Table 2: *H. sapiens* **Recon 1 simulation list.** A complete list of the 288 simulations used to validate Recon 1. Objective column # refers to the column in SI Table 4 that is optimized in the flux balance analysis simulation.

Simulation #	Simulation Name	Objective Column #
1	His -> glu-L	697
2	hista -> im4ac	760
3	his-L -> hista	749
4	hista -> 3mlda	481
5	pro-L -> glu-L	698
6	glu-L -> pro-L	877
7	arg-L -> glu-L (m)	698
8	ATP max aerobic, glc, v0.05	11
9	arg-L -> no	827
10	asp-L + hco3 -> arg-L	553
11	ptrc -> ala-B	537
12	ura -> ala-B	537
13	carn -> ala-B	537
14	msa -> ala-B	537
15	ala-B -> msa	800
16	ptrc -> spmd	904
17	spmd -> sprm	905
18	ala-L -> ala-D	538
19	ala-D -> pyr	881
20	ATP max, anaerobic glc, v0.05	11
21	gln-L(m) -> glu-L(m)	698
22	glu-L(m) -> akg(m)	535
23	cys-L + glu-L + gly -> ghtrd	720
24	gthrd reduces h2o2	719
25	phe-L -> tyr-L	930
26	phe-L -> phpyr	861
27	phe-L -> pheacgln	858
28	phe-L -> peamn	853
29	phe-L -> pacald	842
30	phe-L -> pac	841
31	phe-L -> phaccoa	856
32	selmeth -> selnp	899
33	dna(n) -> dna5mtc(n)	624
34	cys-L -> hyptaur	756
35	hyptaur(c) -> taur(x)	912
36	Lcyst(c) -> taur(x)	912
37	taur(x) -> tchola(x)	913
38	trp-L -> accoa	511
39	trp-L -> srtn	907
40	trp-L -> melatn	791
41	trp-L -> Lfmkynr	495
42	trp-L -> Lkynr	496
43	trp-L -> nformanth	821
44	srtn -> 5moxact	488
45	srtn -> 6hoxmelatn	490
46	srtn -> fna5moxam	659
47	srtn -> nmthsrtn	826

Simulation #	Simulation Name	Objective Column #
48	srtn -> f5hoxkyn	644
49	trp-L -> quln	887
50	trp-L -> id3acald	757
51	trp-L -> anth	550
52	trp-L -> kynate	774
53	tyr-L -> fum + acac	508
54	tyr-L -> T3 + T4	924
55	tyr-L -> 34hpp	479
56	tyr-L -> nrpphr	828
57	tyr-L -> adrnl	530
58	tyr-L -> melanin	790
59	tyr-L -> 4hphac	484
60	tyr-L -> dopa	633
61	dopa -> homoval (1)	751
62	dopa -> homoval (2)	751
63	npphr -> 34dhoxpeg	478
64	adrnl -> 34dhoxpeg	478
65	adrnl -> 34dhoxpeg (2)	478
66	arg -> no	827
67	orn -> ptrc	879
68	orn -> spmd	904
69	orn -> sprm	905
70	arg-L -> pcreat	850
71	arg-L -> creat	593
72	glu5sa -> pro-L	876
73	tyr-L -> T3 + T4 (2)	924
74	adrnl -> 34dhoxpeg (3)	478
75	dmpp -> ggdp	691
76	ipdp(x) -> sql(r)	906
77	coke(r) -> pecgoncoa(r)	854
78	acorn -> orn	839
79	4hpro-LT(m) -> glx(m)	702
80	lys-L [c] -->accoa [m] (via saccrp-L pathway)	513
81	akg[c] --> glu-L[c] via ALATA_L	697
82	akg[c] --> glu-L[c] via ASPTA	697
83	akg[m] --> glu-L[m] via ASPTAm	698
84	glu-L-->gln-L[c]	694
85	gln-L[m]-->glu-L[m]	698
86	4abut --> succ [m]	908
87	glu-L-->4abut	483
88	lys-L[x] -->aacoa [m] (via Lpipecol pathway)	513
89	3pg-->ser-L	900
90	3pg-->gly	704
91	gly --> co2 and nh4 (via glycine cleavage system)	582
92	thr-L --> ppcoa	868
93	ser-L-->cys-L	610
94	choline --> betaine --> glycine	705

Simulation #	Simulation Name	Objective Column #
95	met-L-->cys-L	610
96	cys-L--> 3sala -->so4	901
97	leu-L --> accoa	513
98	ile-L -->accoa	869
99	val-L --> succoa	910
100	gly -->ser-L --> pyr (via SERD_L)	881
101	cystine -->cys-L	610
102	so4 --> PAPS	847
103	o2- --> h2o2 --> o2 + h2o	830
104	ATP production via electron transport chain	560
105	5aop -->pheme	860
106	asp-L-->asn-L	556
107	asp-L --> oaa	835
108	asn-L --> oaa	835
109	asp-L-->ala-B	537
110	pyr<>ala-L	881
111	ala-L-->pyr	881
112	asp-L-->fum (via dcamp)	667
113	asp-L-->fum (via argsuc)	667
114	pheme-->bilirub	565
115	glc -> pyr	46
116	glc -> lac-D	776
117	glc -> lac + atp + h2o	41
118	pyr -> lac-D	776
119	pyr[c] -> accoa[m] + co2[c] + nadh[m]	7
120	etoh -> acald	510
121	acald -> ac	506
122	lac -> glc	31
123	glyc -> glc	31
124	g6p -> ru5p	890
125	g6p -> r5p	889
126	f6p + g3p -> r5p	889
127	udpglcur -> xu5p-D	956
128	fru -> dhap	24
129	fru -> g3p	30
130	gal -> udpgal	942
131	glc -> lcts[g] (2)	777
132	gal -> glc	259
133	pyr -> nad[m] + h[m]	1923
134	pyr -> fad[m] + h[m]	29
135	akg[m[-> oaa[m]	836
136	succoa[m] -> oaa[m]	836
137	fum [m] -> oaa [m]	836
138	ascb -> thrnt	922
139	ascb -> eryth	641
140	ascb -> lyxnt	781
141	ascb -> xylnt	958

Simulation #	Simulation Name	Objective Column #
142	Tyr-ggn -> glygn2	713
143	glygn2 -> glc	31
144	glygn2[e] -> glc[e]	260
145	strch1[e] -> glc[e]	260
146	man6p -> kdn	767
147	man -> gdpmann	690
148	fuc -> gdpfuc	688
149	gdpmann -> gdpfuc	688
150	gam6p -> uacgam	54
151	acgal -> udpacgal	938
152	acgam -> cmpacna	578
153	g1p -> dtdprmn	635
154	glc -> inost	762
155	inost -> xu5p-D	956
156	inost -> pail_hs	845
157	inost -> pail4p_hs	844
158	pail45p -> mi145p	795
159	mi145p -> inost	762
160	inost -> pail45p_hs	843
161	itacon[m] -> pyr[m]	882
162	mescon[m] -> pyr[m]	882
163	hpyr -> 2pg	477
164	hpyr -> glyclt	711
165	xylu-D -> glyclt	711
166	glyclt -> gly	704
167	glyx -> oxa	840
168	glx[m] -> glyclt[m]	712
169	hpyr -> glyc-S	709
170	dhap -> mthgxl	801
171	g3p -> mthgxl	801
172	acetone -> mthgxl	801
173	aact -> mthgxl	801
174	mthgxl -> lac-D	776
175	mthgxl -> 12ppd-S	473
176	12ppd-S -> mthgxl	801
177	12ppd-S -> pyr	881
178	ppcoa[m] -> succoa[m]	910
179	acac[m] -> acetone [m]	516
180	acac[m] -> bhb[m]	564
181	hmgcoa(x)->frdp(x)	663
182	hmgcoa(x)->chsterol(r)	2287
183	hmgcoa(x)-chsterol(r)	1885
184	hmgcoa(x)->xoldiolone(r)	3427
185	hmgcoa(x)->xoltriol(c)	1300
186	xoltriol(m)->thcholstoic(m) v0.05	915
187	pmtcoa(c)->crmp_hs(c)	1886
188	pmtcoa(c)->sphmyln_hs(c)	3920

Simulation #	Simulation Name	Objective Column #
189	galgluside_hs(g) -> gd1c_hs(g)	3985
190	galgluside_hs(g) -> gq1balpha_hs(g)	3974
191	galgluside_hs(g) -> gq1balpha_hs(g) path 2	3973
192	galgluside_hs(g) -> gq1balpha_hs(g) path 3	3979
193	galgluside_hs(g) -> gp1c_hs(g)	3976
194	galgluside_hs(g) -> gd1b2_hs(g)	3972
195	galgluside_hs(g) -> acgagbside_hs(g)	2479
196	galgluside(g) -> galgalgalthcrm_hs(g)	1493
197	galgluside_hs(g) -> acnacngalgbside_hs(g)	3980
198	gluside_hs(g) -> galgluside_hs(g)	1499
199	thcholstoic(x)->gchola(x) v0.05	682
200	thcholstoich(x)->tchola(x) v0.05	913
201	arachd(r) -> txa2(r)	4131
202	glyc(c) + Rtotal(c) -> tag_hs(c) v0.05	911
203	chol(c) + dag_hs(c) -> pe_hs(c)	3653
204	from thm(e) to thmpp(m)	53
205	from thmmp(e) to thmpp(m)	53
206	from thmmp(e) to thmpp(c)	52
207	from thm(c) to thmpp(c)	52
208	from prpp to imp	39
209	from adn(c) to urate(x)	56
210	from imp(c) to urate(x)	56
211	from gsn(c) to urate(x)	56
212	from imp to atp	12
213	from imp to gtp	35
214	from cytd to ala-B	9
215	from cmp to cytd	9
216	from ump to ala-B	9
217	from dcmp to ala-B	9
218	missing dtmp-3aib testing	2
219	from gln-L + HCO3 to UMP(c)	55
220	from ADP(c) to dATP(n)	19
221	from ADP(c) to dATP(n) 2	19
222	from GDP(c) to dGTP(n)	23
223	from CDP(c) to dCTP(n)	21
224	from GDP(c) to dGTP(n) 2	23
225	from UDP(c) to dTTP(n)	27
226	from tyr-L(m) to q10(m)	49
227	val-L-->3aib	480
228	val-L --> succoa	910
229	from pydx(c) to pydx5p(c)	45
230	from hxan(c) to imp(c)	39
231	from gua(c) to gmp(c)	33
232	from ade(c) to amp(c)	10
233	thcholstoic(x) -> gchola(x)	1501
234	thcholstoic(x) -> tchola(x)	1502
235	gln -> nh4 v0.05	342

Simulation #	Simulation Name	Objective Column #
236	R_group	2234
237	arachd(c)->malcoa(m)	2153
238	accoa(c)->pmtcoa(c)->malcoa(m)	42
239	glyc(c) + Rtotal(c) + Rtotal2(c) -> dag_hs(c)	17
240	phytcoa(x)->dmnoncoa(m) v0.05	620
241	frdp -> dolichol_U	627
242	frdp -> dolichol_L	626
243	dolichol_L -> dolmanp_L[r]	629
244	dolichol_U -> dolmanp_U[r]	630
245	dolichol_U -> g3m8mpdol_U[r]	672
246	dolichol_L -> g3m8mpdol_L[r]	670
247	uacgam -> m8masn[r]	784
248	m8masn[r] -> nm4masn[g]	825
249	nm4masn[g] -> l2fn2m2masn[g]	775
250	nm4masn[g] -> s2l2fn2m2masn[g]	891
251	nm4masn[g] -> n2m2nmasn[g]	802
252	s2l2fn2m2masn[l] -> man[l] + acgam[l]	60
253	n2m2nmasn[l] -> man[l] + acgam[l]	60
254	Ser/Thr[g] + udpacgal[g] -> dsTn_antigen[g]	634
255	Ser/Thr[g] + udpacgal[g] -> sTn_antigen[g]	894
256	Ser/Thr[g] + udpacgal[g] -> core2[g]	591
257	Ser/Thr[g] + udpacgal[g] -> core4[g]	592
258	pail_hs -> gpi_prot_hs[r]	715
259	uacgam + udpglcur -> ha[e]	37
260	ha[l] -> acgam[l] + glcur[l]	58
261	Ser-Gly/Ala-X-Gly[er] -> cs_pre[g]	598
262	Ser-Gly/Ala-X-Gly[er] -> cspg_a[g]	599
263	Ser-Gly/Ala-X-Ser[er] -> cspg_b[g]	601
264	Ser-Gly/Ala-X-Gly[er] -> cspg_c[g]	603
265	Ser-Gly/Ala-X-Gly[er] -> cspg_d[g]	605
266	Ser-Gly/Ala-X-Gly[er] -> cspg_e[g]	607
267	core2[g] -> ksii_core2[g]	770
268	core4[g] -> ksii_core4[g]	772
269	l2fn2m2masn[g] -> ksi[g]	768
270	Ser-Gly/Ala-X-Gly[er] -> hspg[g]	753
271	hspg[ly] -> 2 gal[ly] + glcur[ly] + xyl-D[ly]	4
272	cspg_a[ly] -> 2 gal[ly] + glcur[ly] + xyl-D[ly]	4
273	cspg_b[ly] -> 2gal[ly] + glcur[ly] + xyl-D[ly]	4
274	cspg_c[ly] -> 2 gal[ly] + glcur[ly] + xyl-D[ly]	4
275	cspg_d[ly] -> 2 gal[ly] + glcur[ly] + xyl-D[ly]	4
276	cspg_e[ly] -> 2 gal[ly] + glcur[ly] + xyl-D[ly]	4
277	ksi[l] -> man[l] + acgam[l]	60
278	ksii_core2[ly] -> Ser/Thr[ly]	503
279	ksii_core4[ly] -> Ser/Thr[ly]	503
280	Human Recon 1 test mouse biomass 2	4274
281	ATP max, aerobic, citrate v0.05	11
282	ATP max, aerobic, glutamine substrate v0.05	11

Simulation #	Simulation Name	Objective Column #
283	ATP max, aerobic, EtOH substrate v0.05	11
284	ATP max, aerobic, lactate substrate v0.05	11
285	ATP max, aerobic, glutamate v0.05	11
286	ATP max, aerobic, glycine substrate v0.05	11
287	ATP max, aerobic, proline substrate v0.05	11
288	orn -> nh4 v0.05	342