| Peak ID | Measured mass [Da] | Tentative empirical formula (measured mass minus exact ion mass in mDa) | Temp largest signal | Concentration (mean, 10, 50, 90% percentiles) [ng/m3] | LOD [ng/m3] | Fraction of total burden (rank) |
|---|---|---|---|---|---|---|
| m18.0085 | 18.010 | | 200 | 0.32, (0.01, 0.23, 0.75) | 0.015 | 0.029% (346) |
| m18.0321 | 18.033 | $NH_3H^+$ (-0.5) | 150 | 90, (2.4, 79, 177) | n.c. | 8.06% (1) |
| m18.0817 | 18.083 | | 150 | 0.101, (0.004, 0.061, 0.267) | 0.003 | 0.0090% (458) |
| m28.0054 | 28.006 | | 300 | 0.034, (0.000, 0.027, 0.068) | 0.009 | 0.0031% (550) |
| m28.0175 | 28.018 | $CHNH^+$ (0.1) | 300 | 1.16, (0.01, 1.05, 2.29) | 0.267 | 0.104% (173) |
| m28.0301 | 28.031 | | 300 | 0.058, (0.003, 0.050, 0.129) | 0.003 | 0.0052% (506) |
| m31.0174 | 31.018 | $CH_2OH^+$ (0.2) | 300 | 4.0, (0.26, 3.8, 7.3) | 0.961 | 0.36% (58) |
| m32.0519 | 32.053 | | 200 | 0.039, (0.002, 0.028, 0.083) | 0.004 | 0.0035% (542) |
| m33.0332 | 33.034 | $CH_4OH^+$ (0.3) | 200 | 1.22, (0.06, 1.11, 2.18) | 0.089 | 0.109% (163) |
| m34.0358 | 34.036 | $CH_4OH^+$ (-0.5) | 200 | 0.017, (0.002, 0.014, 0.031) | 0.003 | 0.00148% (606) |
| m36.0442 | 36.045 | | 150 | 0.28, (0.01, 0.16, 0.59) | 0.011 | 0.025% (361) |
| m42.0339 | 42.034 | $C_2H_3NH^+$ (0.3) | 250 | 2.2, (0.03, 1.7, 4.7) | n.c. | 0.20% (101) |
| m43.0180 | 43.018 | $C_2H_2OH^+$ (0.3) | 150 | 7.0, (0.19, 5.8, 15.9) | 0.365 | 0.63% (39) |
| m44.0131 | 44.013 | $CHNOH^+$ (0.2) | 300 | 3.6, (0.14, 2.7, 8.6) | 0.313 | 0.33% (65) |
| m44.0495 | 44.050 | $C_2H_5NH^+$ (0.2) | 200 | 0.25, (0.01, 0.22, 0.54) | 0.008 | 0.023% (376) |
| m44.9972 | 44.997 | $CO_2H^+$ (0.2) | 200 | 0.071, (0.003, 0.054, 0.158) | 0.005 | 0.0064% (497) |
| m45.0336 | 45.034 | $C_2H_4OH^+$ (0.2) | 200 | 9.3, (0.53, 9.1, 17.9) | 0.419 | 0.83% (27) |
| m45.9925 | 45.993 | $NO_2^+$ (0.2) | 150 | 0.42, (0.00, 0.20, 0.90) | 0.017 | 0.038% (313) |
| m46.0291 | 46.029 | $CH_3NOH^+$ (0.4) | 200 | 3.3, (0.08, 2.8, 7.0) | 0.031 | 0.29% (75) |
| m46.0648 | 46.065 | $C_2H_7NH^+$ (-0.3) | 200 | 0.090, (0.002, 0.070, 0.207) | 0.002 | 0.0081% (470) |

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| m47.0133 | 47.013 | $CH_2O_2H^+$ (0.6) | 150 | 10.4, (0.46, 10.5, 18.7) | 0.124 | 0.94% (24) |
| m47.0233 | 47.023 | $H_2N_2OH^+$ (-0.7) | 150 | 1.18, (0.08, 1.08, 2.24) | 0.089 | 0.105% (172) |
| m47.0485 | 47.049 | $C_2H_6OH^+$ (-0.6) | 150 | 0.22, (0.01, 0.23, 0.42) | 0.024 | 0.020% (393) |
| m47.9673 | 47.967 | | 250 | 0.045, (0.002, 0.038, 0.098) | 0.002 | 0.0041% (525) |
| m48.0087 | 48.009 | $HNO_2H^+$ (0.7) | 150 | 0.149, (0.009, 0.149, 0.277) | 0.006 | 0.0134% (431) |
| m48.9845 | 48.985 | | 150 | 0.027, (0.002, 0.017, 0.070) | 0.002 | 0.0024% (571) |
| m49.0072 | 49.007 | $HNO_2H^+$ (2.1) | 150 | 0.031, (0.001, 0.028, 0.059) | 0.002 | 0.0027% (560) |
| m49.0285 | 49.028 | $CH_4O_2H^+$ (0.1) | 150 | 0.21, (0.01, 0.15, 0.48) | 0.004 | 0.0191% (398) |
| m51.0446 | 51.044 | | 200 | 0.118, (0.004, 0.082, 0.235) | 0.010 | 0.0106% (448) |
| m51.9955 | 51.995 | | 150 | 0.026, (0.000, 0.021, 0.059) | 0.004 | 0.0023% (574) |
| m52.0184 | 52.018 | $C_3HNH^+$ (0.1) | 350 | 0.070, (0.004, 0.065, 0.132) | 0.015 | 0.0063% (499) |
| m53.0027 | 53.003 | | 150 | 0.011, (0.001, 0.010, 0.023) | 0.004 | 0.00103% (624) |
| m53.0390 | 53.039 | $C_4H_4H^+$ (0.3) | 150 | 0.122, (0.001, 0.090, 0.307) | 0.005 | 0.0109% (446) |
| m53.9927 | 53.993 | | 150 | 0.015, (0.000, 0.011, 0.030) | 0.005 | 0.00130% (616) |
| m54.0344 | 54.034 | $C_3H_3NH^+$ (0.4) | 300 | 0.83, (0.01, 0.62, 1.78) | 0.010 | 0.075% (219) |
| m54.0551 | 54.055 | | 300 | 0.047, (0.000, 0.035, 0.119) | 0.002 | 0.0042% (523) |
| m55.1067 | 55.106 | | 150 | 0.015, (-0.001, 0.008, 0.040) | 0.007 | 0.00130% (615) |
| m56.0233 | 56.023 | $C_3H_2OH^+$ (1.8), $CHN_3H^+$ (-1.3) | 150 | 0.057, (0.002, 0.041, 0.136) | 0.004 | 0.0051% (511) |
| m56.0454 | 56.045 | | 250 | 0.082, (0.001, 0.061, 0.182) | 0.008 | 0.0074% (482) |
| m56.0552 | 56.055 | $C_4H_6H^+$ (-2.6) | 350 | 0.25, (0.00, 0.20, 0.57) | 0.023 | 0.023% (379) |
| m57.0348 | 57.035 | $C_3H_4OH^+$ (1.0) | 250 | 3.5, (0.14, 3.1, 6.6) | 0.114 | 0.31% (69) |

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| m58.0314 | 58.031 | $C_2H_3NOH^+$ (2.3) | 200 | 0.44, (0.02, 0.39, 0.86) | 0.005 | 0.039% (305) |
| m58.0733 | 58.073 | $C_4H_8H^+$ (-0.3) | 150 | 0.22, (-0.03, 0.08, 0.59) | 0.047 | 0.0194% (395) |
| m58.9812 | 58.981 | $CNSH^+$ (-1.6) | 100 | 0.022, (0.001, 0.019, 0.050) | 0.001 | 0.00194% (591) |
| m59.0496 | 59.049 | $C_3H_6OH^+$ (0.1) | 100 | 25, (0.9, 20, 58) | 0.440 | 2.23% (5) |
| m59.9319 | 59.932 | | 100 | 0.011, (0.001, 0.007, 0.023) | 0.002 | 0.00095% (626) |
| m59.9671 | 59.967 | | 100 | 0.007, (0.000, 0.005, 0.017) | 0.001 | 0.00065% (630) |
| m60.0226 | 60.022 | $HN_3OH^+$ (3.0) | 200 | 0.052, (0.002, 0.036, 0.123) | 0.002 | 0.0046% (515) |
| m60.0473 | 60.047 | $C_2H_5NOH^+$ (2.5) | 200 | 3.5, (0.09, 2.9, 7.5) | 0.026 | 0.31% (67) |
| m60.0809 | 60.081 | $C_3H_9NH^+$ (-0.3) | 200 | 0.176, (0.003, 0.143, 0.390) | 0.003 | 0.0158% (415) |
| m60.9869 | 60.987 | | 200 | 0.28, (0.02, 0.24, 0.57) | 0.003 | 0.025% (363) |
| m61.0291 | 61.029 | $C_2H_4O_2H^+$ (0.3) | 200 | 33, (1.6, 30, 65) | 0.214 | 2.99% (3) |
| m61.9805 | 61.980 | $CHOSH^+$ (-2.0) | 200 | 0.024, (0.001, 0.019, 0.056) | 0.005 | 0.0021% (583) |
| m62.0298 | 62.029 | $C_2H_4O_2H^+$ (-2.4) | 200 | 0.92, (0.03, 0.86, 1.79) | 0.009 | 0.082% (199) |
| m63.0015 | 63.001 | | 300 | 0.045, (0.003, 0.039, 0.093) | 0.006 | 0.0040% (527) |
| m63.0256 | 63.025 | $CH_3NO_2H^+$ (-1.9), $C_2H_6SH^+$ (-1.2) | 150 | 0.082, (0.001, 0.074, 0.179) | 0.008 | 0.0074% (481) |
| m63.0438 | 63.043 | $C_2H_6O_2H^+$ (-0.7) | 200 | 0.26, (0.00, 0.20, 0.57) | 0.025 | 0.023% (375) |
| m64.0042 | 64.004 | $HNO_3H^+$ (0.8) | 150 | 0.007, (0.000, 0.004, 0.014) | 0.002 | 0.00061% (631) |
| m64.0421 | 64.042 | $CH_5NO_2H^+$ (2.3) | 200 | 0.022, (0.000, 0.014, 0.046) | 0.002 | 0.0020% (588) |
| m64.9703 | 64.970 | | 250 | 0.028, (0.001, 0.021, 0.058) | 0.001 | 0.0025% (569) |
| m65.0244 | 65.024 | $CH_4O_3H^+$ (0.5), $C_4HNH^+$ (2.3) | 150 | 1.02, (0.03, 0.77, 2.24) | 0.008 | 0.091% (185) |
| m65.0601 | 65.060 | | 150 | 0.038, (0.002, 0.035, 0.074) | 0.003 | 0.0034% (544) |

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| m65.9787 | 65.978 | | 250 | 0.011, (0.000, 0.008, 0.024) | 0.001 | 0.00095% (625) |
| m66.0280 | 66.027 | $CH_4O_3H^+$ (0.8) | 150 | 0.031, (0.001, 0.032, 0.061) | 0.002 | 0.0028% (559) |
| m67.0309 | 67.030 | $C_3H_2N_2H^+$ (1.2) | 150 | 0.025, (0.001, 0.020, 0.056) | 0.003 | 0.0023% (579) |
| m67.0549 | 67.054 | $C_5H_6H^+$ (0.1) | 150 | 0.91, (0.01, 0.70, 2.06) | 0.028 | 0.081% (202) |
| m68.0274 | 68.027 | $C_2HN_3H^+$ (2.5) | 200 | 0.017, (0.002, 0.016, 0.033) | 0.004 | 0.00156% (605) |
| m68.0514 | 68.051 | $C_4H_5NH^+$ (1.3) | 350 | 0.52, (0.01, 0.43, 1.08) | 0.012 | 0.047% (275) |
| m68.9983 | 68.998 | | 150 | 0.039, (0.001, 0.025, 0.088) | 0.002 | 0.0035% (541) |
| m69.0349 | 69.034 | $C_4H_4OH^+$ (0.8) | 150 | 1.49, (0.03, 1.16, 3.33) | 0.080 | 0.134% (136) |
| m70.0064 | 70.006 | | 300 | 0.004, (0.000, 0.003, 0.009) | 0.002 | 0.00035% (638) |
| m70.0317 | 70.031 | $C_3H_3NOH^+$ (2.3) | 200 | 0.27, (0.01, 0.27, 0.51) | 0.006 | 0.024% (368) |
| m70.0715 | 70.071 | $C_5H_8H^+$ (-2.4) | 300 | 0.34, (-0.01, 0.24, 0.80) | 0.021 | 0.030% (335) |
| m71.0169 | 71.016 | | 150 | 0.26, (0.01, 0.19, 0.64) | 0.008 | 0.024% (373) |
| m71.0501 | 71.049 | $C_4H_6OH^+$ (0.3) | 150 | 5.4, (0.23, 4.8, 10.6) | 0.092 | 0.49% (46) |
| m72.0089 | 72.008 | $C_2HNO_2H^+$ (0.2) | 200 | 0.044, (0.001, 0.031, 0.099) | 0.002 | 0.0040% (528) |
| m72.0477 | 72.047 | $C_3H_5NOH^+$ (2.6) | 200 | 0.86, (0.02, 0.73, 1.79) | 0.014 | 0.077% (214) |
| m73.0296 | 73.029 | $C_3H_4O_2H^+$ (0.5) | 200 | 13.1, (1.22, 13.6, 23.9) | 0.125 | 1.18% (17) |
| m73.0514 | 73.051 | $(H_2O)_4H^+$ (1.1), $C_3H_5NOH^+$ (2.9) | 250 | 0.72, (0.03, 0.59, 1.66) | 0.016 | 0.064% (240) |
| m73.0647 | 73.064 | $C_4H_8OH^+$ (-0.8) | 150 | 1.41, (-0.05, 1.23, 3.00) | 0.140 | 0.126% (143) |
| m74.0265 | 74.026 | $C_2H_3NO_2H^+$ (2.1) | 200 | 0.91, (0.06, 0.92, 1.74) | 0.010 | 0.082% (201) |
| m74.0629 | 74.062 | $C_3H_7NOH^+$ (2.1) | 200 | 0.35, (0.01, 0.31, 0.73) | 0.013 | 0.031% (333) |
| m75.0097 | 75.009 | $C_2H_2O_3H^+$ (1.2) | 150 | 0.161, (0.004, 0.146, 0.350) | 0.006 | 0.0144% (424) |
| m75.0445 | 75.044 | $C_3H_6O_2H^+$ (-0.3) | 150 | 5.5, (0.07, 5.5, | 0.293 | 0.50% (45) |

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| | | | | 11.6) | | |
| m75.9962 | 75.995 | | 150 | 0.016, (0.001, 0.011, 0.040) | 0.005 | 0.00143% (612) |
| m76.0429 | 76.042 | $C_2H_5NO_2H^+$ (2.8) | 200 | 0.47, (0.01, 0.32, 1.09) | 0.006 | 0.042% (291) |
| m76.9808 | 76.980 | | 150 | 0.038, (0.002, 0.026, 0.096) | 0.002 | 0.0034% (543) |
| m77.0609 | 77.060 | $C_3H_8O_2H^+$ (0.4) | 150 | 0.155, (0.003, 0.099, 0.371) | 0.006 | 0.0139% (429) |
| m77.9933 | 77.992 | $N_2O_3H^+$ (-2.7) | 150 | 0.005, (0.000, 0.003, 0.011) | 0.002 | 0.00042% (636) |
| m78.9962 | 78.995 | | 150 | 0.185, (0.016, 0.165, 0.353) | 0.063 | 0.0166% (406) |
| m79.0415 | 79.041 | $C_2H_6O_3H^+$ (1.7) | 200 | 0.94, (0.00, 0.51, 2.32) | 0.013 | 0.084% (193) |
| m79.9998 | 79.999 | $HNO_4H^+$ (1.1) | 150 | 0.004, (0.000, 0.003, 0.009) | 0.001 | 0.00039% (637) |
| m80.0149 | 80.014 | $C_4HNOH^+$ (0.9) | 300 | 0.040, (0.001, 0.026, 0.108) | 0.005 | 0.0036% (538) |
| m80.0515 | 80.051 | $C_5H_5NH^+$ (1.2), $CH_6N_2O_2H^+$ (-2.9) | 300 | 0.42, (0.01, 0.37, 0.86) | 0.033 | 0.038% (312) |
| m80.9934 | 80.993 | $HNO_4H^+$ (-2.4) | 150 | 0.048, (0.002, 0.039, 0.099) | 0.012 | 0.0043% (522) |
| m81.0359 | 81.035 | $C_5H_4OH^+$ (1.5), $CH_5NO_3H^+$ (-2.6) | 250 | 0.88, (0.02, 0.63, 2.00) | 0.033 | 0.079% (209) |
| m81.0707 | 81.070 | $C_6H_8H^+$ (-0.1) | 150 | 1.22, (-0.02, 0.89, 3.10) | 0.116 | 0.109% (162) |
| m82.0060 | 82.005 | | 150 | 0.006, (0.000, 0.005, 0.014) | 0.001 | 0.00057% (633) |
| m82.0333 | 82.032 | | 300 | 0.36, (0.02, 0.34, 0.72) | 0.009 | 0.033% (327) |
| m82.0693 | 82.068 | | 300 | 0.58, (0.01, 0.44, 1.32) | 0.008 | 0.052% (266) |
| m82.9464 | 82.946 | | 200 | 0.016, (0.001, 0.009, 0.038) | 0.007 | 0.00140% (614) |
| m83.0152 | 83.014 | $C_4H_2O_2H^+$ (1.5) | 150 | 0.50, (0.00, 0.36, 1.09) | 0.025 | 0.044% (283) |
| m83.0503 | 83.049 | $C_5H_6OH^+$ (0.2) | 150 | 8.6, (0.27, 6.7, 16.9) | 0.189 | 0.77% (33) |
| m84.0227 | 84.022 | $C_2HN_3OH^+$ (2.5) | 150 | 0.012, (-0.001, 0.006, 0.034) | 0.004 | 0.00106% (623) |

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| m84.0486 | 84.048 | | 150 | 1.15, (0.03, 0.96, 2.35) | 0.001 | 0.103% (175) |
| m84.0878 | 84.087 | $C_6H_{10}H^+$ (-2.0) | 300 | 0.31, (-0.01, 0.24, 0.68) | 0.017 | 0.028% (353) |
| m85.0297 | 85.029 | $C_4H_4O_2H^+$ (0.3) | 150 | 8.2, (0.33, 7.4, 16.3) | 0.175 | 0.74% (35) |
| m85.0658 | 85.065 | $C_5H_8OH^+$ (0.1) | 150 | 4.6, (0.15, 4.0, 9.4) | 0.098 | 0.41% (55) |
| m86.0294 | 86.028 | | 200 | 0.65, (0.01, 0.59, 1.32) | 0.006 | 0.058% (255) |
| m86.0627 | 86.062 | $C_4H_7NOH^+$ (1.7) | 200 | 0.97, (0.03, 0.81, 2.05) | 0.014 | 0.087% (191) |
| m87.0452 | 87.044 | $C_4H_6O_2H^+$ (0.2) | 150 | 12.9, (0.42, 11.5, 25.4) | 0.080 | 1.15% (19) |
| m87.0811 | 87.080 | $C_5H_{10}OH^+$ (-0.3) | 200 | 1.90, (0.01, 1.83, 3.96) | 0.060 | 0.170% (109) |
| m87.9261 | 87.925 | | 150 | 0.007, (0.000, 0.005, 0.016) | 0.002 | 0.00061% (632) |
| m87.9629 | 87.962 | | 150 | 0.009, (0.000, 0.007, 0.016) | 0.001 | 0.00077% (629) |
| m87.9976 | 87.997 | | 300 | 0.075, (0.006, 0.069, 0.132) | n.c. | 0.0067% (491) |
| m88.0448 | 88.044 | | 150 | 0.96, (0.03, 0.86, 1.94) | 0.010 | 0.086% (192) |
| m88.0804 | 88.079 | | 200 | 0.28, (0.00, 0.23, 0.59) | 0.012 | 0.025% (364) |
| m88.9810 | 88.980 | | 150 | 0.016, (0.000, 0.011, 0.040) | 0.002 | 0.00143% (613) |
| m89.0322 | 89.031 | | 150 | 0.54, (0.01, 0.34, 1.38) | 0.015 | 0.049% (270) |
| m89.0601 | 89.059 | $C_4H_8O_2H^+$ (-0.6) | 150 | 0.94, (-0.01, 0.86, 2.06) | 0.099 | 0.084% (194) |
| m90.0203 | 90.019 | $C_2H_3NO_3H^+$ (0.7) | 150 | 0.103, (0.001, 0.048, 0.279) | 0.029 | 0.0092% (457) |
| m90.0622 | 90.061 | $C_4H_8O_2H^+$ (-1.9) | 150 | 0.179, (-0.006, 0.118, 0.441) | 0.007 | 0.0161% (410) |
| m90.9969 | 90.996 | | 150 | 0.22, (0.00, 0.22, 0.46) | 0.024 | 0.020% (390) |
| m91.0428 | 91.042 | $C_3H_6O_3H^+$ (2.8) | 250 | 0.128, (0.000, 0.043, 0.363) | n.c. | 0.0114% (440) |
| m92.0587 | 92.058 | $C_7H_6H^+$ (0.1) | 100 | 0.021, (0.000, 0.017, 0.043) | 0.008 | 0.00187% (595) |

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| m92.9588 | 92.958 | | 150 | 0.014, (0.000, 0.012, 0.031) | 0.003 | 0.00127% (618) |
| m93.0123 | 93.011 | | 150 | 0.48, (0.03, 0.45, 0.93) | 0.018 | 0.043% (288) |
| m93.0380 | 93.037 | $C_2H_5NO_3H^+$ (-0.6), $C_3H_8OSH^+$ (0.1) | 150 | 0.24, (0.00, 0.24, 0.48) | 0.031 | 0.021% (385) |
| m93.0705 | 93.069 | $C_7H_8H^+$ (-0.4) | 150 | 1.20, (0.01, 0.94, 2.84) | 0.017 | 0.107% (167) |
| m94.0086 | 94.008 | | 150 | 0.037, (0.002, 0.030, 0.076) | 0.001 | 0.0033% (547) |
| m94.0338 | 94.033 | $CH_4N_2O_3H^+$ (-0.1), $C_2H_7NOSH^+$ (0.7) | 300 | 0.23, (0.02, 0.21, 0.42) | 0.039 | 0.020% (387) |
| m94.0682 | 94.067 | $C_6H_7NH^+$ (2.0), $C_2H_8N_2O_2H^+$ (-2.0) | 300 | 0.57, (0.00, 0.46, 1.36) | 0.008 | 0.051% (267) |
| m94.9929 | 94.992 | | 150 | 0.90, (0.01, 0.66, 1.94) | 0.018 | 0.081% (204) |
| m95.0484 | 95.047 | $C_6H_6OH^+$ (-1.8), $CH_6N_2O_3H^+$ (2.2) | 250 | 2.5, (0.05, 1.9, 5.2) | 0.242 | 0.22% (95) |
| m95.0861 | 95.085 | $C_7H_{10}H^+$ (-0.5) | 150 | 1.26, (-0.07, 0.91, 3.11) | 0.264 | 0.113% (156) |
| m95.9523 | 95.951 | | 150 | 0.012, (0.001, 0.010, 0.027) | 0.003 | 0.00109% (621) |
| m96.0467 | 96.046 | $C_5H_5NOH^+$ (1.3), $CH_6N_2O_3H^+$ (-2.8) | 150 | 1.31, (0.02, 1.21, 2.62) | 0.074 | 0.118% (149) |
| m96.0879 | 96.087 | $C_7H_{10}H^+$ (-2.0) | 150 | 0.34, (0.00, 0.28, 0.77) | 0.033 | 0.031% (334) |
| m96.9621 | 96.961 | | 200 | 0.040, (0.001, 0.033, 0.092) | 0.011 | 0.0036% (537) |
| m96.9909 | 96.990 | $HNO_5H^+$ (0.1) | 150 | 0.23, (0.00, 0.14, 0.59) | 0.004 | 0.020% (389) |
| m97.0297 | 97.029 | $C_5H_4O_2H^+$ (0.2) | 250 | 13.4, (0.88, 13.7, 25.4) | 0.193 | 1.20% (16) |
| m97.0652 | 97.064 | $C_6H_8OH^+$ (-0.6) | 150 | 5.7, (0.21, 4.3, 12.9) | 0.057 | 0.51% (44) |
| m97.9474 | 97.946 | | 200 | 0.025, (0.000, 0.019, 0.055) | 0.002 | 0.0022% (582) |
| m98.0263 | 98.025 | $C_4H_3NO_2H^+$ (1.6) | 300 | 2.7, (0.13, 2.8, 5.1) | 0.020 | 0.24% (86) |
| m98.0623 | 98.061 | $C_5H_7NOH^+$ (1.2) | 150 | 1.42, (0.03, 1.13, 3.00) | 0.069 | 0.127% (140) |

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| m98.1042 | 98.103 | $C_7H_{12}H^+$ (-1.4) | 300 | 0.138, (-0.006, 0.112, 0.293) | 0.027 | 0.0124% (435) |
| m98.9609 | 98.960 | | 200 | 0.44, (0.02, 0.41, 0.88) | 0.020 | 0.040% (304) |
| m99.0091 | 99.008 | $C_4H_2O_3H^+$ (0.4), $H_3NO_5H^+$ (2.6) | 200 | 20, (0.9, 20, 37) | 0.626 | 1.83% (10) |
| m99.0449 | 99.044 | $C_5H_6O_2H^+$ (-0.2) | 150 | 22, (0.7, 18, 45) | 0.466 | 1.96% (7) |
| m99.0803 | 99.079 | $C_6H_{10}OH^+$ (-1.2) | 150 | 3.2, (0.06, 2.9, 7.3) | 0.086 | 0.29% (76) |
| m99.9479 | 99.947 | | 200 | 0.037, (0.002, 0.031, 0.084) | 0.003 | 0.0033% (546) |
| m100.014 | 100.013 | $C_4H_2O_3H^+$ (1.9), $C_2HN_3O_2H^+$ (-1.2) | 200 | 0.84, (0.03, 0.85, 1.61) | 0.062 | 0.076% (217) |
| m100.043 | 100.042 | $C_4H_5NO_2H^+$ (2.6) | 200 | 4.0, (0.04, 3.2, 8.3) | 0.053 | 0.35% (59) |
| m100.077 | 100.076 | $C_5H_9NOH^+$ (0.3) | 150 | 1.25, (0.13, 1.18, 2.37) | 0.113 | 0.112% (157) |
| m100.938 | 100.937 | | 150 | 0.082, (0.000, 0.062, 0.189) | 0.005 | 0.0074% (483) |
| m101.025 | 101.024 | $C_4H_4O_3H^+$ (0.6), $C_7HNH^+$ (2.4) | 150 | 36, (0.3, 32, 77) | 0.125 | 3.23% (2) |
| m101.061 | 101.060 | $C_5H_8O_2H^+$ (0.2) | 150 | 9.2, (0.12, 8.8, 19.7) | 0.460 | 0.83% (28) |
| m101.096 | 101.095 | $C_6H_{12}OH^+$ (-1.2) | 150 | 0.62, (-0.09, 0.51, 1.44) | 0.070 | 0.056% (259) |
| m101.943 | 101.942 | | 150 | 0.026, (0.001, 0.020, 0.056) | 0.005 | 0.0023% (575) |
| m102.026 | 102.025 | $C_4H_4O_3H^+$ (-1.7) | 150 | 1.88, (0.02, 1.60, 4.10) | 0.008 | 0.169% (110) |
| m102.062 | 102.061 | $C_5H_8O_2H^+$ (-2.1) | 150 | 0.89, (0.01, 0.76, 1.99) | 0.040 | 0.080% (206) |
| m102.083 | 102.082 | | 150 | 0.027, (0.000, 0.016, 0.073) | 0.001 | 0.0025% (570) |
| m102.095 | 102.094 | $C_5H_{11}NOH^+$ (2.6) | 150 | 0.129, (-0.003, 0.110, 0.304) | 0.005 | 0.0116% (439) |
| m102.999 | 102.998 | | 150 | 0.084, (0.000, 0.068, 0.193) | 0.005 | 0.0075% (478) |
| m103.041 | 103.040 | $C_4H_6O_3H^+$ (1.0), $C_7H_3NH^+$ (2.8) | 150 | 2.7, (-0.04, 2.2, 5.8) | 0.066 | 0.24% (91) |
| m103.076 | 103.075 | $C_5H_{10}O_2H^+$ (-0.4) | 150 | 0.48, (0.00, 0.44, 1.04) | 0.010 | 0.043% (287) |

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| m104.051 | 104.050 | $C_7H_5NH^+$ (0.5), $C_4H_9NSH^+$ (-2.9) | 300 | 0.47, (0.03, 0.39, 0.99) | 0.016 | 0.042% (293) |
| m104.933 | 104.932 | | 150 | 0.005, (-0.001, 0.003, 0.011) | 0.002 | 0.00043% (635) |
| m104.959 | 104.958 | | 150 | 0.014, (0.000, 0.010, 0.033) | 0.002 | 0.00127% (617) |
| m105.037 | 105.036 | $C_7H_4OH^+$ (2.4), $C_3H_5NO_3H^+$ (-1.6), $C_4H_8OSH^+$ (-0.9) | 150 | 0.47, (0.00, 0.35, 1.19) | 0.091 | 0.042% (295) |
| m106.039 | 106.038 | $C_7H_4OH^+$ (1.1), $C_5H_3N_3H^+$ (-2.0) | 150 | 0.121, (0.004, 0.104, 0.240) | 0.008 | 0.0109% (447) |
| m106.072 | 106.071 | $C_8H_8H^+$ (-2.3), $C_3H_8N_2O_2H^+$ (1.7), $C_4H_{11}NSH^+$ (2.4) | 200 | 0.146, (0.000, 0.118, 0.312) | 0.016 | 0.0131% (432) |
| m106.939 | 106.938 | | 150 | 0.005, (0.000, 0.004, 0.010) | 0.002 | 0.00044% (634) |
| m106.995 | 106.994 | | 150 | 0.22, (0.01, 0.17, 0.46) | 0.004 | 0.020% (394) |
| m107.085 | 107.084 | $C_8H_{10}H^+$ (-1.6), $C_3H_{10}N_2O_2H^+$ (2.4) | 150 | 0.90, (-0.01, 0.70, 2.08) | 0.053 | 0.080% (205) |
| m108.053 | 108.052 | $C_7H_6OH^+$ (-0.5) | 300 | 0.25, (0.02, 0.22, 0.45) | 0.044 | 0.023% (377) |
| m108.083 | 108.082 | $C_7H_9NH^+$ (1.2), $C_3H_{10}N_2O_2H^+$ (-2.9) | 150 | 0.52, (0.01, 0.34, 1.27) | 0.014 | 0.046% (277) |
| m108.961 | 108.960 | | 200 | 0.032, (0.001, 0.030, 0.068) | 0.005 | 0.0029% (554) |
| m109.031 | 109.030 | $C_6H_4O_2H^+$ (1.5), $C_2H_5NO_4H^+$ (-2.5), $C_3H_8O_2SH^+$ (-1.8) | 200 | 1.86, (0.08, 1.68, 3.77) | 0.016 | 0.166% (111) |
| m109.066 | 109.065 | $C_7H_8OH^+$ (0.2) | 150 | 3.8, (0.12, 2.8, 8.8) | 0.155 | 0.34% (61) |
| m109.102 | 109.101 | $C_8H_{12}H^+$ (-0.2) | 150 | 0.88, (-0.05, 0.69, 1.99) | 0.245 | 0.079% (210) |
| m109.958 | 109.957 | | 200 | 0.009, (0.001, 0.006, 0.021) | 0.002 | 0.00083% (628) |
| m110.035 | 110.034 | $C_6H_4O_2H^+$ (2.2), $C_4H_3N_3OH^+$ (-0.9) | 200 | 0.185, (0.008, 0.177, 0.357) | 0.002 | 0.0165% (407) |
| m110.064 | 110.063 | $C_6H_7NOH^+$ (2.9), $C_2H_8N_2O_3H^+$ (-1.2) | 150 | 1.29, (0.02, 0.93, 2.90) | 0.028 | 0.116% (152) |

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| m110.105 | 110.104 | $C_8H_{12}H^+$ (-0.6) | 150 | 0.25, (-0.01, 0.18, 0.59) | 0.029 | 0.022% (382) |
| m111.046 | 111.045 | $C_6H_6O_2H^+$ (0.9) | 200 | 17.6, (0.54, 15.3, 38.0) | 0.132 | 1.57% (12) |
| m111.081 | 111.080 | $C_7H_{10}OH^+$ (-0.5) | 150 | 4.9, (0.10, 3.7, 11.3) | 0.091 | 0.44% (51) |
| m111.956 | 111.955 | | 150 | 0.029, (0.001, 0.020, 0.067) | 0.003 | 0.0026% (566) |
| m112.043 | 112.042 | $C_5H_5NO_2H^+$ (2.7), $CH_6N_2O_4H^+$ (-1.4) | 300 | 0.74, (0.03, 0.56, 1.73) | n.c. | 0.066% (235) |
| m112.079 | 112.078 | $C_6H_9NOH^+$ (2.3) | 150 | 1.02, (0.01, 0.78, 2.27) | 0.013 | 0.092% (184) |
| m112.961 | 112.960 | | 150 | 0.27, (0.01, 0.25, 0.54) | 0.021 | 0.024% (369) |
| m113.026 | 113.025 | $C_5H_4O_3H^+$ (1.7), $CH_5NO_5H^+$ (-2.4) | 200 | 15.3, (0.71, 15.2, 29.3) | 0.308 | 1.37% (14) |
| m113.060 | 113.059 | $C_6H_8O_2H^+$ (-0.7) | 150 | 19.4, (0.38, 16.4, 38.8) | 0.521 | 1.74% (11) |
| m113.097 | 113.096 | $C_7H_{12}OH^+$ (-0.1) | 150 | 2.8, (0.00, 2.3, 6.2) | 0.090 | 0.25% (85) |
| m114.025 | 114.024 | $C_5H_4O_3H^+$ (-2.7) | 200 | 0.93, (0.03, 0.92, 1.86) | 0.019 | 0.084% (195) |
| m114.058 | 114.057 | $C_5H_7NO_2H^+$ (2.0) | 150 | 1.47, (0.05, 1.11, 3.40) | n.c. | 0.132% (137) |
| m114.092 | 114.091 | $C_6H_{11}NOH^+$ (-0.4) | 150 | 0.43, (0.01, 0.32, 1.02) | 0.019 | 0.039% (309) |
| m114.958 | 114.957 | | 150 | 0.081, (0.002, 0.056, 0.189) | 0.002 | 0.0073% (485) |
| m115.040 | 115.039 | $C_5H_6O_3H^+$ (0.0), $C_8H_3NH^+$ (1.8) | 150 | 13.6, (0.04, 12.1, 31.5) | 0.132 | 1.22% (15) |
| m115.076 | 115.075 | $C_6H_{10}O_2H^+$ (-0.4) | 150 | 8.9, (0.09, 7.9, 18.9) | 0.099 | 0.80% (31) |
| m115.112 | 115.111 | $C_7H_{14}OH^+$ (-0.7) | 150 | 0.53, (-0.07, 0.36, 1.41) | 0.065 | 0.048% (273) |
| m116.039 | 116.038 | | 150 | 1.22, (0.00, 0.92, 2.85) | 0.005 | 0.110% (160) |
| m116.078 | 116.077 | $C_6H_{10}O_2H^+$ (-1.7) | 150 | 0.86, (0.01, 0.74, 1.93) | 0.008 | 0.077% (213) |
| m116.115 | 116.114 | $C_7H_{14}OH^+$ (-1.1) | 150 | 0.098, (-0.007, 0.083, 0.234) | 0.008 | 0.0088% (460) |
| m116.909 | 116.908 | | 150 | 0.041, (0.000, 0.028, 0.095) | 0.014 | 0.0037% (535) |

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| m117.021 | 117.020 | $C_4H_4O_4H^+$ (1.8) | 200 | 1.52, (0.06, 1.17, 3.35) | 0.021 | 0.136% (130) |
| m117.056 | 117.055 | $C_5H_8O_3H^+$ (0.4), $C_8H_5NH^+$ (2.2) | 150 | 3.7, (0.03, 3.0, 8.5) | 0.007 | 0.33% (63) |
| m117.091 | 117.090 | $C_6H_{12}O_2H^+$ (-1.0) | 150 | 0.35, (0.01, 0.30, 0.80) | 0.037 | 0.032% (330) |
| m117.959 | 117.958 | | 150 | 0.016, (0.000, 0.012, 0.036) | 0.002 | 0.00145% (609) |
| m118.025 | 118.024 | $C_4H_4O_4H^+$ (2.4), $C_2H_3N_3O_3H^+$ (-0.7) | 150 | 0.21, (0.01, 0.18, 0.47) | 0.007 | 0.0192% (397) |
| m118.078 | 118.077 | | 150 | 0.50, (0.00, 0.36, 1.15) | 0.084 | 0.045% (280) |
| m118.995 | 118.994 | | 150 | 0.31, (0.04, 0.24, 0.66) | 0.041 | 0.028% (350) |
| m119.038 | 119.037 | | 150 | 1.57, (-0.02, 0.92, 3.63) | 0.502 | 0.140% (126) |
| m120.048 | 120.047 | $C_7H_5NOH^+$ (2.6), $C_3H_6N_2O_3H^+$ (-1.4), $C_4H_9NOSH^+$ (-0.7) | 300 | 0.33, (0.01, 0.29, 0.68) | 0.046 | 0.030% (340) |
| m120.091 | 120.090 | $C_9H_{10}H^+$ (1.2) | 200 | 0.46, (-0.02, 0.19, 0.84) | 0.097 | 0.041% (298) |
| m120.903 | 120.902 | | 150 | 0.013, (-0.001, 0.008, 0.034) | 0.006 | 0.00118% (619) |
| m121.066 | 121.065 | $C_8H_8OH^+$ (0.2) | 150 | 3.6, (0.12, 1.6, 8.9) | 1.005 | 0.32% (66) |
| m122.967 | 122.966 | | 150 | 0.079, (0.003, 0.057, 0.201) | 0.012 | 0.0070% (488) |
| m123.046 | 123.045 | $C_7H_6O_2H^+$ (1.0), $C_4H_{10}O_2SH^+$ (-2.4) | 150 | 4.9, (0.06, 4.5, 10.2) | 0.079 | 0.44% (53) |
| m123.079 | 123.078 | $C_8H_{10}OH^+$ (-2.4), $C_3H_{10}N_2O_3H^+$ (1.6) | 150 | 3.4, (0.13, 2.9, 7.8) | 0.024 | 0.31% (70) |
| m123.118 | 123.117 | $C_9H_{14}H^+$ (0.2) | 150 | 0.40, (-0.03, 0.30, 0.96) | 0.241 | 0.036% (317) |
| m124.046 | 124.045 | $C_7H_6O_2H^+$ (-2.3), $C_2H_6N_2O_4H^+$ (1.7), $C_3H_9NO_2SH^+$ (2.4) | 150 | 1.21, (0.02, 1.18, 2.37) | 0.010 | 0.109% (165) |
| m124.079 | 124.078 | $C_7H_9NOH^+$ (2.4), $C_3H_{10}N_2O_3H^+$ (-1.7) | 150 | 0.88, (0.01, 0.63, 2.00) | 0.017 | 0.079% (211) |

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| m124.120 | 124.119 | $C_9H_{14}H^+$ (-1.1) | 150 | 0.117, (-0.006, 0.085, 0.273) | 0.029 | 0.0105% (449) |
| m124.950 | 124.949 | $C_5S_2H^+$ (-2.3) | 150 | 0.086, (0.006, 0.069, 0.181) | 0.006 | 0.0077% (474) |
| m125.026 | 125.025 | $C_6H_4O_3H^+$ (1.8), $C_2H_5NO_5H^+$ (-2.3), $C_3H_8O_3SH^+$ (-1.6) | 250 | 4.3, (0.34, 4.6, 7.1) | 0.097 | 0.38% (57) |
| m125.061 | 125.060 | $C_7H_8O_2H^+$ (0.4) | 150 | 12.1, (0.31, 9.3, 25.2) | 0.161 | 1.08% (20) |
| m125.096 | 125.095 | $C_8H_{12}OH^+$ (-1.0) | 150 | 3.4, (0.02, 2.7, 8.3) | 0.101 | 0.30% (71) |
| m125.963 | 125.962 | | 150 | 0.040, (0.002, 0.036, 0.081) | 0.008 | 0.0036% (536) |
| m126.024 | 126.023 | $CH_4N_2O_5H^+$ (0.5), $C_2H_7NO_3SH^+$ (1.2) | 250 | 0.36, (0.02, 0.37, 0.66) | 0.010 | 0.033% (328) |
| m126.060 | 126.059 | $C_2H_8N_2O_4H^+$ (0.1) | 200 | 2.2, (0.04, 1.8, 4.6) | 0.009 | 0.20% (103) |
| m126.097 | 126.096 | | 150 | 0.61, (0.00, 0.46, 1.37) | 0.012 | 0.055% (261) |
| m126.908 | 126.907 | | 150 | 0.028, (0.001, 0.019, 0.062) | 0.002 | 0.0025% (568) |
| m126.971 | 126.970 | | 150 | 0.21, (0.00, 0.17, 0.44) | 0.008 | 0.0184% (400) |
| m127.041 | 127.040 | $C_6H_6O_3H^+$ (1.1), $C_2H_7NO_5H^+$ (-2.9) | 150 | 8.4, (0.06, 7.8, 17.0) | 0.155 | 0.75% (34) |
| m127.076 | 127.075 | $C_7H_{10}O_2H^+$ (-0.2) | 200 | 20, (0.4, 17, 43) | 0.492 | 1.83% (9) |
| m127.112 | 127.111 | $C_8H_{14}OH^+$ (-0.6) | 150 | 1.62, (-0.07, 1.33, 4.16) | 0.094 | 0.145% (123) |
| m127.949 | 127.948 | | 150 | 0.033, (0.001, 0.024, 0.074) | 0.002 | 0.0029% (553) |
| m127.994 | 127.993 | $CH_2O_7H^+$ (2.4) | 150 | 0.042, (0.002, 0.030, 0.094) | 0.006 | 0.0037% (532) |
| m128.039 | 128.038 | $CH_6N_2O_5H^+$ (-0.2) | 200 | 0.92, (0.01, 0.73, 2.02) | 0.009 | 0.082% (200) |
| m128.076 | 128.075 | | 150 | 2.3, (0.03, 1.9, 5.1) | 0.049 | 0.20% (99) |
| m128.115 | 128.114 | $C_8H_{14}OH^+$ (-1.0) | 150 | 0.31, (0.00, 0.24, 0.73) | 0.012 | 0.028% (351) |
| m128.897 | 128.896 | | 200 | 0.012, (0.001, 0.009, 0.025) | 0.004 | 0.00108% (622) |
| m128.973 | 128.972 | | 150 | 0.158, (0.003, 0.131, 0.348) | 0.025 | 0.0141% (426) |

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| m129.056 | 129.055 | $C_6H_8O_3H^+$ (0.5), $C_9H_5NH^+$ (2.3) | 150 | 11.1, (0.10, 9.2, 24.3) | 0.362 | 0.99% (23) |
| m129.090 | 129.089 | $C_7H_{12}O_2H^+$ (-1.9) | 150 | 5.7, (0.01, 4.6, 13.2) | 0.055 | 0.51% (43) |
| m129.128 | 129.127 | $C_8H_{16}OH^+$ (-0.3) | 150 | 0.30, (-0.04, 0.19, 0.81) | 0.114 | 0.027% (356) |
| m130.055 | 130.054 | | 200 | 1.67, (0.01, 1.19, 3.66) | 0.016 | 0.149% (120) |
| m130.091 | 130.090 | | 150 | 0.72, (0.00, 0.57, 1.75) | 0.009 | 0.065% (238) |
| m130.131 | 130.130 | $C_8H_{16}OH^+$ (-0.6) | 150 | 0.074, (-0.009, 0.050, 0.191) | 0.014 | 0.0066% (493) |
| m131.036 | 131.035 | $C_5H_6O_4H^+$ (1.3) | 150 | 1.54, (0.01, 1.17, 3.31) | 0.089 | 0.138% (129) |
| m131.073 | 131.072 | $C_6H_{10}O_3H^+$ (1.9) | 150 | 2.3, (0.00, 1.5, 5.5) | 0.007 | 0.21% (97) |
| m131.085 | 131.084 | $C_{10}H_{10}H^+$ (-1.4), $C_5H_{10}N_2O_2H^+$ (2.7) | 150 | 0.45, (0.01, 0.35, 1.08) | 0.190 | 0.040% (303) |
| m131.994 | 131.993 | $C_3HNO_5H^+$ (0.4) | 150 | 0.086, (0.003, 0.071, 0.177) | 0.008 | 0.0077% (473) |
| m132.047 | 132.046 | $C_8H_5NOH^+$ (1.8), $C_4H_6N_2O_3H^+$ (-2.3), $C_5H_9NOSH^+$ (-1.6) | 150 | 0.31, (0.00, 0.24, 0.67) | 0.005 | 0.028% (352) |
| m132.084 | 132.083 | $C_9H_9NH^+$ (2.4), $C_5H_{10}N_2O_2H^+$ (-1.7), $C_6H_{13}NSH^+$ (-1.0) | 150 | 0.47, (0.00, 0.33, 1.11) | 0.023 | 0.043% (290) |
| m132.976 | 132.975 | $C_4H_4OS_2H^+$ (-2.4) | 150 | 0.98, (0.01, 0.79, 2.17) | 0.031 | 0.087% (190) |
| m133.007 | 133.006 | $C_2HN_3O_4H^+$ (-1.1) | 150 | 0.35, (0.02, 0.24, 0.81) | 0.053 | 0.031% (332) |
| m133.028 | 133.027 | $C_8H_4O_2H^+$ (-1.2), $C_3H_4N_2O_4H^+$ (2.8) | 50 | 0.010, (-0.001, 0.009, 0.025) | 0.007 | 0.00092% (627) |
| m133.052 | 133.051 | $C_5H_8O_4H^+$ (1.7) | 150 | 5.1, (0.01, 2.6, 14.6) | 0.046 | 0.46% (49) |
| m133.066 | 133.065 | $C_9H_8OH^+$ (0.4), $C_6H_{12}OSH^+$ (-3.0) | 350 | 0.45, (-0.02, 0.34, 0.81) | 0.242 | 0.040% (301) |
| m133.100 | 133.099 | $C_{10}H_{12}H^+$ (-2.0), $C_5H_{12}N_2O_2H^+$ (2.0) | 150 | 1.27, (0.02, 0.99, 2.93) | 0.057 | 0.114% (154) |

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| m133.985 | 133.984 | | 150 | 0.095, (0.005, 0.076, 0.188) | 0.003 | 0.0085% (463) |
| m134.066 | 134.065 | $C_9H_8OH^+$ (-2.9), $C_4H_8N_2O_3H^+$ (1.1), $C_5H_{11}NOSH^+$ (1.8) | 150 | 0.80, (0.01, 0.61, 1.87) | 0.008 | 0.071% (223) |
| m134.102 | 134.101 | $C_5H_{12}N_2O_2H^+$ (0.7), $C_6H_{15}NSH^+$ (1.4) | 150 | 0.23, (0.00, 0.15, 0.59) | 0.012 | 0.021% (386) |
| m134.966 | 134.965 | | 150 | 0.193, (0.007, 0.159, 0.434) | 0.007 | 0.0173% (404) |
| m135.047 | 135.046 | $C_8H_6O_2H^+$ (2.2), $C_4H_7NO_4H^+$ (-1.9), $C_5H_{10}O_2SH^+$ (-1.2) | 250 | 0.79, (0.03, 0.65, 1.64) | 0.054 | 0.071% (225) |
| m135.082 | 135.081 | $C_9H_{10}OH^+$ (0.8), $C_6H_{14}OSH^+$ (-2.6) | 150 | 2.7, (0.36, 2.4, 4.7) | 0.812 | 0.24% (92) |
| m135.117 | 135.116 | $C_{10}H_{14}H^+$ (-0.6) | 150 | 0.73, (-0.02, 0.53, 1.68) | 0.137 | 0.065% (237) |
| m136.044 | 136.043 | $C_3H_6N_2O_4H^+$ (-0.1), $C_4H_9NO_2SH^+$ (0.6) | 250 | 0.45, (0.01, 0.41, 0.91) | 0.013 | 0.040% (302) |
| m136.083 | 136.082 | $C_9H_{10}OH^+$ (-1.5), $C_4H_{10}N_2O_3H^+$ (2.5) | 150 | 0.99, (0.07, 0.80, 2.22) | 0.009 | 0.089% (187) |
| m136.960 | 136.959 | | 150 | 0.122, (0.005, 0.106, 0.243) | 0.024 | 0.0109% (445) |
| m137.029 | 137.028 | $C_3H_5NO_5H^+$ (0.9) | 150 | 0.48, (0.01, 0.33, 0.96) | 0.008 | 0.043% (286) |
| m137.061 | 137.060 | $C_8H_8O_2H^+$ (0.6), $C_5H_{12}O_2SH^+$ (-2.8) | 250 | 5.1, (0.18, 4.4, 11.3) | 0.136 | 0.46% (47) |
| m137.095 | 137.094 | $C_9H_{12}OH^+$ (-1.8), $C_4H_{12}N_2O_3H^+$ (2.2) | 150 | 2.8, (0.06, 2.4, 7.0) | 0.025 | 0.25% (84) |
| m137.965 | 137.964 | | 150 | 0.031, (0.001, 0.026, 0.064) | 0.004 | 0.0028% (557) |
| m138.015 | 138.014 | $C_3H_4O_6H^+$ (2.9), $CH_3N_3O_5H^+$ (-0.3) | 300 | 0.115, (0.003, 0.084, 0.262) | 0.021 | 0.0103% (451) |
| m138.059 | 138.058 | $C_3H_8N_2O_4H^+$ (-0.8), $C_4H_{11}NO_2SH^+$ (0.0) | 200 | 1.50, (0.02, 1.30, 3.02) | 0.011 | 0.135% (133) |
| m138.094 | 138.093 | $C_8H_{11}NOH^+$ (1.9), $C_4H_{12}N_2O_3H^+$ (-2.1) | 150 | 0.70, (0.01, 0.52, 1.46) | 0.006 | 0.062% (243) |

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| m138.136 | 138.135 | $C_{10}H_{16}H^+$ (-0.5) | 300 | 0.026, (-0.003, 0.020, 0.060) | 0.016 | 0.0024% (573) |
| m138.965 | 138.964 | | 150 | 0.34, (0.01, 0.28, 0.70) | 0.006 | 0.030% (337) |
| m139.041 | 139.040 | $C_7H_6O_3H^+$ (1.3), $C_3H_7NO_5H^+$ (-2.8), $C_4H_{10}O_3SH^+$ (-2.0) | 150 | 9.8, (0.39, 8.6, 19.3) | 0.183 | 0.88% (25) |
| m139.075 | 139.074 | $C_8H_{10}O_2H^+$ (-1.1), $C_3H_{10}N_2O_4H^+$ (3.0) | 200 | 11.5, (0.35, 9.3, 27.4) | 0.442 | 1.03% (21) |
| m139.112 | 139.111 | $C_9H_{14}OH^+$ (-0.4) | 150 | 2.2, (0.01, 2.1, 5.0) | 0.120 | 0.20% (102) |
| m139.674 | 139.673 | | 150 | 0.024, (0.000, 0.017, 0.053) | 0.004 | 0.0021% (584) |
| m139.979 | 139.978 | | 150 | 0.093, (0.002, 0.077, 0.204) | 0.008 | 0.0084% (467) |
| m140.039 | 140.038 | $C_2H_6N_2O_5H^+$ (0.0) | 150 | 1.10, (0.04, 0.98, 2.23) | 0.008 | 0.099% (179) |
| m140.074 | 140.073 | $C_7H_9NO_2H^+$ (2.7), $C_3H_{10}N_2O_4H^+$ (-1.4) | 200 | 2.6, (0.03, 2.1, 5.7) | 0.012 | 0.23% (94) |
| m140.114 | 140.113 | $C_9H_{14}OH^+$ (-1.8) | 150 | 0.46, (0.00, 0.36, 1.08) | 0.010 | 0.041% (297) |
| m140.982 | 140.981 | $C_6H_4S_2H^+$ (-1.4) | 150 | 0.43, (0.01, 0.34, 0.87) | 0.035 | 0.039% (310) |
| m141.056 | 141.055 | $C_7H_8O_3H^+$ (0.7), $C_{10}H_5NH^+$ (2.5) | 150 | 23, (0.4, 18, 46) | 0.261 | 2.02% (6) |
| m141.090 | 141.089 | $C_8H_{12}O_2H^+$ (-1.7) | 150 | 7.3, (0.10, 5.4, 17.3) | 0.074 | 0.65% (37) |
| m141.127 | 141.126 | $C_9H_{16}OH^+$ (-1.1) | 150 | 0.89, (-0.05, 0.77, 2.16) | 0.055 | 0.080% (207) |
| m141.960 | 141.959 | | 150 | 0.057, (0.002, 0.042, 0.127) | 0.005 | 0.0051% (509) |
| m142.057 | 142.056 | $C_7H_8O_3H^+$ (-1.6), $C_2H_8N_2O_5H^+$ (2.4) | 150 | 2.3, (0.02, 1.7, 5.2) | 0.081 | 0.21% (96) |
| m142.090 | 142.089 | | 150 | 1.51, (0.01, 1.16, 3.26) | 0.018 | 0.135% (132) |
| m142.927 | 142.926 | | 150 | 0.058, (0.001, 0.041, 0.126) | 0.003 | 0.0052% (507) |
| m142.996 | 142.995 | $C_5H_2O_5H^+$ (-2.1) | 150 | 0.23, (0.01, 0.20, 0.54) | 0.009 | 0.020% (388) |
| m143.038 | 143.037 | $C_4H_6N_4SH^+$ (-1.2) | 150 | 1.22, (0.00, 0.75, 2.76) | 0.044 | 0.109% (161) |

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| m143.072 | 143.071 | $C_7H_{10}O_3H^+$ (1.1), $C_{10}H_7NH^+$ (2.9) | 150 | 9.5, (0.07, 8.3, 21.0) | 0.271 | 0.85% (26) |
| m143.106 | 143.105 | $C_8H_{14}O_2H^+$ (-1.3) | 100 | 2.7, (-0.04, 2.0, 6.7) | 0.009 | 0.24% (90) |
| m143.934 | 143.933 | | 150 | 0.026, (0.000, 0.016, 0.050) | 0.004 | 0.0023% (577) |
| m144.037 | 144.036 | $C_6H_6O_4H^+$ (-0.9) | 150 | 0.42, (0.00, 0.32, 0.89) | 0.021 | 0.037% (315) |
| m144.071 | 144.070 | | 150 | 1.19, (0.00, 0.93, 2.56) | 0.033 | 0.107% (168) |
| m144.109 | 144.108 | $C_8H_{14}O_2H^+$ (-1.6) | 150 | 0.43, (-0.01, 0.29, 0.99) | 0.017 | 0.039% (308) |
| m144.146 | 144.145 | $C_9H_{18}OH^+$ (-1.0) | 150 | 0.041, (-0.009, 0.030, 0.106) | 0.022 | 0.0037% (534) |
| m145.009 | 145.008 | $C_8HNO_2H^+$ (-3.0), $C_3HN_3O_4H^+$ (1.1), $C_4H_4N_2O_2SH^+$ (1.8) | 150 | 0.155, (0.007, 0.100, 0.344) | 0.046 | 0.0139% (428) |
| m145.053 | 145.052 | $C_6H_8O_4H^+$ (2.9), $C_4H_8N_4SH^+$ (-1.8) | 150 | 3.3, (0.01, 2.2, 7.4) | 0.122 | 0.30% (74) |
| m145.122 | 145.121 | $C_8H_{16}O_2H^+$ (-0.9) | 150 | 0.88, (0.00, 0.68, 2.02) | 0.128 | 0.079% (208) |
| m145.973 | 145.972 | | 150 | 0.016, (0.000, 0.011, 0.037) | 0.001 | 0.00147% (607) |
| m146.010 | 146.009 | $C_4H_3NO_5H^+$ (1.0) | 150 | 0.085, (0.006, 0.072, 0.181) | 0.004 | 0.0076% (477) |
| m146.059 | 146.058 | $C_9H_7NOH^+$ (-1.6), $C_4H_7N_3O_3H^+$ (2.4) | 150 | 0.66, (0.00, 0.43, 1.41) | 0.026 | 0.060% (250) |
| m146.124 | 146.123 | $C_8H_{16}O_2H^+$ (-2.2) | 150 | 0.28, (0.00, 0.20, 0.66) | 0.012 | 0.026% (360) |
| m146.979 | 146.978 | | 150 | 0.20, (0.01, 0.12, 0.47) | 0.058 | 0.0181% (401) |
| m147.047 | 147.046 | $C_9H_6O_2H^+$ (2.4), $C_5H_7NO_4H^+$ (-1.7), $C_6H_{10}O_2SH^+$ (-1.0) | 150 | 1.51, (0.06, 1.45, 2.90) | 0.023 | 0.135% (131) |
| m147.078 | 147.077 | $C_{10}H_{10}OH^+$ (-3.0), $C_5H_{10}N_2O_3H^+$ (1.0), $C_8H_7N_3H^+$ (2.8) | 150 | 1.90, (0.02, 1.49, 4.24) | 0.014 | 0.170% (108) |
| m147.116 | 147.115 | $C_{11}H_{14}H^+$ (-1.4), $C_6H_{14}N_2O_2H^+$ (2.6) | 200 | 0.31, (-0.02, 0.23, 0.75) | 0.048 | 0.028% (349) |

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| m147.982 | 147.981 | | 150 | 0.042, (0.004, 0.029, 0.092) | 0.004 | 0.0038% (531) |
| m148.042 | 148.041 | $C_8H_5NO_2H^+$ (2.2), $C_4H_6N_2O_4H^+$ (-1.9), $C_5H_9NO_2SH^+$ (-1.2) | 300 | 1.25, (0.01, 1.08, 2.51) | 0.029 | 0.112% (158) |
| m149.026 | 149.025 | $C_8H_4O_3H^+$ (2.2), $C_4H_5NO_5H^+$ (-1.9) | 150 | 9.1, (-0.51, 8.7, 19.8) | 0.049 | 0.82% (29) |
| m149.095 | 149.094 | $C_{10}H_{12}OH^+$ (-1.6), $C_5H_{12}N_2O_3H^+$ (2.4) | 150 | 3.5, (0.05, 2.8, 7.9) | 0.031 | 0.31% (68) |
| m149.980 | 149.979 | | 150 | 0.024, (0.000, 0.012, 0.067) | 0.005 | 0.0021% (585) |
| m150.029 | 150.029 | $C_8H_4O_3H^+$ (1.8), $C_6H_3N_3O_2H^+$ (-1.3) | 150 | 0.74, (-0.04, 0.69, 1.62) | 0.004 | 0.067% (232) |
| m150.055 | 150.055 | $C_8H_7NO_2H^+$ (-0.5) | 200 | 0.77, (0.00, 0.63, 1.65) | 0.012 | 0.069% (226) |
| m150.094 | 150.094 | $C_9H_{11}NOH^+$ (2.2), $C_5H_{12}N_2O_3H^+$ (-1.9) | 150 | 0.77, (0.01, 0.57, 1.82) | 0.009 | 0.069% (229) |
| m150.135 | 150.135 | $C_{11}H_{16}H^+$ (-1.3), $C_6H_{16}N_2O_2H^+$ (2.7) | 150 | 0.097, (-0.001, 0.071, 0.209) | 0.016 | 0.0087% (462) |
| m150.970 | 150.970 | | 150 | 0.181, (0.007, 0.156, 0.387) | 0.012 | 0.0162% (409) |
| m151.042 | 151.042 | $C_8H_6O_3H^+$ (2.5), $C_4H_7NO_5H^+$ (-1.5), $C_5H_{10}O_3SH^+$ (-0.8) | 250 | 1.56, (0.03, 1.39, 3.02) | 0.041 | 0.140% (128) |
| m151.076 | 151.076 | $C_9H_{10}O_2H^+$ (0.2) | 150 | 4.5, (0.08, 3.3, 10.3) | 0.074 | 0.41% (56) |
| m151.110 | 151.110 | $C_{10}H_{14}OH^+$ (-2.2), $C_5H_{14}N_2O_3H^+$ (1.8) | 150 | 2.8, (0.04, 2.5, 6.0) | 0.030 | 0.26% (83) |
| m151.939 | 151.939 | | 150 | 0.012, (0.001, 0.008, 0.028) | 0.003 | 0.00112% (620) |
| m151.978 | 151.978 | | 150 | 0.050, (-0.001, 0.043, 0.107) | 0.014 | 0.0045% (521) |
| m152.040 | 152.040 | $C_8H_6O_3H^+$ (-2.8), $C_3H_6N_2O_5H^+$ (1.2) | 150 | 0.32, (0.00, 0.29, 0.64) | 0.005 | 0.029% (344) |
| m152.076 | 152.076 | $C_4H_{10}N_2O_4H^+$ (0.8), $C_5H_{13}NO_2SH^+$ (1.6) | 200 | 1.30, (0.01, 0.95, 2.83) | 0.011 | 0.117% (150) |

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| m152.114 | 152.114 | $C_{10}H_{14}OH^+$ (-1.6), $C_5H_{14}N_2O_3H^+$ (2.5) | 150 | 0.52, (0.01, 0.41, 1.09) | 0.009 | 0.046% (278) |
| m153.022 | 153.022 | $C_4H_8O_4SH^+$ (-0.1) | 250 | 0.69, (0.00, 0.74, 1.23) | 0.035 | 0.062% (246) |
| m153.057 | 153.057 | $C_8H_8O_3H^+$ (1.9), $C_4H_9NO_5H^+$ (-2.1), $C_5H_{12}O_3SH^+$ (-1.4) | 150 | 6.9, (0.16, 5.6, 14.5) | 0.137 | 0.62% (40) |
| m153.091 | 153.091 | $C_9H_{12}O_2H^+$ (-0.5) | 150 | 7.8, (0.03, 5.6, 18.1) | 0.146 | 0.70% (36) |
| m153.126 | 153.126 | $C_{10}H_{16}OH^+$ (-1.8) | 150 | 1.37, (-0.03, 1.06, 3.22) | 0.052 | 0.123% (146) |
| m153.692 | 153.692 | | 150 | 0.026, (0.000, 0.019, 0.059) | 0.005 | 0.0023% (578) |
| m153.923 | 153.923 | | 150 | 0.026, (0.000, 0.018, 0.053) | 0.004 | 0.0023% (576) |
| m154.013 | 154.013 | $C_6H_3NO_4H^+$ (-0.9) | 350 | 0.157, (0.000, 0.150, 0.305) | 0.014 | 0.0141% (427) |
| m154.057 | 154.057 | $C_8H_8O_3H^+$ (-1.4), $C_3H_8N_2O_5H^+$ (2.6) | 150 | 1.07, (0.02, 0.80, 2.38) | 0.023 | 0.096% (180) |
| m154.089 | 154.089 | $C_8H_{11}NO_2H^+$ (2.3), $C_4H_{12}N_2O_4H^+$ (-1.8) | 150 | 1.69, (0.01, 1.17, 3.91) | 0.023 | 0.151% (119) |
| m154.930 | 154.930 | | 150 | 0.094, (0.001, 0.063, 0.214) | 0.003 | 0.0084% (466) |
| m155.031 | 155.031 | $C_{10}H_3NOH^+$ (-1.5), $C_5H_3N_3O_3H^+$ (2.5) | 150 | 1.59, (-0.01, 0.39, 4.86) | 0.101 | 0.143% (125) |
| m155.072 | 155.072 | $C_8H_{10}O_3H^+$ (1.3), $C_4H_{11}NO_5H^+$ (-2.8) | 150 | 16.3, (0.09, 12.3, 37.7) | 0.140 | 1.46% (13) |
| m155.143 | 155.143 | $C_{10}H_{18}OH^+$ (-0.4) | 150 | 3.1, (-0.06, 2.4, 7.3) | 0.086 | 0.28% (80) |
| m155.921 | 155.921 | | 150 | 0.032, (0.000, 0.021, 0.073) | 0.004 | 0.0028% (556) |
| m156.032 | 156.032 | $C_6H_5NO_4H^+$ (2.5) | 150 | 0.21, (0.00, 0.12, 0.63) | 0.019 | 0.0192% (396) |
| m156.072 | 156.072 | $C_8H_{10}O_3H^+$ (-2.0), $C_3H_{10}N_2O_5H^+$ (2.0) | 150 | 2.7, (0.01, 1.8, 6.1) | 0.016 | 0.24% (87) |
| m157.051 | 157.051 | $C_7H_8O_4H^+$ (1.1), $C_{10}H_5NOH^+$ (2.9) | 150 | 21, (0.0, 16, 49) | 0.164 | 1.86% (8) |

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| m157.085 | 157.085 | $C_8H_{12}O_3H^+$ (-1.3), $C_{11}H_9NH^+$ (0.5) | 150 | 7.1, (0.05, 5.8, 16.5) | 0.374 | 0.64% (38) |
| m157.121 | 157.121 | $C_9H_{16}O_2H^+$ (-1.7) | 150 | 1.11, (-0.07, 0.87, 2.78) | 0.196 | 0.099% (178) |
| m157.660 | 157.660 | | 150 | 0.030, (0.000, 0.021, 0.069) | 0.003 | 0.0027% (563) |
| m158.055 | 158.055 | $C_7H_8O_4H^+$ (1.8), $C_5H_7N_3O_3H^+$ (-1.4) | 150 | 2.0, (0.02, 1.5, 4.6) | 0.042 | 0.179% (105) |
| m158.094 | 158.094 | $C_{11}H_{11}NH^+$ (-2.8), $C_6H_{11}N_3O_2H^+$ (1.2) | 150 | 1.42, (0.00, 1.02, 3.34) | 0.022 | 0.127% (141) |
| m158.158 | 158.158 | | 150 | 0.072, (-0.009, 0.054, 0.197) | 0.035 | 0.0065% (496) |
| m158.997 | 158.997 | | 150 | 0.69, (0.02, 0.64, 1.34) | 0.095 | 0.062% (247) |
| m159.046 | 159.046 | $C_{10}H_6O_2H^+$ (1.6), $C_6H_7NO_4H^+$ (-2.5), $C_7H_{10}O_2SH^+$ (-1.8) | 150 | 0.183, (-0.004, 0.112, 0.488) | 0.056 | 0.0164% (408) |
| m159.066 | 159.066 | $C_7H_{10}O_4H^+$ (0.5), $C_{10}H_7NOH^+$ (2.3) | 150 | 4.9, (-0.05, 2.2, 12.8) | 0.031 | 0.44% (54) |
| m159.120 | 159.120 | $C_{12}H_{14}H^+$ (2.8), $C_8H_{15}NO_2H^+$ (-1.2), $C_9H_{18}SH^+$ (-0.5) | 150 | 0.76, (-0.03, 0.40, 2.05) | 0.054 | 0.068% (230) |
| m159.982 | 159.982 | | 100 | 0.037, (0.004, 0.034, 0.072) | 0.002 | 0.0034% (545) |
| m160.071 | 160.071 | $C_7H_{10}O_4H^+$ (2.2), $C_5H_9N_3O_3H^+$ (-1.0) | 150 | 0.75, (0.00, 0.47, 1.71) | 0.029 | 0.067% (231) |
| m160.123 | 160.123 | $C_{12}H_{14}H^+$ (2.5) | 150 | 0.27, (0.00, 0.16, 0.65) | 0.014 | 0.024% (370) |
| m160.976 | 160.976 | | 100 | 0.107, (0.008, 0.070, 0.223) | 0.020 | 0.0096% (455) |
| m161.059 | 161.059 | $C_{10}H_8O_2H^+$ (-1.0) | 150 | 3.0, (0.13, 2.8, 5.8) | n.c. | 0.27% (81) |
| m161.982 | 161.982 | | 100 | 0.027, (0.004, 0.022, 0.056) | 0.003 | 0.0024% (572) |
| m162.059 | 162.059 | $C_5H_8N_2O_4H^+$ (-0.3), $C_6H_{11}NO_2SH^+$ (0.4) | 150 | 0.81, (0.01, 0.67, 1.65) | 0.019 | 0.073% (222) |

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| m162.098 | 162.098 | $C_{11}H_{12}OH^+$ (-1.7), $C_6H_{12}N_2O_3H^+$ (2.3) | 200 | 0.28, (-0.01, 0.22, 0.65) | 0.066 | 0.025% (365) |
| m162.936 | 162.936 | | 250 | 0.023, (-0.001, 0.018, 0.051) | 0.013 | 0.0021% (586) |
| m163.043 | 163.043 | $C_5H_7NO_5H^+$ (-0.3) | 150 | 3.2, (0.07, 3.0, 6.0) | 0.011 | 0.29% (78) |
| m163.075 | 163.075 | $C_{10}H_{10}O_2H^+$ (-0.6) | 150 | 2.7, (0.13, 2.3, 6.0) | 0.199 | 0.24% (88) |
| m163.111 | 163.111 | $C_{11}H_{14}OH^+$ (-1.0) | 150 | 0.72, (0.00, 0.61, 1.60) | 0.028 | 0.065% (239) |
| m163.979 | 163.979 | | 150 | 0.033, (0.000, 0.025, 0.068) | 0.001 | 0.0030% (551) |
| m164.042 | 164.042 | $C_9H_6O_3H^+$ (-0.5) | 150 | 0.47, (0.00, 0.43, 0.95) | 0.038 | 0.042% (292) |
| m164.076 | 164.076 | $C_{10}H_{10}O_2H^+$ (-2.9), $C_5H_{10}N_2O_4H^+$ (1.1), $C_6H_{13}NO_2SH^+$ (1.8) | 200 | 0.99, (0.02, 0.79, 2.14) | 0.028 | 0.089% (189) |
| m164.113 | 164.113 | $C_{11}H_{14}OH^+$ (-2.3), $C_6H_{14}N_2O_3H^+$ (1.7) | 150 | 0.27, (0.00, 0.19, 0.67) | 0.006 | 0.025% (367) |
| m165.022 | 165.022 | | 150 | 0.59, (0.00, 0.57, 1.24) | 0.041 | 0.053% (265) |
| m165.057 | 165.057 | $C_9H_8O_3H^+$ (2.2), $C_5H_9NO_5H^+$ (-1.9), $C_6H_{12}O_3SH^+$ (-1.2) | 200 | 1.90, (0.05, 1.65, 3.66) | 0.098 | 0.171% (107) |
| m165.091 | 165.091 | $C_{10}H_{12}O_2H^+$ (-0.2) | 150 | 5.1, (0.06, 3.7, 12.4) | 0.106 | 0.46% (48) |
| m165.972 | 165.972 | | 200 | 0.018, (0.000, 0.013, 0.039) | 0.004 | 0.00166% (600) |
| m166.020 | 166.020 | $C_8H_4O_4H^+$ (-1.8), $C_5H_3N_5SH^+$ (1.6) | 150 | 0.087, (0.001, 0.081, 0.171) | 0.005 | 0.0078% (471) |
| m166.055 | 166.055 | $C_4H_8N_2O_5H^+$ (0.9), $C_5H_{11}NO_3SH^+$ (1.6) | 200 | 0.45, (0.00, 0.37, 0.95) | 0.003 | 0.041% (299) |
| m166.091 | 166.091 | $C_5H_{12}N_2O_4H^+$ (0.5) | 150 | 1.18, (0.00, 0.74, 2.74) | 0.014 | 0.106% (171) |
| m166.907 | 166.907 | | 150 | 0.039, (0.001, 0.027, 0.092) | 0.004 | 0.0035% (540) |
| m166.965 | 166.965 | | 150 | 0.126, (0.002, 0.087, 0.298) | 0.013 | 0.0113% (441) |

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| m167.037 | 167.037 | $C_8H_6O_4H^+$ (3.0), $C_5H_{10}O_4SH^+$ (-0.4) | 200 | 1.01, (0.00, 0.96, 2.02) | 0.022 | 0.090% (186) |
| m167.072 | 167.072 | $C_9H_{10}O_3H^+$ (1.6), $C_5H_{11}NO_5H^+$ (-2.5), $C_6H_{14}O_3SH^+$ (-1.8) | 150 | 6.2, (0.07, 4.3, 13.6) | 0.255 | 0.56% (42) |
| m167.104 | 167.104 | $C_{10}H_{14}O_2H^+$ (-2.8), $C_5H_{14}N_2O_4H^+$ (1.2) | 150 | 4.9, (-0.01, 3.8, 11.6) | 0.112 | 0.44% (52) |
| m168.035 | 168.035 | $C_8H_6O_4H^+$ (-2.4) | 150 | 0.165, (0.002, 0.145, 0.339) | 0.006 | 0.0148% (419) |
| m168.073 | 168.073 | $C_9H_{10}O_3H^+$ (-0.8) | 150 | 1.32, (0.01, 0.86, 2.84) | 0.035 | 0.118% (147) |
| m168.104 | 168.104 | $C_9H_{13}NO_2H^+$ (2.0), $C_5H_{14}N_2O_4H^+$ (-2.1) | 150 | 0.93, (0.00, 0.62, 2.20) | 0.021 | 0.083% (198) |
| m168.903 | 168.903 | | 150 | 0.044, (0.001, 0.026, 0.098) | 0.003 | 0.0039% (530) |
| m169.053 | 169.053 | $C_5H_{12}O_4SH^+$ (0.0) | 200 | 3.8, (0.01, 2.6, 8.4) | 0.105 | 0.34% (60) |
| m169.085 | 169.085 | $C_9H_{12}O_3H^+$ (-1.0), $C_{12}H_9NH^+$ (0.8), $C_4H_{12}N_2O_5H^+$ (3.0) | 150 | 9.1, (0.05, 6.4, 21.3) | 0.045 | 0.82% (30) |
| m169.120 | 169.120 | $C_{10}H_{16}O_2H^+$ (-2.4) | 150 | 1.72, (-0.03, 1.32, 4.22) | 0.078 | 0.154% (118) |
| m169.158 | 169.158 | $C_{11}H_{20}OH^+$ (-0.8) | 150 | 0.21, (0.00, 0.15, 0.49) | 0.022 | 0.0188% (399) |
| m170.055 | 170.055 | $C_8H_8O_4H^+$ (2.0), $C_6H_7N_3O_3H^+$ (-1.1) | 200 | 0.71, (0.01, 0.43, 1.76) | 0.013 | 0.064% (241) |
| m170.086 | 170.086 | $C_4H_{12}N_2O_5H^+$ (0.7) | 150 | 1.83, (0.00, 1.11, 4.30) | 0.025 | 0.164% (112) |
| m170.926 | 170.926 | | 150 | 0.100, (0.003, 0.072, 0.222) | 0.029 | 0.0090% (459) |
| m171.067 | 171.067 | $C_8H_{10}O_4H^+$ (1.7) | 150 | 26, (0.0, 20, 58) | 0.351 | 2.33% (4) |
| m171.137 | 171.137 | $C_{10}H_{18}O_2H^+$ (-1.0) | 150 | 3.8, (-0.11, 2.9, 9.6) | 0.278 | 0.34% (62) |
| m171.974 | 171.974 | | 300 | 0.165, (0.013, 0.129, 0.363) | 0.020 | 0.0148% (421) |
| m172.069 | 172.069 | $C_8H_{10}O_4H^+$ (0.4), $C_6H_9N_3O_3H^+$ (-2.7) | 150 | 3.2, (0.01, 2.3, 7.0) | 0.058 | 0.29% (77) |

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| m172.140 | 172.140 | $C_{10}H_{18}O_2H^+$ (-1.4) | 150 | 0.69, (-0.01, 0.46, 1.65) | 0.036 | 0.062% (245) |
| m172.959 | 172.959 | | 150 | 0.33, (0.00, 0.23, 0.84) | 0.032 | 0.029% (342) |
| m173.049 | 173.049 | | 150 | 3.3, (0.00, 1.5, 9.3) | 0.034 | 0.30% (72) |
| m173.077 | 173.077 | $C_{11}H_9NOH^+$ (-2.1), $C_6H_9N_3O_3H^+$ (2.0), $C_7H_{12}N_2OSH^+$ (2.7) | 150 | 3.7, (-0.04, 2.1, 8.4) | 0.050 | 0.33% (64) |
| m173.153 | 173.153 | $C_{10}H_{20}O_2H^+$ (-0.6) | 150 | 0.99, (-0.06, 0.91, 2.23) | 0.184 | 0.089% (188) |
| m173.970 | 173.970 | | 150 | 0.143, (0.009, 0.113, 0.309) | 0.004 | 0.0128% (433) |
| m174.054 | 174.054 | $C_{10}H_7NO_2H^+$ (-1.0) | 150 | 0.39, (0.00, 0.24, 0.97) | 0.023 | 0.035% (319) |
| m174.080 | 174.080 | | 150 | 0.90, (0.00, 0.50, 2.15) | 0.011 | 0.081% (203) |
| m174.155 | 174.155 | $C_{10}H_{20}O_2H^+$ (-2.0) | 150 | 0.27, (0.00, 0.22, 0.61) | 0.023 | 0.024% (371) |
| m175.044 | 175.044 | $C_6H_7NO_5H^+$ (1.0) | 150 | 0.74, (0.02, 0.68, 1.50) | 0.018 | 0.066% (233) |
| m175.067 | 175.067 | $C_9H_7N_3OH^+$ (-2.5), $C_5H_{10}N_4OSH^+$ (2.2) | 150 | 1.81, (0.01, 1.28, 4.27) | 0.041 | 0.162% (113) |
| m175.147 | 175.147 | $C_{13}H_{18}H^+$ (-1.1), $C_8H_{18}N_2O_2H^+$ (2.9) | 150 | 0.43, (-0.02, 0.34, 1.04) | 0.071 | 0.039% (311) |
| m175.975 | 175.975 | | 300 | 0.020, (0.000, 0.016, 0.046) | 0.011 | 0.00180% (597) |
| m176.042 | 176.042 | $C_{10}H_6O_3H^+$ (-0.3) | 250 | 0.085, (0.002, 0.085, 0.174) | 0.004 | 0.0077% (476) |
| m176.071 | 176.071 | $C_{10}H_9NO_2H^+$ (0.4) | 150 | 0.63, (0.00, 0.43, 1.42) | 0.009 | 0.056% (258) |
| m176.151 | 176.151 | $C_{13}H_{18}H^+$ (-0.4) | 150 | 0.165, (-0.005, 0.110, 0.407) | 0.012 | 0.0148% (420) |
| m177.056 | 177.056 | $C_{10}H_8O_3H^+$ (1.4), $C_6H_9NO_5H^+$ (-2.6) | 150 | 1.49, (-0.02, 1.41, 3.00) | 0.110 | 0.134% (135) |
| m177.087 | 177.087 | $C_6H_{12}N_2O_4H^+$ (0.1), $C_9H_9N_3OH^+$ (1.9) | 200 | 1.41, (0.00, 1.16, 3.18) | 0.096 | 0.127% (142) |
| m178.058 | 178.058 | $C_{10}H_8O_3H^+$ (0.1) | 150 | 0.25, (0.00, 0.23, 0.49) | 0.014 | 0.022% (380) |

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| m178.083 | 178.083 | $C_5H_{11}N_3O_4H^+$ (0.8) | 150 | 0.66, (0.00, 0.45, 1.52) | 0.009 | 0.059% (251) |
| m178.167 | 178.167 | $C_{13}H_{20}H^+$ (0.0) | 150 | 0.064, (-0.005, 0.044, 0.154) | 0.026 | 0.0057% (503) |
| m178.908 | 178.908 | | 150 | 0.031, (0.000, 0.021, 0.077) | 0.005 | 0.0028% (558) |
| m179.039 | 179.039 | $C_7H_6N_4SH^+$ (0.5) | 200 | 1.15, (0.00, 1.00, 2.30) | 0.026 | 0.103% (174) |
| m179.087 | 179.087 | $C_{14}H_{10}H^+$ (1.6), $C_{10}H_{11}NO_2H^+$ (-2.5), $C_5H_{11}N_3O_4H^+$ (1.5), $C_{11}H_{14}SH^+$ (-1.8 | 100 | 0.52, (0.00, 0.33, 1.18) | 0.023 | 0.047% (276) |
| m179.972 | 179.972 | | 150 | 0.033, (0.002, 0.025, 0.078) | 0.011 | 0.0030% (552) |
| m180.091 | 180.091 | $C_{14}H_{10}H^+$ (2.3) | 150 | 0.60, (0.00, 0.44, 1.37) | 0.065 | 0.053% (264) |
| m181.009 | 181.009 | $C_{11}HNO_2H^+$ (-2.2), $C_6HN_3O_4H^+$ (1.8), $C_4H_8N_2O_2S_2H^+$ (-0.8) | 150 | 1.27, (0.01, 1.06, 2.60) | 0.011 | 0.114% (155) |
| m181.100 | 181.100 | $C_{14}H_{12}H^+$ (-1.0), $C_9H_{12}N_2O_2H^+$ (3.0), $C_5H_{13}N_3O_4H^+$ (-1.1) | 150 | 8.8, (0.16, 7.1, 20.6) | 0.510 | 0.79% (32) |
| m182.008 | 182.008 | $C_7H_3NO_5H^+$ (-0.2) | 150 | 0.33, (0.01, 0.28, 0.65) | 0.035 | 0.030% (339) |
| m182.104 | 182.104 | $C_{14}H_{12}H^+$ (-0.3), $C_6H_{15}NO_5H^+$ (1.9) | 150 | 1.76, (0.02, 1.23, 3.81) | 0.090 | 0.157% (116) |
| m182.937 | 182.937 | | 150 | 0.016, (-0.001, 0.007, 0.033) | 0.006 | 0.00145% (610) |
| m182.988 | 182.988 | | 150 | 0.66, (0.00, 0.58, 1.30) | 0.088 | 0.059% (252) |
| m183.083 | 183.083 | $C_{13}H_{10}OH^+$ (2.8), $C_9H_{11}NO_3H^+$ (-1.3), $C_4H_{11}N_3O_5H^+$ (2.7), $C_{10}H_{14}OSH^+$ (-0.6) | 150 | 12.9, (0.15, 7.9, 30.0) | 0.138 | 1.16% (18) |
| m183.173 | 183.173 | $C_{12}H_{22}OH^+$ (-1.1) | 150 | 1.50, (-0.04, 1.04, 3.63) | 0.057 | 0.134% (134) |

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| m184.001 | 184.001 | $C_{10}HNO_3H^+$ (-1.7), $C_5HN_3O_5H^+$ (2.3) | 150 | 0.37, (0.00, 0.26, 0.80) | 0.012 | 0.033% (325) |
| m184.086 | 184.086 | $C_{13}H_{10}OH^+$ (2.4), $C_{11}H_9N_3H^+$ (-0.7) | 150 | 2.3, (0.02, 1.3, 5.2) | 0.019 | 0.20% (100) |
| m184.935 | 184.935 | | 150 | 0.022, (0.001, 0.017, 0.046) | 0.005 | 0.0020% (589) |
| m184.986 | 184.986 | | 150 | 0.47, (0.00, 0.39, 0.90) | 0.009 | 0.042% (294) |
| m185.082 | 185.082 | $C_9H_{12}O_4H^+$ (1.4) | 150 | 11.1, (-0.02, 7.3, 26.6) | 0.298 | 0.99% (22) |
| m185.151 | 185.151 | $C_{11}H_{20}O_2H^+$ (-2.4) | 150 | 2.2, (-0.04, 1.6, 5.2) | 0.136 | 0.20% (104) |
| m185.938 | 185.938 | | 150 | 0.030, (0.000, 0.019, 0.073) | 0.003 | 0.0027% (564) |
| m186.083 | 186.083 | $C_9H_{12}O_4H^+$ (-0.9) | 150 | 1.79, (0.00, 1.15, 4.14) | 0.065 | 0.161% (115) |
| m186.192 | 186.192 | $C_{12}H_{24}OH^+$ (-1.1) | 150 | 0.080, (-0.004, 0.054, 0.206) | 0.020 | 0.0071% (486) |
| m186.934 | 186.934 | | 150 | 0.060, (0.000, 0.038, 0.137) | 0.005 | 0.0054% (504) |
| m187.062 | 187.062 | $C_8H_{10}O_5H^+$ (2.2), $C_9H_{14}S_2H^+$ (1.3) | 150 | 4.9, (-0.01, 2.4, 12.9) | 0.079 | 0.44% (50) |
| m187.151 | 187.151 | $C_{10}H_{19}NO_2H^+$ (-0.9), $C_{11}H_{22}SH^+$ (-0.2) | 150 | 1.13, (-0.03, 0.70, 2.62) | 0.067 | 0.102% (176) |
| m187.971 | 187.971 | | 150 | 0.059, (0.001, 0.043, 0.125) | 0.005 | 0.0053% (505) |
| m188.063 | 188.063 | $C_8H_{10}O_5H^+$ (-0.1) | 150 | 1.21, (0.00, 0.62, 2.95) | 0.038 | 0.108% (166) |
| m189.024 | 189.024 | | 150 | 0.74, (0.02, 0.69, 1.55) | 0.012 | 0.066% (234) |
| m189.076 | 189.076 | $C_8H_{12}O_5H^+$ (0.6), $C_{11}H_9NO_2H^+$ (2.4), $C_9H_{16}S_2H^+$ (-0.3) | 150 | 2.7, (0.00, 2.1, 6.6) | 0.040 | 0.24% (89) |
| m189.126 | 189.126 | $C_{13}H_{16}OH^+$ (-1.1), $C_8H_{16}N_2O_3H^+$ (3.0) | 150 | 0.42, (-0.01, 0.29, 1.00) | 0.028 | 0.037% (314) |
| m189.979 | 189.979 | | 150 | 0.080, (0.003, 0.069, 0.164) | 0.007 | 0.0071% (487) |

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| m190.055 | 190.055 | $C_{11}H_8O_3H^+$ (-2.6), $C_6H_8N_2O_5H^+$ (1.4) | 250 | 0.159, (0.002, 0.153, 0.326) | 0.008 | 0.0142% (425) |
| m190.083 | 190.083 | $C_{11}H_{11}NO_2H^+$ (-2.9), $C_6H_{11}N_3O_4H^+$ (1.1) | 150 | 0.62, (0.00, 0.39, 1.40) | 0.008 | 0.055% (260) |
| m190.166 | 190.166 | $C_{14}H_{20}H^+$ (-0.8) | 150 | 0.117, (-0.006, 0.075, 0.263) | 0.022 | 0.0105% (450) |
| m190.968 | 190.968 | | 150 | 1.57, (-0.01, 0.88, 4.50) | 0.213 | 0.140% (127) |
| m191.069 | 191.069 | $C_{11}H_{10}O_3H^+$ (-0.9), $C_{14}H_7NH^+$ (0.9) | 150 | 1.61, (0.00, 1.33, 3.35) | 0.132 | 0.144% (124) |
| m191.102 | 191.102 | $C_7H_{14}N_2O_4H^+$ (-0.2), $C_{10}H_{11}N_3OH^+$ (1.6) | 150 | 1.06, (-0.02, 0.76, 2.52) | 0.057 | 0.095% (181) |
| m191.972 | 191.972 | | 150 | 0.179, (0.003, 0.114, 0.484) | 0.019 | 0.0160% (411) |
| m192.070 | 192.070 | $C_6H_{10}N_2O_5H^+$ (0.8), $C_7H_{13}NO_3SH^+$ (1.5) | 150 | 0.57, (0.00, 0.42, 1.25) | 0.015 | 0.051% (268) |
| m192.965 | 192.965 | | 150 | 1.27, (0.00, 0.81, 3.45) | 0.187 | 0.114% (153) |
| m193.052 | 193.052 | $C_{10}H_8O_4H^+$ (2.9), $C_7H_{12}O_4SH^+$ (-0.5) | 150 | 0.88, (0.00, 0.70, 1.80) | 0.026 | 0.078% (212) |
| m193.088 | 193.088 | $C_{11}H_{12}O_3H^+$ (2.5), $C_7H_{13}NO_5H^+$ (-1.6), $C_8H_{16}O_3SH^+$ (-0.9) | 200 | 0.84, (0.00, 0.63, 1.86) | 0.018 | 0.075% (218) |
| m193.118 | 193.118 | $C_7H_{16}N_2O_4H^+$ (0.2), $C_{10}H_{13}N_3OH^+$ (2.0) | 150 | 1.19, (-0.04, 0.87, 2.83) | 0.061 | 0.106% (169) |
| m193.969 | 193.969 | | 150 | 0.133, (0.001, 0.088, 0.348) | 0.024 | 0.0119% (438) |
| m194.095 | 194.095 | $C_{14}H_{11}NH^+$ (-1.0) | 200 | 0.60, (0.02, 0.45, 1.32) | 0.004 | 0.054% (263) |
| m194.121 | 194.121 | $C_7H_{16}N_2O_4H^+$ (-0.2) | 150 | 0.195, (0.001, 0.123, 0.484) | 0.010 | 0.0175% (402) |
| m194.961 | 194.961 | | 150 | 0.34, (0.00, 0.22, 0.88) | 0.048 | 0.030% (336) |
| m195.073 | 195.073 | $C_9H_{10}N_2O_3H^+$ (-2.9), $C_{12}H_7N_3H^+$ (-1.1) | 150 | 1.79, (-0.01, 1.27, 3.85) | 0.045 | 0.161% (114) |

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| m195.101 | 195.101 | $C_{11}H_{14}O_3H^+$ (-0.1), $C_{14}H_{11}NH^+$ (1.7) | 150 | 2.3, (0.05, 1.6, 5.5) | 0.072 | 0.21% (98) |
| m195.965 | 195.965 | | 150 | 0.058, (0.000, 0.041, 0.134) | 0.007 | 0.0052% (508) |
| m196.091 | 196.092 | $C_7H_{14}O_6H^+$ (1.8), $C_5H_{13}N_3O_5H^+$ (-1.3) | 200 | 0.52, (0.00, 0.31, 1.22) | 0.029 | 0.047% (274) |
| m196.099 | 196.100 | $C_{10}H_{13}NO_3H^+$ (2.7), $C_6H_{14}N_2O_5H^+$ (-1.4) | 150 | 0.26, (0.01, 0.16, 0.60) | 0.019 | 0.023% (374) |
| m196.958 | 196.959 | | 150 | 0.126, (0.005, 0.086, 0.296) | 0.004 | 0.0113% (442) |
| m197.095 | 197.096 | $C_{14}H_{12}OH^+$ (-0.5), $C_5H_{13}N_3O_5H^+$ (-0.6) | 150 | 3.1, (0.10, 1.7, 7.7) | 0.810 | 0.28% (79) |
| m197.949 | 197.950 | | 150 | 0.022, (0.000, 0.016, 0.049) | 0.006 | 0.00193% (593) |
| m198.099 | 198.100 | $C_{14}H_{12}OH^+$ (0.1) | 150 | 0.68, (0.01, 0.35, 1.72) | 0.142 | 0.061% (248) |
| m198.956 | 198.957 | | 150 | 0.115, (-0.002, 0.081, 0.259) | 0.010 | 0.0103% (452) |
| m199.052 | 199.053 | $C_{16}H_6H^+$ (-1.6), $C_{11}H_6N_2O_2H^+$ (2.4), $C_7H_7N_3O_4H^+$ (-1.7) | 150 | 2.6, (0.01, 1.9, 5.9) | 0.038 | 0.23% (93) |
| m199.095 | 199.096 | $C_{10}H_{14}O_4H^+$ (-0.9), $C_{13}H_{11}NOH^+$ (0.9) | 150 | 6.7, (0.00, 3.9, 16.2) | 0.055 | 0.60% (41) |
| m199.938 | 199.939 | | 150 | 0.025, (-0.001, 0.015, 0.061) | 0.008 | 0.0022% (580) |
| m200.062 | 200.063 | $C_9H_{10}O_5H^+$ (-0.8) | 150 | 0.29, (0.00, 0.23, 0.62) | 0.009 | 0.026% (359) |
| m200.097 | 200.098 | $C_{10}H_{14}O_4H^+$ (-2.2), $C_7H_{13}N_5SH^+$ (1.2) | 150 | 1.32, (0.00, 0.67, 3.16) | 0.010 | 0.118% (148) |
| m200.171 | 200.172 | $C_{12}H_{22}O_2H^+$ (-1.0) | 150 | 0.154, (-0.005, 0.092, 0.386) | 0.047 | 0.0138% (430) |
| m201.078 | 201.079 | $C_9H_{12}O_5H^+$ (2.9) | 150 | 3.0, (0.00, 2.0, 6.9) | 0.065 | 0.27% (82) |
| m201.170 | 201.171 | $C_{11}H_{21}NO_2H^+$ (2.8) | 150 | 0.73, (0.00, 0.49, 1.64) | 0.024 | 0.066% (236) |
| m201.935 | 201.936 | | 150 | 0.022, (-0.001, 0.014, 0.054) | 0.006 | 0.00195% (590) |

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| m202.084 | 202.085 | $C_{12}H_{11}NO_2H^+$ (-1.6), $C_7H_{11}N_3O_4H^+$ (2.4) | 150 | 0.79, (-0.01, 0.47, 1.87) | 0.012 | 0.071% (224) |
| m202.171 | 202.172 | | 150 | 0.29, (-0.01, 0.19, 0.73) | 0.034 | 0.026% (357) |
| m203.092 | 203.093 | $C_9H_{14}O_5H^+$ (1.3), $C_{10}H_{18}S_2H^+$ (0.4) | 150 | 1.66, (0.00, 1.24, 3.77) | 0.054 | 0.149% (121) |
| m204.095 | 204.096 | $C_9H_{14}O_5H^+$ (1.0), $C_7H_{13}N_3O_4H^+$ (-2.2) | 150 | 0.48, (0.00, 0.28, 1.10) | 0.010 | 0.043% (285) |
| m204.181 | 204.182 | $C_{15}H_{22}H^+$ (-1.1), $C_{10}H_{22}N_2O_2H^+$ (3.0) | 150 | 0.073, (-0.002, 0.045, 0.176) | 0.026 | 0.0065% (495) |
| m204.988 | 204.989 | $C_5H_4N_2O_5SH^+$ (-2.6) | 150 | 0.33, (0.00, 0.30, 0.67) | 0.017 | 0.030% (341) |
| m205.084 | 205.085 | $C_{12}H_{12}O_3H^+$ (-1.2), $C_{15}H_9NH^+$ (0.6), $C_7H_{12}N_2O_5H^+$ (2.8) | 150 | 1.74, (-0.03, 1.36, 4.07) | 0.065 | 0.156% (117) |
| m205.936 | 205.937 | | 150 | 0.017, (0.000, 0.012, 0.039) | 0.006 | 0.00157% (604) |
| m206.086 | 206.087 | $C_{12}H_{12}O_3H^+$ (-2.5), $C_7H_{12}N_2O_5H^+$ (1.5) | 150 | 0.46, (0.00, 0.33, 1.02) | 0.013 | 0.042% (296) |
| m207.032 | 207.033 | $C_7H_{10}O_5SH^+$ (0.6) | 150 | 0.53, (-0.01, 0.41, 1.12) | 0.019 | 0.048% (272) |
| m207.101 | 207.102 | $C_{12}H_{14}O_3H^+$ (0.2), $C_{15}H_{11}NH^+$ (2.0) | 150 | 1.38, (0.00, 0.95, 3.17) | 0.032 | 0.124% (144) |
| m207.132 | 207.133 | $C_8H_{18}N_2O_4H^+$ (-1.1), $C_{11}H_{15}N_3OH^+$ (0.7) | 150 | 0.54, (-0.02, 0.34, 1.30) | 0.068 | 0.048% (271) |
| m207.934 | 207.935 | | 150 | 0.018, (0.000, 0.013, 0.044) | 0.006 | 0.00165% (601) |
| m208.076 | 208.077 | $C_{14}H_9NOH^+$ (1.1), $C_{10}H_{10}N_2O_3H^+$ (-2.9), $C_{11}H_{13}NOSH^+$ (-2.2) | 150 | 0.56, (0.01, 0.46, 1.19) | 0.021 | 0.050% (269) |
| m208.936 | 208.937 | | 150 | 0.036, (0.000, 0.022, 0.095) | 0.016 | 0.0033% (548) |

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| m209.062 | 209.063 | $C_7H_{12}O_7H^+$ (-2.7), $C_{10}H_9NO_4H^+$ (-0.9), $C_{11}H_{12}O_2SH^+$ (-0.2) | 150 | 1.23, (0.09, 0.92, 2.63) | 0.068 | 0.110% (159) |
| m209.151 | 209.152 | $C_{13}H_{20}O_2H^+$ (-1.8), $C_8H_{20}N_2O_4H^+$ (2.3) | 150 | 1.65, (-0.11, 1.13, 4.18) | 0.129 | 0.148% (122) |
| m209.936 | 209.937 | | 150 | 0.016, (-0.001, 0.009, 0.040) | 0.008 | 0.00145% (611) |
| m210.067 | 210.068 | $C_7H_{12}O_7H^+$ (-1.1), $C_{12}H_7N_3OH^+$ (1.7) | 150 | 0.41, (0.01, 0.23, 1.01) | 0.015 | 0.036% (316) |
| m210.153 | 210.154 | $C_8H_{20}N_2O_4H^+$ (0.9) | 150 | 0.44, (-0.02, 0.24, 1.13) | 0.030 | 0.039% (306) |
| m211.077 | 211.078 | $C_{14}H_{10}O_2H^+$ (2.5), $C_{10}H_{11}NO_4H^+$ (-1.5), $C_{11}H_{14}O_2SH^+$ (-0.8) | 150 | 1.44, (0.02, 1.20, 2.90) | 0.230 | 0.129% (139) |
| m211.204 | 211.205 | $C_{14}H_{26}OH^+$ (-0.7) | 150 | 0.35, (0.00, 0.25, 0.84) | 0.072 | 0.032% (331) |
| m211.967 | 211.968 | | 150 | 0.032, (0.000, 0.022, 0.073) | 0.005 | 0.0029% (555) |
| m212.081 | 212.082 | $C_7H_{14}O_7H^+$ (-2.7), $C_{12}H_9N_3OH^+$ (0.1) | 150 | 0.66, (0.03, 0.46, 1.44) | 0.040 | 0.059% (253) |
| m213.079 | 213.080 | | 150 | 3.3, (0.00, 2.1, 8.2) | 0.044 | 0.30% (73) |
| m213.169 | 213.170 | $C_{12}H_{21}NO_2H^+$ (2.1) | 150 | 0.70, (-0.02, 0.47, 1.76) | 0.141 | 0.063% (242) |
| m213.936 | 213.937 | | 150 | 0.020, (-0.001, 0.014, 0.045) | 0.007 | 0.00179% (598) |
| m214.087 | 214.088 | $C_{13}H_{11}NO_2H^+$ (1.7), $C_9H_{12}N_2O_4H^+$ (-2.4), $C_{10}H_{15}NO_2SH^+$ (-1.6) | 150 | 0.77, (-0.01, 0.54, 1.75) | 0.010 | 0.069% (228) |
| m214.170 | 214.171 | | 150 | 0.165, (-0.003, 0.106, 0.392) | 0.025 | 0.0147% (422) |
| m214.924 | 214.925 | | 150 | 0.031, (-0.001, 0.020, 0.069) | 0.007 | 0.0027% (562) |
| m215.035 | 215.036 | $C_{12}H_6O_4H^+$ (2.1), $C_9H_{10}O_4SH^+$ (-1.3) | 150 | 0.38, (0.00, 0.27, 0.85) | 0.013 | 0.034% (321) |

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| m215.093 | 215.094 | $C_{10}H_{14}O_5H^+$ (2.6), $C_{11}H_{18}S_2H^+$ (1.7) | 150 | 1.98, (-0.01, 1.10, 4.99) | 0.047 | 0.178% (106) |
| m215.964 | 215.965 | | 150 | 0.031, (0.001, 0.025, 0.066) | 0.003 | 0.0027% (561) |
| m216.098 | 216.099 | $C_{13}H_{13}NO_2H^+$ (-2.9), $C_8H_{13}N_3O_4H^+$ (1.1) | 150 | 0.61, (0.00, 0.34, 1.46) | 0.006 | 0.055% (262) |
| m217.044 | 217.045 | $C_{15}H_5NOH^+$ (-2.7), $C_{10}H_5N_3O_3H^+$ (1.3) | 150 | 0.32, (0.00, 0.22, 0.72) | 0.016 | 0.029% (345) |
| m217.108 | 217.109 | $C_{10}H_{16}O_5H^+$ (2.0) | 150 | 1.19, (-0.03, 0.99, 2.69) | 0.048 | 0.106% (170) |
| m217.947 | 217.948 | | 150 | 0.030, (0.001, 0.026, 0.062) | 0.006 | 0.0027% (565) |
| m218.047 | 218.048 | | 150 | 0.075, (0.000, 0.046, 0.170) | 0.007 | 0.0067% (492) |
| m218.112 | 218.113 | $C_{10}H_{16}O_5H^+$ (2.7), $C_8H_{15}N_3O_4H^+$ (-0.5) | 150 | 0.37, (-0.01, 0.25, 0.83) | 0.010 | 0.033% (326) |
| m219.049 | 219.050 | $C_8H_{10}O_7H^+$ (0.2), $C_{11}H_7NO_4H^+$ (2.0), $C_9H_{14}O_2S_2H^+$ (-0.7) | 150 | 0.29, (0.00, 0.20, 0.66) | 0.043 | 0.026% (358) |
| m219.098 | 219.099 | $C_{13}H_{14}O_3H^+$ (-2.5), $C_{16}H_{11}NH^+$ (-0.7), $C_8H_{14}N_2O_5H^+$ (1.6) | 200 | 0.50, (-0.01, 0.35, 1.14) | 0.010 | 0.044% (282) |
| m219.135 | 219.136 | $C_{14}H_{18}O_2H^+$ (-1.8), $C_9H_{18}N_2O_4H^+$ (2.2) | 150 | 0.85, (-0.02, 0.64, 1.89) | 0.082 | 0.076% (216) |
| m219.947 | 219.948 | | 150 | 0.018, (0.000, 0.014, 0.040) | 0.006 | 0.00162% (602) |
| m220.053 | 220.054 | $C_8H_{10}O_7H^+$ (0.9), $C_{10}H_9N_3OSH^+$ (0.2) | 150 | 0.195, (0.000, 0.122, 0.474) | 0.009 | 0.0175% (403) |
| m221.080 | 221.081 | $C_{12}H_{12}O_4H^+$ (0.3), $C_{15}H_9NOH^+$ (2.1) | 150 | 0.93, (0.00, 0.62, 2.15) | 0.033 | 0.083% (196) |
| m221.153 | 221.154 | $C_{14}H_{20}O_2H^+$ (0.6), $C_{11}H_{24}O_2SH^+$ (-2.8) | 150 | 1.03, (-0.03, 0.62, 2.58) | 0.197 | 0.093% (183) |
| m222.156 | 222.157 | $C_{14}H_{20}O_2H^+$ (0.2), $C_{12}H_{19}N_3OH^+$ (-2.9) | 150 | 0.30, (-0.01, 0.18, 0.78) | 0.039 | 0.027% (355) |

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| m222.938 | 222.939 | | 150 | 0.045, (0.000, 0.033, 0.104) | 0.010 | 0.0040% (526) |
| m223.094 | 223.095 | $C_{12}H_{14}O_4H^+$ (-1.3), $C_{15}H_{11}NOH^+$ (0.5) | 150 | 1.38, (-0.08, 0.92, 3.36) | 0.149 | 0.123% (145) |
| m223.166 | 223.167 | $C_{14}H_{22}O_2H^+$ (-2.0), $C_9H_{22}N_2O_4H^+$ (2.0) | 150 | 0.49, (-0.01, 0.30, 1.25) | 0.119 | 0.044% (284) |
| m224.069 | 224.070 | $C_{14}H_9NO_2H^+$ (-0.4), $C_7H_9N_7SH^+$ (-1.0) | 150 | 0.28, (-0.01, 0.16, 0.72) | 0.027 | 0.025% (362) |
| m225.047 | 225.048 | $C_9H_8N_2O_5H^+$ (-2.3), $C_{12}H_5N_3O_2H^+$ (-0.5) | 150 | 0.22, (-0.02, 0.12, 0.53) | 0.059 | 0.020% (392) |
| m225.113 | 225.114 | $C_{12}H_{16}O_4H^+$ (2.1), $C_9H_{20}O_4SH^+$ (-1.2) | 150 | 1.29, (0.00, 0.76, 3.12) | 0.021 | 0.116% (151) |
| m225.148 | 225.149 | $C_{13}H_{20}O_3H^+$ (0.8), $C_{16}H_{17}NH^+$ (2.5) | 150 | 0.50, (-0.01, 0.37, 1.17) | 0.261 | 0.045% (281) |
| m226.048 | 226.049 | $C_{13}H_7NO_3H^+$ (-0.6), $C_{16}H_4N_2H^+$ (1.2) | 150 | 0.083, (-0.010, 0.051, 0.193) | 0.014 | 0.0074% (480) |
| m226.110 | 226.111 | | 150 | 0.33, (0.00, 0.18, 0.79) | 0.011 | 0.029% (343) |
| m226.152 | 226.153 | $C_{13}H_{20}O_3H^+$ (1.4), $C_{11}H_{19}N_3O_2H^+$ (-1.7) | 150 | 0.098, (-0.001, 0.064, 0.238) | 0.050 | 0.0088% (461) |
| m226.942 | 226.943 | | 200 | 0.018, (-0.002, 0.011, 0.048) | 0.005 | 0.00161% (603) |
| m227.088 | 227.089 | $C_{11}H_{14}O_5H^+$ (-2.1), $C_{14}H_{11}NO_2H^+$ (-0.3), $C_{15}H_{14}SH^+$ (0.4) | 150 | 1.46, (-0.01, 0.83, 3.62) | 0.079 | 0.131% (138) |
| m228.042 | 228.043 | $C_{16}H_5NOH^+$ (-1.0), $C_{11}H_5N_3O_3H^+$ (3.0) | 150 | 0.029, (0.000, 0.020, 0.066) | 0.007 | 0.0026% (567) |
| m228.094 | 228.095 | $C_{11}H_{14}O_5H^+$ (0.6), $C_9H_{13}N_3O_4H^+$ (-2.5) | 150 | 0.38, (0.00, 0.22, 0.90) | 0.019 | 0.034% (323) |
| m229.081 | 229.082 | $C_{17}H_9NH^+$ (-1.7), $C_9H_{12}N_2O_5H^+$ (0.5), $C_{12}H_9N_3O_2H^+$ (2.3), $C_{13}H_{12}N_2SH^+$ (3.0) | 200 | 0.45, (0.01, 0.26, 1.07) | 0.006 | 0.041% (300) |

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| m229.099 | 229.100 | $C_{18}H_{12}H^+$ (-0.8), $C_9H_{13}N_3O_4H^+$ (-0.8), $C_{10}H_{16}N_2O_2SH^+$ (-0.1) | 150 | 0.83, (-0.06, 0.45, 2.20) | 0.062 | 0.074% (220) |
| m230.105 | 230.106 | $C_{18}H_{12}H^+$ (1.9) | 150 | 0.37, (0.00, 0.20, 0.88) | 0.015 | 0.033% (324) |
| m230.201 | 230.202 | | 150 | 0.087, (-0.001, 0.063, 0.238) | 0.009 | 0.0078% (472) |
| m231.025 | 231.026 | $C_{12}H_6O_5H^+$ (-2.4), $C_{15}H_3NO_2H^+$ (-0.6) | 150 | 0.190, (0.002, 0.147, 0.418) | 0.018 | 0.0170% (405) |
| m231.093 | 231.094 | $C_{16}H_{10}N_2H^+$ (2.8), $C_{12}H_{11}N_3O_2H^+$ (-1.3), $C_{13}H_{14}N_2SH^+$ (-0.6) | 150 | 0.64, (0.00, 0.44, 1.47) | 0.015 | 0.058% (256) |
| m231.135 | 231.136 | $C_{15}H_{18}O_2H^+$ (-1.5), $C_{10}H_{18}N_2O_4H^+$ (2.5) | 150 | 0.142, (-0.003, 0.082, 0.375) | 0.067 | 0.0127% (434) |
| m233.153 | 233.155 | $C_{15}H_{20}O_2H^+$ (0.9), $C_{12}H_{24}O_2SH^+$ (-2.5) | 150 | 0.83, (-0.05, 0.53, 2.08) | 0.069 | 0.074% (221) |
| m234.158 | 234.160 | $C_{15}H_{20}O_2H^+$ (2.6), $C_{13}H_{19}N_3OH^+$ (-0.6) | 150 | 0.22, (-0.01, 0.14, 0.55) | 0.015 | 0.020% (391) |
| m235.168 | 235.170 | $C_{15}H_{22}O_2H^+$ (0.3) | 150 | 1.11, (-0.05, 0.72, 2.83) | 0.107 | 0.100% (177) |
| m236.171 | 236.173 | $C_{15}H_{22}O_2H^+$ (0.0) | 150 | 0.25, (-0.01, 0.15, 0.63) | 0.024 | 0.023% (378) |
| m237.144 | 237.146 | $C_{14}H_{20}O_3H^+$ (-2.9), $C_{17}H_{17}NH^+$ (-1.1), $C_9H_{20}N_2O_5H^+$ (1.1), $C_{12}H_{17}N_3O_2H^+$ (2.9) | 150 | 1.21, (-0.01, 0.64, 2.98) | 0.113 | 0.109% (164) |
| m238.113 | 238.115 | $C_{13}H_{16}O_4H^+$ (-0.8), $C_{10}H_{15}N_5SH^+$ (2.6) | 150 | 0.32, (-0.01, 0.18, 0.83) | 0.025 | 0.028% (348) |
| m239.064 | 239.066 | $C_{18}H_7NH^+$ (-2.8), $C_{10}H_{10}N_2O_5H^+$ (-0.6), $C_{13}H_7N_3O_2H^+$ (1.2), $C_6H_{14}N_4O_2S_2H^+$ (2.6) | 150 | 0.39, (0.00, 0.25, 0.87) | 0.037 | 0.035% (318) |

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| m239.128 | 239.130 | $C_{13}H_{18}O_4H^+$ (1.9), $C_{10}H_{22}O_4SH^+$ (-1.5) | 150 | 0.39, (0.00, 0.16, 1.05) | 0.007 | 0.035% (320) |
| m241.103 | 241.105 | $C_{12}H_{16}O_5H^+$ (-2.3), $C_{15}H_{13}NO_2H^+$ (-0.5), $C_{16}H_{16}SH^+$ (0.2) | 150 | 1.05, (-0.02, 0.60, 2.76) | 0.064 | 0.094% (182) |
| m242.087 | 242.089 | $C_{15}H_{12}O_3H^+$ (-0.5) | 150 | 0.24, (0.00, 0.14, 0.60) | 0.011 | 0.022% (383) |
| m243.116 | 243.118 | $C_{19}H_{14}H^+$ (1.0), $C_{10}H_{15}N_3O_4H^+$ (0.9), $C_{11}H_{18}N_2O_2SH^+$ (1.6) | 150 | 0.63, (-0.03, 0.36, 1.64) | 0.056 | 0.056% (257) |
| m246.118 | 246.120 | $C_{15}H_{16}O_3H^+$ (-0.7) | 150 | 0.174, (-0.005, 0.098, 0.422) | 0.011 | 0.0156% (416) |
| m246.957 | 246.959 | | 150 | 0.042, (-0.002, 0.028, 0.107) | 0.009 | 0.0037% (533) |
| m247.170 | 247.172 | $C_{16}H_{22}O_2H^+$ (2.7), $C_{12}H_{23}NO_4H^+$ (-1.4), $C_{13}H_{26}O_2SH^+$ (-0.7) | 150 | 0.48, (-0.04, 0.30, 1.22) | 0.061 | 0.043% (289) |
| m248.173 | 248.175 | $C_{16}H_{22}O_2H^+$ (2.3), $C_{14}H_{21}N_3OH^+$ (-0.8) | 150 | 0.095, (-0.003, 0.054, 0.244) | 0.013 | 0.0085% (465) |
| m249.184 | 249.186 | $C_{16}H_{24}O_2H^+$ (1.1), $C_{13}H_{28}O_2SH^+$ (-2.3) | 150 | 0.77, (-0.04, 0.48, 2.02) | 0.069 | 0.069% (227) |
| m250.123 | 250.125 | $C_{17}H_{15}NOH^+$ (2.4), $C_{13}H_{16}N_2O_3H^+$ (-1.7) | 150 | 0.123, (-0.001, 0.070, 0.264) | 0.014 | 0.0110% (444) |
| m250.186 | 250.188 | $C_{16}H_{24}O_2H^+$ (-0.3) | 150 | 0.081, (-0.004, 0.050, 0.212) | 0.013 | 0.0073% (484) |
| m251.003 | 251.005 | | 150 | 0.069, (-0.002, 0.043, 0.161) | 0.013 | 0.0062% (500) |
| m251.172 | 251.174 | $C_{14}H_{22}N_2O_2H^+$ (-1.4) | 150 | 0.93, (-0.06, 0.53, 2.44) | 0.093 | 0.083% (197) |
| m252.160 | 252.162 | $C_{14}H_{21}NO_3H^+$ (2.6), $C_{10}H_{22}N_2O_5H^+$ (-1.4) | 150 | 0.25, (-0.01, 0.14, 0.66) | 0.029 | 0.022% (381) |
| m253.002 | 253.004 | | 150 | 0.069, (-0.004, 0.048, 0.169) | 0.019 | 0.0062% (501) |
| m253.140 | 253.142 | $C_{14}H_{20}O_4H^+$ (-1.4), $C_{17}H_{17}NOH^+$ (0.4) | 150 | 0.86, (-0.01, 0.42, 2.15) | 0.042 | 0.077% (215) |

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| m254.005 | 254.007 | $C_{13}H_3NO_5H^+$ (-1.3) | 150 | 0.021, (-0.001, 0.014, 0.051) | 0.008 | 0.00186% (596) |
| m254.999 | 255.001 | $C_{12}H_2N_2O_5H^+$ (-2.5) | 150 | 0.035, (-0.001, 0.022, 0.090) | 0.018 | 0.0032% (549) |
| m255.121 | 255.123 | $C_{13}H_{18}O_5H^+$ (0.4), $C_{16}H_{15}NO_2H^+$ (2.2) | 150 | 0.67, (-0.02, 0.33, 1.76) | 0.049 | 0.060% (249) |
| m255.230 | 255.232 | $C_{16}H_{30}O_2H^+$ (0.3) | 150 | 0.38, (0.01, 0.21, 0.95) | 0.065 | 0.034% (322) |
| m256.122 | 256.124 | $C_{13}H_{18}O_5H^+$ (-1.9) | 150 | 0.171, (-0.005, 0.084, 0.426) | 0.014 | 0.0153% (418) |
| m257.026 | 257.028 | $C_{10}H_8O_8H^+$ (-1.0), $C_{13}H_5NO_5H^+$ (0.8), $C_6H_{12}N_2O_5S_2H^+$ (2.2) | 150 | 0.051, (-0.002, 0.036, 0.123) | 0.011 | 0.0045% (518) |
| m257.107 | 257.109 | $C_{18}H_{12}N_2H^+$ (1.9), $C_{14}H_{13}N_3O_2H^+$ (-2.2), $C_{15}H_{16}N_2SH^+$ (-1.5) | 150 | 0.43, (-0.02, 0.22, 1.10) | 0.042 | 0.039% (307) |
| m259.019 | 259.021 | $C_{13}H_6O_6H^+$ (-2.4), $C_{16}H_3NO_3H^+$ (-0.6), $C_9H_{10}N_2O_3S_2H^+$ (0.7) | 150 | 0.054, (-0.003, 0.043, 0.118) | 0.010 | 0.0048% (512) |
| m259.107 | 259.109 | $C_{19}H_{14}OH^+$ (-2.5), $C_{14}H_{14}N_2O_3H^+$ (1.6), $C_{10}H_{15}N_3O_5H^+$ (-2.5), $C_{11}H_{18}N_2O_3SH^+$ (-1.8) | 200 | 0.24, (-0.01, 0.17, 0.59) | 0.084 | 0.022% (384) |
| m260.109 | 260.111 | $C_{14}H_{14}N_2O_3H^+$ (0.2), $C_{15}H_{17}NOSH^+$ (0.9) | 150 | 0.104, (-0.003, 0.057, 0.260) | 0.017 | 0.0093% (456) |
| m261.116 | 261.118 | | 200 | 0.34, (-0.01, 0.22, 0.87) | 0.099 | 0.030% (338) |
| m262.118 | 262.120 | $C_{18}H_{15}NOH^+$ (-2.3), $C_{13}H_{15}N_3O_3H^+$ (1.7) | 200 | 0.092, (-0.004, 0.052, 0.212) | 0.022 | 0.0082% (468) |
| m263.123 | 263.125 | $C_{15}H_{18}O_4H^+$ (-2.4), $C_{18}H_{15}NOH^+$ (-0.6) | 200 | 0.36, (-0.02, 0.20, 0.86) | 0.082 | 0.032% (329) |
| m264.127 | 264.129 | $C_{15}H_{18}O_4H^+$ (-1.7) | 150 | 0.138, (-0.006, 0.068, 0.327) | 0.028 | 0.0124% (436) |

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| m265.142 | 265.144 | $C_{15}H_{20}O_4H^+$ (1.0), $C_{18}H_{17}NOH^+$ (2.8) | 150 | 0.65, (-0.03, 0.34, 1.57) | 0.067 | 0.059% (254) |
| m266.174 | 266.176 | $C_{15}H_{23}NO_3H^+$ (1.4), $C_{11}H_{24}N_2O_5H^+$ (-2.7) | 150 | 0.083, (0.000, 0.048, 0.186) | 0.037 | 0.0075% (479) |
| m267.155 | 267.158 | $C_{15}H_{22}O_4H^+$ (-1.6), $C_{18}H_{19}NOH^+$ (0.2) | 150 | 0.69, (-0.04, 0.33, 1.79) | 0.070 | 0.062% (244) |
| m269.136 | 269.139 | $C_{14}H_{20}O_5H^+$ (0.2), $C_{17}H_{17}NO_2H^+$ (2.0) | 150 | 0.51, (-0.02, 0.24, 1.44) | 0.041 | 0.046% (279) |
| m270.139 | 270.142 | $C_{14}H_{20}O_5H^+$ (-0.1) | 150 | 0.044, (-0.003, 0.020, 0.136) | 0.023 | 0.0039% (529) |
| m270.236 | 270.239 | | 150 | 0.051, (-0.002, 0.026, 0.135) | 0.009 | 0.0046% (517) |
| m271.150 | 271.153 | $C_{14}H_{22}O_5H^+$ (-1.4), $C_{17}H_{19}NO_2H^+$ (0.4) | 150 | 0.178, (0.001, 0.115, 0.368) | 0.057 | 0.0160% (413) |
| m273.127 | 273.130 | $C_{20}H_{16}OH^+$ (2.3), $C_{16}H_{17}NO_3H^+$ (-1.8), $C_{11}H_{17}N_3O_5H^+$ (2.3), $C_{17}H_{20}OSH^+$ (-1.1) | 150 | 0.26, (0.00, 0.16, 0.68) | 0.067 | 0.024% (372) |
| m274.130 | 274.133 | $C_{20}H_{16}OH^+$ (2.0), $C_{18}H_{15}N_3H^+$ (-1.1) | 150 | 0.075, (-0.001, 0.039, 0.188) | 0.016 | 0.0068% (490) |
| m275.132 | 275.135 | $C_{18}H_{15}N_3H^+$ (-2.5) | 200 | 0.172, (0.001, 0.105, 0.392) | 0.034 | 0.0154% (417) |
| m275.163 | 275.166 | $C_{17}H_{22}O_3H^+$ (1.6), $C_{13}H_{23}NO_5H^+$ (-2.5), $C_{14}H_{26}O_3SH^+$ (-1.8) | 150 | 0.078, (-0.010, 0.044, 0.194) | 0.040 | 0.0070% (489) |
| m276.140 | 276.143 | $C_{15}H_{18}N_2O_3H^+$ (0.4) | 150 | 0.085, (-0.002, 0.052, 0.190) | 0.024 | 0.0077% (475) |
| m277.137 | 277.140 | $C_{19}H_{17}NOH^+$ (-1.8), $C_{14}H_{17}N_3O_3H^+$ (2.2), $C_{15}H_{20}N_2OSH^+$ (2.9) | 150 | 0.32, (-0.01, 0.19, 0.76) | 0.077 | 0.029% (347) |
| m278.137 | 278.140 | $C_{15}H_{19}NO_4H^+$ (1.2), $C_{18}H_{16}N_2OH^+$ (3.0) | 150 | 0.064, (-0.001, 0.032, 0.137) | 0.015 | 0.0058% (502) |

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| m278.186 | 278.189 | $C_{20}H_{23}NH^+$ (-1.5), $C_{15}H_{23}N_3O_2H^+$ (2.6) | 150 | 0.023, (-0.002, 0.014, 0.062) | 0.012 | 0.0021% (587) |
| m279.159 | 279.162 | $C_{16}H_{22}O_4H^+$ (2.8) | 150 | 0.31, (-0.02, 0.23, 0.73) | 0.095 | 0.028% (354) |
| m280.162 | 280.165 | $C_{16}H_{22}O_4H^+$ (2.5), $C_{14}H_{21}N_3O_3H^+$ (-0.6) | 150 | 0.074, (-0.004, 0.055, 0.167) | 0.022 | 0.0066% (494) |
| m283.043 | 283.046 | $C_{12}H_{10}O_8H^+$ (1.2), $C_{15}H_7NO_5H^+$ (3.0) | 150 | 0.126, (-0.001, 0.101, 0.279) | 0.030 | 0.0113% (443) |
| m284.042 | 284.045 | $C_{19}H_6O_3H^+$ (2.7), $C_{17}H_5N_3O_2H^+$ (-0.4) | 200 | 0.021, (-0.001, 0.017, 0.045) | 0.011 | 0.00192% (594) |
| m285.026 | 285.029 | $C_{17}H_4N_2O_3H^+$ (-0.4), $C_{20}HN_3H^+$ (1.4) | 150 | 0.040, (0.000, 0.026, 0.091) | 0.015 | 0.0036% (539) |
| m285.259 | 285.262 | $C_{17}H_{33}NO_2H^+$ (0.3), $C_{18}H_{36}SH^+$ (1.0) | 200 | 0.114, (0.014, 0.089, 0.264) | 0.055 | 0.0102% (453) |
| m287.142 | 287.145 | $C_{21}H_{18}OH^+$ (2.1), $C_{17}H_{19}NO_3H^+$ (-2.0), $C_{12}H_{19}N_3O_5H^+$ (2.1), $C_{18}H_{22}OSH^+$ (-1.3) | 150 | 0.178, (-0.009, 0.097, 0.460) | 0.035 | 0.0160% (412) |
| m288.146 | 288.149 | $C_{21}H_{18}OH^+$ (2.8), $C_{19}H_{17}N_3H^+$ (-0.3) | 150 | 0.070, (-0.002, 0.030, 0.162) | 0.012 | 0.0063% (498) |
| m295.078 | 295.081 | $C_{14}H_{14}O_7H^+$ (0.2), $C_{17}H_{11}NO_4H^+$ (2.0), $C_{18}H_{14}O_2SH^+$ (2.7) | 200 | 0.177, (-0.004, 0.134, 0.413) | 0.063 | 0.0158% (414) |
| m300.065 | 300.069 | $C_{15}H_{10}N_2O_5H^+$ (-1.0) | 150 | 0.047, (0.003, 0.035, 0.106) | 0.022 | 0.0042% (524) |
| m301.059 | 301.063 | $C_{23}H_8OH^+$ (-2.2), $C_{18}H_8N_2O_3H^+$ (1.8), $C_{14}H_9N_3O_5H^+$ (-2.2) | 150 | 0.057, (0.005, 0.040, 0.128) | 0.025 | 0.0051% (510) |
| m306.187 | 306.191 | $C_{22}H_{24}OH^+$ (-2.6), $C_{17}H_{24}N_2O_3H^+$ (1.5) | 150 | 0.054, (-0.003, 0.031, 0.141) | 0.015 | 0.0048% (513) |
| m306.924 | 306.928 | | 150 | 0.019, (-0.003, 0.018, 0.045) | 0.008 | 0.00172% (599) |

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| m308.923 | 308.927 | | 150 | 0.025, (-0.003, 0.024, 0.054) | 0.012 | 0.0022% (581) |
| m309.094 | 309.098 | $C_{15}H_{16}O_7H^+$ (1.0), $C_{18}H_{13}NO_4H^+$ (2.8) | 200 | 0.161, (0.001, 0.104, 0.385) | 0.045 | 0.0144% (423) |
| m310.919 | 310.923 | | 150 | 0.016, (-0.001, 0.014, 0.036) | 0.006 | 0.00146% (608) |
| m311.094 | 311.098 | $C_{20}H_{11}N_3OH^+$ (-2.9) | 150 | 0.27, (0.00, 0.18, 0.72) | 0.054 | 0.025% (366) |
| m331.039 | 331.044 | $C_{16}H_{10}O_8H^+$ (-1.2), $C_{19}H_7NO_5H^+$ (0.6) | 200 | 0.110, (-0.002, 0.079, 0.271) | 0.037 | 0.0099% (454) |
| m343.049 | 343.054 | $C_{28}H_6H^+$ (-0.2), $C_{19}H_7N_3O_4H^+$ (-0.2) | 200 | 0.052, (-0.001, 0.029, 0.140) | 0.017 | 0.0046% (516) |
| m345.053 | 345.058 | $C_{17}H_{12}O_8H^+$ (-2.4), $C_{20}H_9NO_5H^+$ (-0.6) | 200 | 0.091, (-0.001, 0.055, 0.232) | 0.024 | 0.0081% (469) |
| m357.059 | 357.065 | $C_{24}H_8N_2O_2H^+$ (-1.3) | 150 | 0.134, (0.000, 0.130, 0.285) | 0.018 | 0.0120% (437) |
| m358.055 | 358.061 | $C_{25}H_8O_3H^+$ (2.6), $C_{23}H_7N_3O_2H^+$ (-0.5) | 150 | 0.050, (-0.001, 0.048, 0.110) | 0.013 | 0.0045% (520) |
| m359.044 | 359.050 | $C_{28}H_6OH^+$ (0.5), $C_{19}H_7N_3O_5H^+$ (0.4), $C_{12}H_{14}N_4O_5S_2H^+$ (1.8) | 150 | 0.050, (0.000, 0.039, 0.110) | 0.021 | 0.0045% (519) |
| m373.086 | 373.092 | $C_{19}H_{16}O_8H^+$ (0.3), $C_{22}H_{13}NO_5H^+$ (2.1) | 150 | 0.053, (-0.003, 0.042, 0.124) | 0.018 | 0.0048% (514) |
| m374.083 | 374.089 | $C_{26}H_{12}O_3H^+$ (-0.1) | 150 | 0.022, (-0.003, 0.017, 0.055) | 0.012 | 0.00193% (592) |
| m391.283 | 391.290 | | 300 | 0.095, (-0.005, 0.024, 0.256) | 0.016 | 0.0085% (464) |