

Accurate Masses of iTRAQ Ions and Known Interference Ions

label	Formula	$\Delta(R_{400}=7500)$	$\Delta(m/z)_{\text{interf}}$	m/z calc.	published‡	$\Delta, \text{ppm}^\dagger$
m-I	$\text{C}_5\text{H}_9\text{N}_2\text{O}$	0.008016	-0.036386	113.070939	113.070965	-0.2270
iTRAQ 113(8-plex)	$\text{C}_6\text{H}_{13}\text{N}_2$	0.008019		113.107325	113.107326	-0.0102
iTRAQ 114(4+8-plex)	$\text{C}_5^{13}\text{CH}_{13}\text{N}_2$	0.008126		114.110680	114.110681	-0.0115
m-II*	$\text{C}_5\text{H}_{11}\text{N}_2\text{O}$	0.008231	-0.021125	115.086589	115.086616	-0.2311
iTRAQ 115(4+8-plex)	$\text{C}_5^{13}\text{CH}_{13}\text{N}^{15}\text{N}$	0.008233		115.107715	115.107714	0.0050
m-III**	$\text{C}_4^{13}\text{C}_2\text{H}_{13}\text{N}_2$	0.008234	0.006320	115.114035	115.114033	0.0132
m-IV(1)*	$\text{C}_5\text{H}_{10}\text{NO}_2$	0.008337	-0.040464	116.070605	116.070650	-0.3878
m-A	$\text{C}_2^{13}\text{C}_4\text{H}_{10}\text{NO}$	0.008339	-0.021960	116.089110	116.089114	-0.0369
iTRAQ 116(4+8-plex)	$\text{C}_4^{13}\text{C}_2\text{H}_{13}\text{N}^{15}\text{N}$	0.008341		116.111069	116.111068	0.0122
m-IV(2)	$^{13}\text{C}_4\text{CH}_8\text{NO}_2$	0.008553	-0.043085	118.068374	118.068373	0.0108
iTRAQ 118(8-plex)	$\text{C}_4^{13}\text{C}_3\text{H}_{13}^{15}\text{N}_2$	0.008557		118.111459	118.111460	-0.0072
m-B**	$\text{C}_2^{13}\text{C}_4\text{H}_{13}\text{N}^{15}\text{N}$	0.008558	0.006320	118.117779	118.117777	0.0177
m-V	$\text{C}_8\text{H}_7\text{O}$	0.008660	-0.065673	119.049141	119.049186	-0.3758
m-IV	$^{13}\text{C}_6\text{H}_{10}^{15}\text{NO}$	0.008664	-0.021960	119.092854	119.092820	0.2879
iTRAQ 119(8-plex)	$\text{C}_2^{13}\text{C}_4\text{H}_{13}^{15}\text{N}_2$	0.008667		119.114814	119.114817	-0.0253
iTRAQ 121(8-plex)	$^{13}\text{C}_6\text{H}_{13}^{15}\text{N}_2$	0.008887		121.121524		

* 2 Interference peaks shown in Thermo App Note 421, Figure 6.

** Peaks, which probably originated from iTRAQ and cannot be resolved by Orbitrap with standard ms/ms spectrum resolution settings, $R(400)=7500$.

† (calculated – published) in ppm

‡ Published m/z are from "An insight into iTRAQ: where do we stand now?", Fig. 3;
Anal Bioanal Chem (2012) 404:1011–1027 (DOI 10.1007/s00216-012-5918-6)

Calculated m/z: exact masses of isotopes are from

http://physics.nist.gov/cgi-bin/Compositions/stand_alone.pl?ele=&ascii=ascii&isotype=some

Mass of the electron in u is from <http://physics.nist.gov/cgi-bin/cuu/Value?meu>

^1H	1.00782503207	^{14}N	14.0030740048
^2H	2.014101778	^{15}N	15.0001088982
^{12}C	12	^{16}O	15.99491461956
^{13}C	13.0033548378	^{18}O	17.9991610
m_e	0.00054857990946		