Supplementary file 2. Relative abundances of intact C2 and C3 fragments in proteinogenic amino acids.

Table 1 - First series of labeling experiments

	Strain											
	X-33 control				X-33 *ROL* 1-copy				X-33 *ROL 2*-copy			
C atom	$f^{(1)}$	$f^{(2)}$	$f^{(2*)}$	$f^{(3)}$	$f^{(1)}$	$f^{(2)}$	$f^{(2*)}$	$f^{(3)}$	$f^{(1)}$	$f^{(2)}$	$f^{(2*)}$	$f^{(3)}$
Ala-Cα	0.224	0.153	0.104	0.518	0.211	0.148	0.069	0.572	0.23	0.137	0.072	0.561
Ala-Cβ	0.356	0.644	-	-	0.31	0.69	-	-	0.313	0.687	-	-
Arg-Cβ	0.673	0.327	-	0	0.646	0.36	-	0	0.723	0.254	-	0
Arg-Cδ	0.401	0.599	-	-	0.329	0.671	-	-	0.315	0.685	-	-
Asp-Cα	0.46	0.146	0.272	0.133	0.41	0.156	0.289	0.146	0.445	0.125	0.291	0.14
Asp-Cβ	0.502	0.224	0.204	0.070	0.429	0.227	0.254	0.09	0.465	0.183	0.278	0.07
Glu-Cα	0.459	0.208	0.252	0.08	0.468	0.192	0.303	0.036	0.459	0.189	0.279	0.073
Glu-Cβ	0.729	0.271	-	0	0.67	0.329	-	0	0.736	0.34	-	0
Glu-Cγ	0.389	0	0.611	0	0.289	0.009	0.701	0	0.288	0	0.721	0
Gly-Cα	0.465	0.535	-	-	0.45	0.55	-	-	0.42	0.58	-	-
His-Cα	0.174	0.077	0.074	0.674	0.19	0.045	0.036	0.728	0.224	0	0.065	0.739
His-Cβ	0.371	0.449	0	0.181	0.259	0.439	0.001	0.301	0.352	0.492	0	0.19
His-$C\delta^2$	0.571	0.429	-	-	0.508	0.492	-	-	0.538	0.462	-	-
Ile-Cα	0.623	0	0.377	0	0.572	0	0.428	0	0.604	0	0.4	0
Ile-$C\gamma^1$	0.733	0.267	-	0	0.574	0.354	-	0	0.734	0.302	-	0
Ile-$C\gamma^2$	0.425	0.575	-	-	0.313	0.687	-	-	0.33	0.67	-	-
Ile-Cδ	0.761	0.239	-	-	0.66	0.34	-	-	0.763	0.237	-	-
Leu-Cα	0.405	0	0.595	0	0.349	0	0.651	0	0.365	0	0.625	0
Leu-Cβ	1	0	-	0	0.895	0.105	-	0	1	0	-	0
Leu-$C\delta^1$	0.435	0.565	-	-	0.37	0.63	-	-	0.35	0.65	-	-
Leu-$C\delta^2$	1	0	-	-	0.982	0.018	-	-	1	0	-	-
Lys-Cα	0.366	0	0.634	0	0.366	0	0.633	0	0.319	0	0.681	0
Lys-Cβ	0.754	0.145	-	-	0.7	0.294	-	-	0.769	0.227	-	-
Lys-Cγ	0.719	0.281	-	-	0.689	0.308	-	-	0.741	0.259	-	-
Lys-Cδ	0.411	0.589	-	-	0.32	0.68	-	-	0.306	0.694	-	-
Lys-Cε	0.402	0.598	-	-	0.328	0.672	-	-	0.329	0.671	-	-
Met-Cα	0.414	0.177	0.227	0.181	0.424	0.126	0.243	0.207	0.382	0.161	0.281	0.176
Phe-Cα	0.265	0.16	0.123	0.451	0.228	0.138	0.073	0.562	0.267	0.118	0.032	0.582
Phe-Cβ	0.382	0.618	0	0	0.305	0.695	0	0	0.276	0.724	0	0
Pro-Cα	0.492	0.202	0.241	0.065	0.391	0.207	0.286	0.117	0.448	0.195	0.289	0.067
Pro-Cβ	0.626	0.352	-	0.021	0.48	0.373	-	0.147	0.708	0.237	-	0.055
Pro-Cγ	0.407	0.593	-	0	0.302	0.664	-	0.034	0.312	0.688	-	0
Pro-Cδ	0.4	0.6	-	-	0.324	0.676	-	-	0.309	0.691	-	-
Ser-Cα	0.328	0.094	0.265	0.313	0.271	0.101	0.24	0.388	0.285	0.075	0.241	0.399
Ser-Cβ	0.628	0.372	-	-	0.546	0.454	-	-	0	1	-	-
Thr-Cα	0.48	0.155	0.242	0.123	0.417	0.162	0.28	0.142	0.478	0.129	0.26	0.134

Thr-Cβ	0.461	0.314	0.155	0.07	0.387	0.378	0.133	0.102	0.448	0.339	0.163	0.04
Thr-$C\gamma^2$	0.689	0.311	-	-	0.622	0.378	-	-	0.63	0.37	-	-
Tyr-Cα	0.256	0.152	0.136	0.456	0.229	0.139	0.104	0.528	0.26	0.116	0.051	0.573
Tyr-Cβ	0.402	0.598	-	-	0.302	0.698	-	-	0.318	0.682	-	-
Tyr-$C\delta^x$	0.336	0.664	-	0	0.281	0.719	-	0	0.28	0.721	-	0
Tyr-$C\varepsilon^x$	0.56	0.07	0.108	0.256	0.519	0.062	0.13	0.289	0.519	0.047	0.108	0.325
Val-Cα	0.435	0	0.565	0	0.365	0	0.623	0.011	0.373	0	0.627	0
Val-$C\gamma^1$	0.428	0.572	-	-	0.996	0	-	-	0.315	0.685	-	-
Val-$C\gamma^2$	1	0	-	-	0.937	0.062	-	-	0.992	0.008	-	-

The first column indicates the carbon for which the ^{13}C fines structure was observed. The *f*-values were calculated as described in Syzperski (1995) and are given for the chemostat cultivations of *P. pastoris* at $\mu = 0.09h^{-1}$ on glucose-methanol mixtures. Note that, for the terminal carbons, $f^{(2*)}$ and $f^{(3)}$ are not defined, and in case where $f^{(2*)}$ is not given for a mid-chain carbon, the carbon-carbon scalar coupling constants are similar and the two doublets cannot be distinguished.

Table 2 - Second series of labeling experiments

	Strain											
	X-33 control				X-33 *ROL* 1-copy				X-33 *ROL* 2-copy			
C atom	$f^{(1)}$	$f^{(2)}$	$f^{(2*)}$	$f^{(3)}$	$f^{(1)}$	$f^{(2)}$	$f^{(2*)}$	$f^{(3)}$	$f^{(1)}$	$f^{(2)}$	$f^{(2*)}$	$f^{(3)}$
Ala-Cα	0.241	0.205	0.099	0.456	0.237	0.186	0.07	0.507	0.261	0.156	0.051	0.532
Ala-Cβ	0.333	0.667	-	-	0.334	0.666	-	-	0.342	0.658	-	-
Arg-Cβ	0.656	0.335	-	0	0.666	0.304	-	0	0.657	0.318	-	0.025
Arg-Cδ	0.403	0.597	-	-	0.378	0.622	-	-	0.372	0.628	-	-
Asp-Cα	0.464	0.167	0.23	0.139	0.404	0.161	0.278	0.157	0.483	0.108	0.274	0.135
Asp-Cβ	0.449	0.234	0.254	0.063	0.379	0.256	0.271	0.094	0.494	0.164	0.267	0.075
Glu-Cα	0.420	0.247	0.258	0.075	0.388	0.233	0.276	0.103	0.501	0.173	0.274	0.052
Glu-Cβ	0.646	0.354	-	0	0.636	0.364	-	0	0.772	0.229	-	0
Glu-Cγ	0.345	0	0.646	0	0.325	0	0.665	0	0.368	0	0.632	0
Gly-Cα	0.433	0.567	-	-	0.434	0.566	-	-	0.447	0.553	-	-
His-Cα	0.184	0.054	0.073	0.690	0.191	0.049	0.080	0.68	0.245	0.016	0.062	0.677
His-Cβ	0.263	0.451	0	0.286	0.306	0.426	0	0.268	0.329	0.465	0	0.205
His-$C\delta^2$	0.554	0.446	-	-	0.637	0.363	-	-	0.587	0.413	-	-
Ile-Cα	0.598	0	0.402	0	0.582	0	0.418	-	0.604	0	0.396	0

Ile-Cγ^1	0.708	0.257	-	0	0.658	0.295	-	0	0.699	0.301	-	0
Ile-Cγ^2	0.401	0.599	-	-	0.335	0.665	-	-	0.351	0.649	-	-
Ile-Cδ	0.744	0.256	-	-	0.713	0.287	-	-	0.694	0.306	-	-
Leu-Cα	0.401	0	0.599	0	0.369	0	0.631	0	0.384	0	0.616	0
Leu-Cβ	0.94	0.027	-	0.033	0.99	0	-	0.01	0.99	0	-	0.01
Leu-Cδ^1	0.449	0.551	-	-	0.361	0.639	-	-	0.381	0.619	-	-
Leu-Cδ^2	0.981	0.019	-	-	0.927	0.073	-	-	1	0	-	-
Lys-Cα	0.314	0.024	0.662	0	0.384	0	0.592	0.024	0.366	0	0.634	
Lys-Cβ	0.682	0.273	-	0.045	0.385	0.593	-	0.022	0.756	0.199	-	0.018
Lys-Cγ	0.654	0.305	-	0.041	0.649	0.317	-	0.034	0.71	0.29	-	0
Lys-Cδ	0.397	0.603	-	-	0.362	0.044	0.594	0	0.37	0.017	0.613	-
Lys-Cε	0.401	0.599	-	-	0.37	0.63	-	-	0.373	0.627	-	-
Met-Cα	0.403	0.119	0.256	0.222	0.43	0.128	0.243	0.199	0.45	0.098	0.291	0.162
Phe-Cα	0.237	0.162	0.143	0.458	0.257	0.129	0.105	0.51	0.282	0.11	0.067	0.54
Phe-Cβ	0.378	0.622	0	0	0.338	0.662	0	0	0.351	0.649	0	0
Pro-Cα	0.498	0.236	0.216	0.050	0.437	0.206	0.248	0.135	0.499	0.166	0.262	0.074
Pro-Cβ	0.668	0.33	-	0.002	0.656	0.344	-	0	0.744	0.256	-	0
Pro-Cγ	0.408	0.592	-	0	0.372	0.617	-	0.011	0.374	0.616	-	0
Pro-Cδ	0.405	0.595	-	-	0.367	0.633	-	-	0.377	0.623	-	-
Ser-Cα	0.274	0.116	0.254	0.356	0.268	0.094	0.262	0.376	0.333	0.072	0.236	0.352
Ser-Cβ	0.559	0.441	-	-	0.557	0.443	-	-	0.586	0.414	-	-
Thr-Cα	0.471	0.142	0.253	0.135	0.443	0.176	0.238	0.143	0.502	0.116	0.271	0.11
Thr-Cβ	0.449	0.156	0.33	0.066	0.409	0.35	0.15	0.091	0.489	0.306	0.146	0.059
Thr-Cγ^2	0.654	0.346	-	-	0.582	0.418	-	-	0.673	0.327	-	-
Tyr-Cα	0.236	0.177	0.134	0.452	0.22	0.145	0.093	0.542	0.288	0.12	0.0721	0.521
Tyr-Cβ	0.394	0.606	0	0	0.36	0.64	0	0	0.347	0.653	0	0
Tyr-Cδ^x	0.339	0.661	-	0	0.259	0.672	-	0.04	0.309	0.691	-	0
Tyr-Cε^x	0.469	0.071	0.139	0.321	0.523	0.056	0.136	0.285	0.586	0.03	0.107	0.277
Val-Cα	0.415	0	0.585	0	0.384	0	0.616	0	0.393	0	0.607	0
Val-Cγ^1	0.405	0.595	-	-	0.374	0.626	-	-	0.408	0.592	-	-
Val-Cγ^2	0.947	0.053	-	-	1	0	-	-	0.978	0.022	-	-

The first column indicates the carbon for which the ^{13}C fines structure was observed. The *f*-values were calculated as described in Szyperski (1995) and are given for the chemostat cultivations of *P. pastoris* at $\mu = 0.09h^{-1}$ on glucose-methanol mixtures. Note that, for the terminal carbons, $f^{(2*)}$ and $f^{(3)}$ are not defined, and in case where $f^{(2*)}$ is not given for a mid-chain carbon, the carbon-carbon scalar coupling constants are similar and the two doublets cannot be distinguished.