

Elemental Composition Report

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

119 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 25-25 H: 0-200 N: 0-10 O: 0-10 F: 3-3

Minimum: -1.5

Maximum: 5.0 7.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

456.1922 456.1899 2.3 5.0 13.5 29.8 C25 H25 N3 O2 F3

M+CH3CNH

146.0623 1.683e2

147.0883 1.301e2

148.0588 1.002e2

148.6208 3.038e0

149.2249 6.555e1

150.1905 2.083e2

151.1403 7.430e2

152.1167 2.592e2

153.1055 1.133e2

154.0883 7.170e1

155.0651 5.724e1

156.0675 1.310e2

157.0959 6.143e1

158.0844 5.266e1

159.0097 6.257e1

160.0672 5.485e1

161.0121 7.190e1

161.5547 5.063e0

162.0914 4.876e2

163.0811 1.383e2

164.1100 8.380e1

164.6177 1.013e0

165.1977 6.184e1

166.1300 5.552e1

167.0526 5.730e1

167.7003 1.013e1

168.3893 5.243e1

169.1863 4.831e1

170.1132 8.822e1

171.0820 9.886e1

171.6084 1.013e0

172.1666 1.444e2

173.0944 9.537e1

174.0878 6.076e1

175.0148 8.066e1

175.6341 1.823e1

176.2993 9.095e1

177.1147 5.187e1

178.0659 7.354e1

179.0173 9.875e1

180.0445 8.128e1

181.0992 8.668e1

182.0342 5.266e1

182.9409 1.629e2

184.0368 8.895e1

185.0551 7.690e1

186.1240 5.772e1

186.6582 1.013e0

187.1742 6.278e1

188.1850 8.648e1

189.1815 6.278e1

189.7575 7.089e0

190.3586 1.148e2

191.1206 5.800e1

191.9406 8.886e1

192.5357 5.063e0

193.1478 6.172e1

194.1533 6.539e1

195.0361 4.759e1

195.9944 1.041e2

196.9834 9.019e1

197.4932 1.013e0

198.0580 6.785e1

199.0312 1.706e2

200.0132 2.348e2

201.0009 7.461e1

201.5096 1.013e0

202.0778 7.190e1

202.5831 1.013e0

203.1233 1.776e2

204.1264 7.634e1

205.1147 6.152e1

206.1447 1.322e2

207.1053 6.684e1

208.0585 2.513e2

209.0465 1.147e2

210.1385 8.361e1

211.1087 7.660e1

212.0868 9.026e1

212.5952 1.013e0

213.0959 7.087e1

213.9936 1.581e2

214.5375 1.013e0

215.0761 7.089e1

216.0319 7.890e1

216.5387 2.025e0

217.0932 8.016e1

218.0902 6.157e1

219.0398 3.799e1

220.0923 6.392e1

221.0809 5.063e1

221.5885 1.013e0

222.1023 1.270e2

223.0595 1.041e2

224.0271 8.310e2

225.0393 2.567e2

226.0246 2.156e2

227.0104 8.299e1

228.0104 3.700e2

228.9935 8.955e1

230.0145 8.950e1

230.5881 9.114e0

231.1640 6.987e1

232.1067 4.456e1

233.0365 5.734e1

233.5756 4.051e0

234.1136 1.642e2

235.1089 8.734e1

236.0727 3.949e1

237.0304 1.146e2

237.5894 4.051e0

238.1939 6.020e1

239.0502 4.476e1

239.9237 5.873e1

240.5343 9.114e0

241.1534 8.255e1

242.1200 1.674e2

243.1068 9.003e1

244.0819 8.885e1

245.0572 6.106e1

246.0165 9.253e1

246.5323 1.013e0

247.0338 6.085e1

248.1224 6.493e1

248.6237 1.013e0

249.1492 8.506e1

250.0485 4.057e1

250.9868 6.987e1

251.5017 1.013e0

252.0373 5.750e1

253.0390 5.266e1

254.0262 5.367e1

254.5774 4.051e0

255.1451 7.387e1

256.1100 6.188e1

256.9497 4.759e1

257.4604 2.025e0

258.0474 5.791e1

259.0731 6.418e1

260.0500 4.226e1

261.0217 6.611e1

261.9928 5.367e1

262.5275 1.013e0

263.0778 5.837e1

263.6055 1.013e0

264.1854 4.389e1

265.1289 5.749e1

266.0980 4.557e1

267.1278 7.432e1

268.1071 5.671e1

268.6329 5.063e0

269.2173 6.705e1

270.1476 5.273e1

271.0470 6.684e1

272.0986 8.709e1

273.1130 5.668e1

273.9958 7.226e1

274.5189 4.168e0

275.0399 8.907e1

275.5928 2.025e0

276.1217 6.142e1

276.6665 3.038e0

277.2561 5.873e1

278.1192 8.447e1

279.1265 1.170e2

280.1370 6.623e1

281.1283 5.570e1

282.1341 5.975e1

283.1242 7.190e1

284.1261 5.360e1

285.1128 5.408e1

286.1004 4.845e1

287.0957 7.006e1

287.6140 1.013e0

288.1377 8.422e1

288.6652 5.063e0

289.2096 6.616e1

290.1085 4.253e1

291.1308 6.832e1

292.1170 5.063e1

293.1115 6.926e1

294.0931 4.861e1

295.0645 8.481e1

295.5775 1.013e0

296.1054 5.450e1

296.6803 4.051e0

297.2368 1.004e2

298.2189 6.592e1

299.1319 3.747e1

300.0431 6.442e1

301.0686 7.341e1

302.0334 7.276e1

302.9857 1.282e2

303.6209 9.114e0

304.2386 1.164e2

305.1852 1.061e2

305.7023 1.013e0

306.2276 7.418e1

307.2124 5.649e1

308.1416 4.947e1

308.7319 4.051e0

309.3063 5.367e1

310.2130 3.443e1

311.1038 4.231e1

311.6548 2.025e0

312.1643 6.257e1

313.1056 7.188e1

314.1152 5.962e1

315.1483 4.759e1

316.1162 5.479e1

317.0673 6.794e1

318.0853 5.468e1

319.0952 5.960e1

320.0783 5.913e1

320.5997 2.025e0

321.1478 8.386e1

322.2192 4.967e1

323.1927 7.315e1

324.1122 5.055e1

324.6492 2.025e0

325.1905 7.277e1

325.7270 5.063e0

326.3195 1.164e2

327.1915 6.713e1

328.0962 5.493e1

329.0554 8.348e1

330.0705 6.103e1

331.0926 6.275e1

331.6884 6.076e0

332.2656 9.575e1

333.2165 7.634e1

334.1455 6.248e1

335.1225 5.775e1

335.6609 4.051e0

336.2073 5.959e1

337.1663 6.009e1

338.1216 6.302e1

339.1931 6.367e1

339.7162 1.013e0

340.2654 4.998e1

341.2609 9.007e1

342.2112 6.846e1

343.1771 6.582e1

344.1359 6.883e1

345.1112 8.082e1

346.0982 9.071e1

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348.1110 7.491e1

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350.7584 2.025e0

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354.0641 6.322e1

355.1258 7.167e1

356.1600 5.911e1

357.1566 6.136e1

358.0981 6.996e1

359.0491 5.230e1

360.1745 5.331e1

361.0903 5.426e1

362.1231 5.748e1

363.1024 4.942e1

364.1297 5.701e1

365.1732 4.980e1

366.2427 6.955e1

367.1523 5.534e1

367.6763 4.051e0

368.2645 1.441e2

368.7725 2.025e0

369.3000 1.333e2

370.2316 6.144e1

370.8040 2.025e0

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372.3257 1.801e2

373.2428 8.401e1

374.2280 7.490e1

375.1466 5.074e1

376.1457 4.882e1

377.1259 5.740e1

378.1047 4.395e1

379.0625 5.619e1

379.7447 5.063e0

380.3171 7.944e1

381.2672 5.389e1

382.1811 6.191e1

383.1602 7.363e1

384.1748 6.296e1

385.2531 1.119e2

386.2803 5.688e1

387.1946 6.192e1

387.7201 3.038e0

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389.1662 5.108e1

390.2018 5.756e1

390.7184 3.038e0

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392.2037 7.140e1

393.1307 7.199e1

393.6614 3.038e0

394.2691 5.822e1

395.2060 5.442e1

396.1678 5.810e1

396.6819 1.013e0

397.1995 6.426e1

398.1871 5.217e1

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399.7434 5.063e0

400.3287 1.084e2

401.2245 6.464e1

402.1805 7.266e1

403.1673 5.991e1

404.1726 3.949e1

405.1725 5.270e1

405.6858 1.013e0

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409.1991 5.971e1

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423.6229 3.038e0

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426.7513 2.025e0

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458.1992 9.091e1

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459.7488 1.013e0

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461.1955 5.064e1

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467.2992 5.302e1

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521.8069 4.051e0

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523.3579 4.974e1

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525.8542 7.089e0

526.4716 6.200e1

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530.2316 4.967e1

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532.1947 5.012e1

533.1985 7.142e1

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534.8428 9.114e0

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536.5073 5.492e1

537.3932 4.675e1

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555.8609 1.013e0

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566.7316 3.038e0

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569.7822 3.038e0

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571.2496 4.404e1

571.9015 5.063e0

572.5151 4.759e1

573.3875 3.634e1

574.3889 4.162e1

575.4350 5.515e1

576.4283 4.018e1

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577.8687 1.013e0

578.3848 4.044e1

579.3176 3.949e1

580.3130 5.138e1

581.3388 4.109e1

581.9028 6.076e0

582.4825 4.314e1

583.4182 4.063e1

584.3853 5.646e1

585.3224 5.473e1

585.8984 2.025e0

586.4213 4.230e1

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588.4590 4.385e1

589.3572 3.695e1

589.8591 1.013e0

590.3806 4.471e1

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592.3293 5.406e1

593.2148 4.694e1

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596.2415 4.035e1

597.2241 4.927e1

598.2759 4.735e1

598.7985 2.025e0

599.3682 5.405e1

599.8895 2.025e0

600.4494 5.916e1

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602.4256 5.227e1

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604.3276 4.031e1

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618.8804 2.025e0

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620.3828 3.522e1

621.3072 5.453e1

622.2885 3.440e1

623.2662 4.152e1

623.7909 4.051e0

624.3655 4.002e1

625.2883 4.826e1