



|       |       |      |     |       |              |              |       |              |              |       |              |              |       |
|-------|-------|------|-----|-------|--------------|--------------|-------|--------------|--------------|-------|--------------|--------------|-------|
| Ile   | M-85  | 2-6  | 0   | 0.009 | <i>0.005</i> | 0.001        | 0.006 | <i>0.002</i> | 0.000        | 0.007 | <i>0.002</i> | 0.001        |       |
|       |       |      | 1   | 0.082 | <i>0.073</i> | 0.004        | 0.041 | <i>0.034</i> | 0.002        | 0.046 | <i>0.033</i> | 0.005        |       |
|       |       |      | 2   | 0.220 | <i>0.245</i> | 0.004        | 0.195 | <i>0.204</i> | 0.003        | 0.128 | <i>0.137</i> | 0.002        |       |
|       |       |      | 3   | 0.387 | <i>0.355</i> | 0.008        | 0.486 | <i>0.482</i> | 0.009        | 0.320 | <i>0.297</i> | 0.017        |       |
|       |       |      | 4   | 0.218 | <i>0.246</i> | 0.010        | 0.226 | <i>0.230</i> | 0.002        | 0.316 | <i>0.335</i> | 0.006        |       |
|       | M-159 | 2-6  | 0   | 0.009 | <i>0.005</i> | 0.001        | 0.006 | <i>0.002</i> | 0.000        | 0.006 | <i>0.002</i> | 0.001        |       |
|       |       |      | 1   | 0.081 | <i>0.073</i> | 0.003        | 0.042 | <i>0.034</i> | 0.002        | 0.045 | <i>0.033</i> | 0.005        |       |
|       |       |      | 2   | 0.220 | <i>0.246</i> | 0.004        | 0.195 | <i>0.203</i> | 0.003        | 0.129 | <i>0.137</i> | 0.002        |       |
|       |       |      | 3   | 0.388 | <i>0.356</i> | 0.009        | 0.485 | <i>0.482</i> | 0.009        | 0.321 | <i>0.298</i> | 0.016        |       |
|       |       |      | 4   | 0.220 | <i>0.247</i> | 0.010        | 0.227 | <i>0.230</i> | 0.002        | 0.316 | <i>0.336</i> | 0.006        |       |
| Ser   | M-57  | 1-3  | 0   | 0.396 | <i>0.383</i> | 0.006        | 0.323 | <i>0.310</i> | 0.005        | 0.136 | <i>0.127</i> | 0.005        |       |
|       |       |      | 1   | 0.329 | <i>0.334</i> | 0.002        | 0.349 | <i>0.352</i> | 0.001        | 0.299 | <i>0.296</i> | 0.004        |       |
|       |       |      | 2   | 0.270 | <i>0.281</i> | 0.006        | 0.320 | <i>0.329</i> | 0.004        | 0.522 | <i>0.525</i> | 0.007        |       |
|       |       |      | 3   | 0.006 | <i>0.008</i> | 0.001        | 0.008 | <i>0.012</i> | 0.001        | 0.043 | <i>0.048</i> | 0.002        |       |
|       |       |      | 4   | 0.006 | <i>0.008</i> | 0.001        | 0.008 | <i>0.012</i> | 0.001        | 0.043 | <i>0.048</i> | 0.002        |       |
|       | M-85  | 2-3  | 0   | 0.395 | <i>0.392</i> | 0.005        | 0.323 | <i>0.321</i> | 0.004        | 0.144 | <i>0.139</i> | 0.004        |       |
|       |       |      | 1   | 0.334 | <i>0.331</i> | 0.002        | 0.355 | <i>0.352</i> | 0.002        | 0.316 | <i>0.313</i> | 0.004        |       |
|       |       |      | 2   | 0.271 | <i>0.278</i> | 0.006        | 0.322 | <i>0.328</i> | 0.005        | 0.539 | <i>0.542</i> | 0.008        |       |
|       | M-159 | 2-3  | 0   | 0.399 | <i>0.392</i> | 0.005        | 0.325 | <i>0.320</i> | 0.004        | 0.146 | <i>0.139</i> | 0.003        |       |
|       |       |      | 1   | 0.331 | <i>0.332</i> | 0.002        | 0.352 | <i>0.352</i> | 0.001        | 0.314 | <i>0.313</i> | 0.004        |       |
|       | f302  | 1-2  | 0   | 0.559 | <i>0.559</i> | 0.006        | 0.502 | <i>0.498</i> | 0.005        | 0.285 | <i>0.275</i> | 0.008        |       |
|       |       |      | 1   | 0.428 | <i>0.429</i> | 0.006        | 0.482 | <i>0.486</i> | 0.005        | 0.657 | <i>0.661</i> | 0.007        |       |
|       |       |      | 2   | 0.012 | <i>0.013</i> | 0.000        | 0.017 | <i>0.017</i> | 0.000        | 0.058 | <i>0.061</i> | 0.001        |       |
|       | Phe   | M-57 | 1-9 | 0     | 0.127        | <i>0.084</i> | 0.015 | 0.094        | <i>0.051</i> | 0.012 | 0.057        | <i>0.006</i> | 0.018 |
|       |       |      |     | 1     | 0.088        | <i>0.087</i> | 0.005 | 0.073        | <i>0.066</i> | 0.002 | 0.034        | <i>0.017</i> | 0.004 |
| 2     |       |      |     | 0.243 | <i>0.257</i> | 0.005        | 0.210 | <i>0.211</i> | 0.001        | 0.090 | <i>0.072</i> | 0.001        |       |
| 3     |       |      |     | 0.149 | <i>0.164</i> | 0.001        | 0.152 | <i>0.167</i> | 0.002        | 0.108 | <i>0.110</i> | 0.001        |       |
| 4     |       |      |     | 0.236 | <i>0.230</i> | 0.006        | 0.253 | <i>0.255</i> | 0.005        | 0.196 | <i>0.225</i> | 0.006        |       |
| 5     |       |      |     | 0.078 | <i>0.079</i> | 0.003        | 0.100 | <i>0.109</i> | 0.003        | 0.168 | <i>0.192</i> | 0.005        |       |
| 6     |       |      |     | 0.074 | <i>0.061</i> | 0.003        | 0.107 | <i>0.091</i> | 0.003        | 0.242 | <i>0.206</i> | 0.010        |       |
| 7     |       |      |     | 0.004 | <i>0.005</i> | 0.002        | 0.010 | <i>0.009</i> | 0.002        | 0.092 | <i>0.060</i> | 0.003        |       |
| 8     |       |      |     | 0.000 | <i>0.000</i> | 0.000        | 0.001 | <i>0.000</i> | 0.000        | 0.013 | <i>0.006</i> | 0.000        |       |
| f302  |       | 1-2  | 0   | 0.505 | <i>0.498</i> | 0.014        | 0.459 | <i>0.451</i> | 0.011        | 0.288 | <i>0.273</i> | 0.021        |       |
|       |       |      | 1   | 0.477 | <i>0.484</i> | 0.012        | 0.520 | <i>0.527</i> | 0.010        | 0.654 | <i>0.660</i> | 0.016        |       |
|       |       |      | 2   | 0.018 | <i>0.015</i> | 0.003        | 0.021 | <i>0.019</i> | 0.002        | 0.058 | <i>0.061</i> | 0.005        |       |
| M-159 |       | 2-9  | 0   | 0.128 | <i>0.086</i> | 0.015        | 0.095 | <i>0.053</i> | 0.011        | 0.058 | <i>0.007</i> | 0.018        |       |
|       |       |      | 1   | 0.088 | <i>0.087</i> | 0.004        | 0.073 | <i>0.066</i> | 0.002        | 0.035 | <i>0.018</i> | 0.003        |       |
|       |       |      | 2   | 0.245 | <i>0.261</i> | 0.004        | 0.212 | <i>0.216</i> | 0.001        | 0.094 | <i>0.077</i> | 0.002        |       |
|       |       |      | 3   | 0.148 | <i>0.161</i> | 0.001        | 0.150 | <i>0.165</i> | 0.002        | 0.109 | <i>0.113</i> | 0.001        |       |
|       |       |      | 4   | 0.237 | <i>0.231</i> | 0.009        | 0.254 | <i>0.257</i> | 0.004        | 0.202 | <i>0.235</i> | 0.007        |       |
|       |       |      | 5   | 0.075 | <i>0.074</i> | 0.003        | 0.098 | <i>0.102</i> | 0.003        | 0.167 | <i>0.188</i> | 0.005        |       |
|       |       |      | 6   | 0.075 | <i>0.060</i> | 0.003        | 0.108 | <i>0.090</i> | 0.003        | 0.247 | <i>0.206</i> | 0.010        |       |
|       |       |      | 7   | 0.004 | <i>0.003</i> | 0.000        | 0.008 | <i>0.006</i> | 0.001        | 0.080 | <i>0.046</i> | 0.002        |       |

|     |       |     |       |              |              |       |              |              |       |              |              |       |
|-----|-------|-----|-------|--------------|--------------|-------|--------------|--------------|-------|--------------|--------------|-------|
|     |       |     | 8     | 0.000        | <i>0.000</i> | 0.000 | 0.001        | <i>0.000</i> | 0.000 | 0.007        | <i>0.003</i> | 0.000 |
| Asx | M-57  | 1-4 | 0     | 0.114        | <i>0.098</i> | 0.010 | 0.102        | <i>0.087</i> | 0.002 | 0.046        | <i>0.036</i> | 0.002 |
|     |       |     | 1     | 0.192        | <i>0.188</i> | 0.004 | 0.186        | <i>0.181</i> | 0.001 | 0.133        | <i>0.122</i> | 0.007 |
|     |       |     | 2     | 0.647        | <i>0.651</i> | 0.010 | 0.655        | <i>0.659</i> | 0.002 | 0.707        | <i>0.708</i> | 0.004 |
|     |       |     | 3     | 0.047        | <i>0.045</i> | 0.004 | 0.055        | <i>0.051</i> | 0.001 | 0.110        | <i>0.120</i> | 0.004 |
|     |       |     | 4     | 0.000        | <i>0.001</i> | 0.001 | 0.001        | <i>0.001</i> | 0.000 | 0.004        | <i>0.005</i> | 0.001 |
|     | M-85  | 2-4 | 0     | 0.114        | <i>0.101</i> | 0.011 | 0.102        | <i>0.091</i> | 0.002 | 0.048        | <i>0.040</i> | 0.002 |
|     |       |     | 1     | 0.197        | <i>0.197</i> | 0.004 | 0.192        | <i>0.190</i> | 0.002 | 0.140        | <i>0.136</i> | 0.006 |
|     |       |     | 2     | 0.667        | <i>0.669</i> | 0.012 | 0.679        | <i>0.681</i> | 0.003 | 0.755        | <i>0.756</i> | 0.006 |
|     |       |     | 3     | 0.023        | <i>0.019</i> | 0.003 | 0.027        | <i>0.024</i> | 0.001 | 0.057        | <i>0.057</i> | 0.002 |
|     |       |     | 0     | 0.115        | <i>0.100</i> | 0.010 | 0.103        | <i>0.090</i> | 0.002 | 0.050        | <i>0.039</i> | 0.003 |
|     | M-159 | 2-4 | 1     | 0.196        | <i>0.195</i> | 0.005 | 0.190        | <i>0.188</i> | 0.001 | 0.140        | <i>0.135</i> | 0.006 |
|     |       |     | 2     | 0.661        | <i>0.664</i> | 0.013 | 0.674        | <i>0.676</i> | 0.002 | 0.747        | <i>0.749</i> | 0.006 |
|     |       |     | 3     | 0.028        | <i>0.019</i> | 0.003 | 0.032        | <i>0.024</i> | 0.000 | 0.063        | <i>0.057</i> | 0.003 |
|     | f302  | 1-2 | 0     | 0.214        | <i>0.230</i> | 0.013 | 0.201        | <i>0.216</i> | 0.002 | 0.118        | <i>0.120</i> | 0.005 |
| 1   |       |     | 0.755 | <i>0.750</i> | 0.011        | 0.763 | <i>0.759</i> | 0.003        | 0.814 | <i>0.813</i> | 0.002        |       |
| 2   |       |     | 0.031 | <i>0.029</i> | 0.002        | 0.036 | <i>0.032</i> | 0.001        | 0.068 | <i>0.078</i> | 0.003        |       |
| Glx | M-57  | 1-4 | 0     | 0.006        | <i>0.002</i> | 0.001 | 0.005        | <i>0.003</i> | 0.000 | 0.004        | <i>0.002</i> | 0.001 |
|     |       |     | 1     | 0.101        | <i>0.084</i> | 0.008 | 0.093        | <i>0.084</i> | 0.002 | 0.045        | <i>0.039</i> | 0.003 |
|     |       |     | 2     | 0.233        | <i>0.229</i> | 0.004 | 0.220        | <i>0.220</i> | 0.002 | 0.163        | <i>0.163</i> | 0.007 |
|     |       |     | 3     | 0.614        | <i>0.618</i> | 0.008 | 0.633        | <i>0.635</i> | 0.002 | 0.684        | <i>0.684</i> | 0.005 |
|     |       |     | 4     | 0.044        | <i>0.029</i> | 0.004 | 0.048        | <i>0.041</i> | 0.000 | 0.101        | <i>0.104</i> | 0.006 |
|     | M-159 | 2-4 | 5     | 0.001        | <i>0.000</i> | 0.000 | 0.002        | <i>0.001</i> | 0.000 | 0.004        | <i>0.004</i> | 0.001 |
|     |       |     | 0     |              |              |       | 0.006        | <i>0.003</i> | 0.000 | 0.005        | <i>0.002</i> | 0.001 |
|     |       |     | 1     |              |              |       | 0.100        | <i>0.087</i> | 0.002 | 0.054        | <i>0.043</i> | 0.004 |
|     |       |     | 2     |              |              |       | 0.233        | <i>0.226</i> | 0.002 | 0.184        | <i>0.176</i> | 0.005 |
|     |       |     | 3     |              |              |       | 0.638        | <i>0.642</i> | 0.004 | 0.708        | <i>0.710</i> | 0.008 |
|     |       |     | 4     |              |              |       | 0.023        | <i>0.019</i> | 0.001 | 0.049        | <i>0.054</i> | 0.002 |
|     |       |     | 0     |              |              |       |              |              |       |              |              |       |
|     |       |     | 1     |              |              |       |              |              |       |              |              |       |
|     |       |     | 2     |              |              |       |              |              |       |              |              |       |
| Tyr | f302  | 1-2 | 0     | 0.484        | <i>0.500</i> | 0.008 | 0.435        | <i>0.454</i> | 0.005 | 0.255        | <i>0.280</i> | 0.008 |
|     |       |     | 1     | 0.503        | <i>0.486</i> | 0.007 | 0.546        | <i>0.530</i> | 0.004 | 0.687        | <i>0.676</i> | 0.005 |
|     |       |     | 2     | 0.014        | <i>0.015</i> | 0.002 | 0.019        | <i>0.019</i> | 0.001 | 0.058        | <i>0.062</i> | 0.003 |

Values are corrected for the natural abundances of all atoms except for the carbons in the amino acid backbones. AA: amino acid; Frag: fragment; C: Carbons in fragment; x+: increase in mass due to  $^{13}\text{C}$  incorporation and is equal to the number of  $^{13}\text{C}$  atoms in the amino acid fragment backbone; Ave: average fraction of the amino acid fragment having the specified mass; sim: simulated fraction of the amino acid fragment having the specified mass from the optimized fit; SD: measured mass isotopomer standard deviation; Asx: aspartate and asparagine; Glx: glutamate and glutamine.