nd
366	Iso	Ssa	hydrogen ç	3			nd
367	Iso	Suc	hydrogen ç	1	-0.00121	nlform	
368	Iso	Suc	hydrogen ç	2	0.000358	nlform	
369	Iso	Suc	hydrogen ç	3	0.000148	nlform	
370	Mal	Mal	hydrogen ç	1	0.040324	linform	
371	Mal	Mal	hydrogen ç	2	0.080925	linform	
372	Mal	Mal	hydrogen ç	3	0.085346	linform	
373	Mal	Pyr	hydrogen ç	1	0.002009	linform	
374	Mal	Pyr	hydrogen ç	2	-0.0008	linform	
375	Mal	Pyr	hydrogen ç	3	0.00325	linform	

376	Mal	Suc	hydrogen p	1	0.000996	linform	
377	Mal	Suc	hydrogen p	2	0.000896	linform	
378	Mal	Suc	hydrogen p	3	8.70E-05	linform	
379	Suc	Aco	hydrogen p	1	0.013674	exdc	
380	Suc	Aco	hydrogen p	2	0.012143	exdc	
381	Suc	Aco	hydrogen p	3	0.008535	exdc	
382	Suc	Pyr	hydrogen p	1			nd
383	Suc	Pyr	hydrogen p	2			nd
384	Suc	Pyr	hydrogen p	3			nd
385	Suc	Suc	hydrogen p	1			nd
386	Suc	Suc	hydrogen p	1	0.000315	linform	
387	Suc	Suc	hydrogen p	2			nd
388	Suc	Suc	hydrogen p	2	0.000167	linform	
389	Suc	Suc	hydrogen p	3			nd
390	Suc	Suc	hydrogen p	3	0.000201	linform	
391	Aco	Pyr	hydrogen p	1			nd
392	Aco	Pyr	hydrogen p	2			nd
393	Aco	Pyr	hydrogen p	3			nd
394	Aco	Ssa	hydrogen p	1			nd
395	Aco	Ssa	hydrogen p	2			nd
396	Aco	Ssa	hydrogen p	3			nd
397	Aco	Suc	hydrogen p	1			no reliable decrease
398	Aco	Suc	hydrogen p	2			no reliable decrease
399	Aco	Suc	hydrogen p	3			no reliable decrease
400	Akg	Akg	hydrogen p	1	0.005462	linform	
401	Akg	Akg	hydrogen p	2	-0.01542	linform	
402	Akg	Akg	hydrogen p	3	0.011416	linform	
403	Akg	Mal	hydrogen p	1	-0.00306	linform	
404	Akg	Mal	hydrogen p	2	-0.00127	linform	
405	Akg	Mal	hydrogen p	3	-0.00062	linform	
406	Akg	Pyr	hydrogen p	1	-0.00099	linform	
407	Akg	Pyr	hydrogen p	2	0.000287	linform	
408	Akg	Pyr	hydrogen p	3	0.001601	linform	
409	Akg	Suc	hydrogen p	1	0.069192	linform	
410	Akg	Suc	hydrogen p	2	-0.01891	linform	
411	Akg	Suc	hydrogen p	3	0.100414	linform	
412	Cit	Cit	hydrogen p	1	0.024689	linform	low qual
413	Cit	Cit	hydrogen p	2	-8.03E-06	linform	low qual
414	Cit	Cit	hydrogen p	3	0.005166	linform	low qual
415	Cit	Pyr	hydrogen p	1	-0.00208	linform	low qual
416	Cit	Pyr	hydrogen p	2	0.000414	linform	low qual
417	Cit	Pyr	hydrogen p	3	-0.00086	linform	low qual
418	Cit	Suc	hydrogen p	1	-3.47E-05	linform	
419	Cit	Suc	hydrogen p	2	0.000114	linform	
420	Cit	Suc	hydrogen p	3	0.000661	linform	
421	Fum	Fum	hydrogen p	1	0.072776	linform	
422	Fum	Fum	hydrogen p	2	0.098182	linform	

423	Fum	Fum	hydrogen ç	3	0.022677	linform	
424	Fum	Pyr	hydrogen ç	1	-0.00036	linform	
425	Fum	Pyr	hydrogen ç	2	0.000438	linform	
426	Fum	Pyr	hydrogen ç	3	0.00069	linform	
427	Fum	Suc	hydrogen ç	1	0.003474	linform	
428	Fum	Suc	hydrogen ç	2	0.000988	linform	
429	Fum	Suc	hydrogen ç	3	0.00097	linform	
430	Iso	Aco	hydrogen ç	1	-4.99E-06	linform	unreliable
431	Iso	Aco	hydrogen ç	2	4.52E-05	linform	unreliable
432	Iso	Aco	hydrogen ç	3	3.21E-05	linform	unreliable
433	Iso	Akg	hydrogen ç	1			nd
434	Iso	Akg	hydrogen ç	2			nd
435	Iso	Akg	hydrogen ç	3			nd
436	Iso	Cit	hydrogen ç	1	-0.0244	nlform	
437	Iso	Cit	hydrogen ç	2	-0.01887	nlform	
438	Iso	Cit	hydrogen ç	3	-0.02529	nlform	
439	Iso	Pyr	hydrogen ç	1			nd
440	Iso	Pyr	hydrogen ç	2			nd
441	Iso	Pyr	hydrogen ç	3			nd
442	Iso	Ssa	hydrogen ç	1			nd
443	Iso	Ssa	hydrogen ç	2			nd
444	Iso	Ssa	hydrogen ç	3			nd
445	Iso	Suc	hydrogen ç	1	0.000857	nlform	
446	Iso	Suc	hydrogen ç	2	0.000103	nlform	
447	Iso	Suc	hydrogen ç	3	1.56E-05	lform	
448	Mal	Mal	hydrogen ç	1	0.070443	linform	
449	Mal	Mal	hydrogen ç	2	0.115035	linform	
450	Mal	Mal	hydrogen ç	3	0.026317	linform	
451	Mal	Pyr	hydrogen ç	1	-0.00082	linform	
452	Mal	Pyr	hydrogen ç	2	-0.0004	linform	
453	Mal	Pyr	hydrogen ç	3	0.000994	linform	
454	Mal	Suc	hydrogen ç	1	-0.00084	linform	
455	Mal	Suc	hydrogen ç	2	0.000343	linform	
456	Mal	Suc	hydrogen ç	3	0.000515	linform	
457	Suc	Aco	hydrogen ç	1	0.003966	exdc	
458	Suc	Aco	hydrogen ç	2	0.015326	exdc	
459	Suc	Aco	hydrogen ç	3	0.021581	exdc	
460	Suc	Pyr	hydrogen ç	1			nd
461	Suc	Pyr	hydrogen ç	2			nd
462	Suc	Pyr	hydrogen ç	3			nd
463	Suc	Suc	hydrogen ç	1	1.81E-07	linform	low quality
464	Suc	Suc	hydrogen ç	1			nd
465	Suc	Suc	hydrogen ç	2	5.85E-07	linform	low quality
466	Suc	Suc	hydrogen ç	2			nd
467	Suc	Suc	hydrogen ç	3	5.85E-07	linform	low quality
468	Suc	Suc	hydrogen ç	3			nd
469	Aco	Pyr	hydrogen ç	1			nd

470	Aco	Pyr	hydrogen ç	2		nd
471	Aco	Pyr	hydrogen ç	3		nd
472	Aco	Ssa	hydrogen ç	1		nd
473	Aco	Ssa	hydrogen ç	2		nd
474	Aco	Ssa	hydrogen ç	3		nd
475	Aco	Suc	hydrogen ç	1		no reliable decrease
476	Aco	Suc	hydrogen ç	2		no reliable decrease
477	Aco	Suc	hydrogen ç	3		no reliable decrease
478	Akg	Akg	hydrogen ç	1	0.010214	linform
479	Akg	Akg	hydrogen ç	2	0.048385	linform
480	Akg	Akg	hydrogen ç	3	0.016832	linform
481	Akg	Mal	hydrogen ç	1	0.001194	linform
482	Akg	Mal	hydrogen ç	2	0.002872	linform
483	Akg	Mal	hydrogen ç	3	0.004257	linform
484	Akg	Pyr	hydrogen ç	1	-0.00218	linform
485	Akg	Pyr	hydrogen ç	2	-0.00046	linform
486	Akg	Pyr	hydrogen ç	3	-0.00068	linform
487	Akg	Suc	hydrogen ç	1	0.07787	linform
488	Akg	Suc	hydrogen ç	2	0.088904	linform
489	Akg	Suc	hydrogen ç	3	0.145998	linform
490	Cit	Cit	hydrogen ç	1	0.033828	linform low qual
491	Cit	Cit	hydrogen ç	2	0.001663	linform low qual
492	Cit	Cit	hydrogen ç	3	0.01456	linform low qual
493	Cit	Pyr	hydrogen ç	1	0.000425	linform low qual
494	Cit	Pyr	hydrogen ç	2	4.76E-05	linform low qual
495	Cit	Pyr	hydrogen ç	3	-0.00112	linform low qual
496	Cit	Suc	hydrogen ç	1	0.000415	linform
497	Cit	Suc	hydrogen ç	2	0.000168	linform
498	Cit	Suc	hydrogen ç	3	0.000111	linform
499	Fum	Fum	hydrogen ç	1	0.045535	linform
500	Fum	Fum	hydrogen ç	2	0.032039	linform
501	Fum	Fum	hydrogen ç	3	0.09357	linform
502	Fum	Pyr	hydrogen ç	1	-9.10E-05	linform
503	Fum	Pyr	hydrogen ç	2	0.000957	linform
504	Fum	Pyr	hydrogen ç	3	-0.00257	linform
505	Fum	Suc	hydrogen ç	1	-0.00012	linform
506	Fum	Suc	hydrogen ç	2	-0.0001	linform
507	Fum	Suc	hydrogen ç	3	-0.0001	linform
508	Iso	Aco	hydrogen ç	1	6.74E-06	linform unreliable
509	Iso	Aco	hydrogen ç	2	3.03E-05	linform unreliable
510	Iso	Aco	hydrogen ç	3	-2.57E-06	linform unreliable
511	Iso	Akg	hydrogen ç	1		nd
512	Iso	Akg	hydrogen ç	2		nd
513	Iso	Akg	hydrogen ç	3		nd
514	Iso	Cit	hydrogen ç	1	-0.01808	nlform
515	Iso	Cit	hydrogen ç	2	-0.01647	nlform
516	Iso	Cit	hydrogen ç	3	-0.02696	nlform

517	Iso	Pyr	hydrogen ç	1			nd
518	Iso	Pyr	hydrogen ç	2			nd
519	Iso	Pyr	hydrogen ç	3			nd
520	Iso	Ssa	hydrogen ç	1	4.47E-07	linform	
521	Iso	Ssa	hydrogen ç	2	6.66E-07	linform	
522	Iso	Ssa	hydrogen ç	3	1.12E-06	linform	
523	Iso	Suc	hydrogen ç	1			nd
524	Iso	Suc	hydrogen ç	2			nd
525	Iso	Suc	hydrogen ç	3			nd
526	Mal	Mal	hydrogen ç	1	0.023334	linform	
527	Mal	Mal	hydrogen ç	2	0.03639	linform	
528	Mal	Mal	hydrogen ç	3	-0.02328	linform	
529	Mal	Pyr	hydrogen ç	1	-0.00032	linform	
530	Mal	Pyr	hydrogen ç	2	0.001574	linform	
531	Mal	Pyr	hydrogen ç	3	-0.00059	linform	
532	Mal	Suc	hydrogen ç	1	0.001059	linform	
533	Mal	Suc	hydrogen ç	2	0.000359	linform	
534	Mal	Suc	hydrogen ç	3	0.00067	linform	
535	Suc	Aco	hydrogen ç	1			nd
536	Suc	Aco	hydrogen ç	2	0.003838	exdc	
537	Suc	Aco	hydrogen ç	3	0.008763	exdc	
538	Suc	Pyr	hydrogen ç	1			nd
539	Suc	Pyr	hydrogen ç	2			nd
540	Suc	Pyr	hydrogen ç	3			nd
541	Suc	Suc	hydrogen ç	1	7.38E-07	linform	low quality
542	Suc	Suc	hydrogen ç	1			nd
543	Suc	Suc	hydrogen ç	2	9.52E-07	linform	low quality
544	Suc	Suc	hydrogen ç	2			nd
545	Suc	Suc	hydrogen ç	3	1.47E-06	linform	low quality
546	Suc	Suc	hydrogen ç	3			nd