

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

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

Elements Used:

C: 19-19 H: 0-200 N: 0-10 O: 0-10 S: 0-1 F: 3-3

Minimum: -1.5

Maximum: 5.0 7.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula

415.0832 415.0827 0.5 1.2 9.5 44.1 C19 H18 O5 S F3

151.9473 2.051e2

152.9230 2.073e2

153.7046 9.946e1

154.4978 2.299e2

155.0975 4.289e1

155.6847 1.927e2

156.5976 1.368e2

157.5070 1.775e2

158.4737 1.671e2

159.0891 4.193e1

159.7272 2.116e2

160.3665 3.222e1

160.9345 2.104e2

161.8881 1.734e2

162.8177 1.698e2

163.6145 1.247e2

164.4249 2.176e2

165.1863 9.565e1

165.9257 1.972e2

166.6313 7.252e1

167.3671 1.973e2

168.0518 5.699e1

168.7273 1.696e2

169.3461 3.768e1

169.9708 1.117e2

170.9028 1.896e2

171.8069 1.787e2

172.5950 7.225e1

173.3144 2.008e2

174.1592 1.316e2

175.0272 2.315e2

175.9425 2.500e2

176.7543 1.227e2

177.6526 1.890e2

178.6484 6.920e2

179.4835 3.302e2

180.2215 7.819e1

180.9328 2.088e2

181.9502 1.701e2

182.5980 5.323e1

183.2712 2.269e2

184.1165 9.447e1

184.8855 1.845e2

185.9422 2.425e2

186.9589 1.886e2

187.9547 1.726e2

188.9158 2.153e2

189.8213 1.626e2

190.3880 2.862e1

190.9819 3.994e2

191.8607 1.643e2

192.7317 2.046e2

193.4387 7.617e1

194.1620 2.049e2

194.8116 4.560e1

195.4282 1.954e2

195.9519 3.016e0

196.5163 1.751e2

197.4827 1.643e2

198.5015 1.824e2

199.4691 1.904e2

200.0109 2.204e1

200.5578 1.893e2

201.0868 1.542e0

201.6176 1.742e2

202.4814 8.735e1

203.2959 1.920e2

204.1995 1.409e2

205.0607 1.704e2

205.5663 8.114e0

206.1151 1.540e2

206.6649 1.222e1

207.2194 2.165e2

208.2916 1.562e2

209.2298 1.587e2

209.9254 4.000e1

210.6012 1.219e2

211.1746 1.688e1

211.7346 1.473e2

212.2808 7.133e0

212.8428 1.397e2

213.7728 7.957e1

214.6292 1.258e2

215.6282 1.525e2

216.3970 6.094e1

217.1533 1.374e2

218.1839 2.427e2

219.1232 1.411e2

219.8794 7.034e1

220.6848 1.358e2

221.3857 3.056e1

222.0014 1.226e2

222.7436 5.250e1

223.5321 1.275e2

224.3146 4.862e1

224.9936 2.294e2

225.7192 5.872e1

226.4358 1.505e2

227.4726 1.086e2

228.2074 1.403e1

228.8656 1.525e2

229.3985 1.001e1

229.9616 1.350e2

230.7412 8.109e1

231.6148 1.379e2

232.3042 2.319e1

232.9172 1.483e2

233.5636 3.259e1

234.1775 1.411e2

235.0593 1.051e2

235.9866 3.573e2

236.9244 1.670e2

237.7817 8.968e1

238.6336 1.608e2

239.6062 1.168e2

240.5141 1.446e2

241.4751 1.776e2

242.0191 7.027e0

242.5822 1.550e2

243.5522 1.369e2

244.2513 5.706e1

244.9269 1.520e2

245.8372 9.937e1

246.7740 1.739e2

247.6630 1.311e2

248.2815 2.684e1

248.9513 1.355e2

249.6470 6.395e1

250.4338 1.700e2

251.4516 1.618e2

252.4385 1.355e2

253.3758 1.650e2

253.9245 1.070e1

254.5340 1.588e2

255.4690 1.238e2

256.3751 1.595e2

257.3088 1.494e2

258.1154 1.193e2

258.9937 2.038e2

259.9978 1.503e2

260.5312 9.178e0

261.0598 1.672e2

261.8805 6.793e1

262.5994 1.663e2

263.3254 7.785e1

264.1285 1.522e2

264.6357 1.465e0

265.1960 3.345e2

265.7951 2.281e1

266.3925 1.970e2

266.9386 1.152e1

267.5123 1.442e2

268.2285 3.483e1

268.8725 2.009e2

269.8292 1.346e2

270.4825 3.587e1

271.1144 1.389e2

272.0807 1.472e2

272.9291 9.630e1

273.9006 1.770e2

274.4427 9.408e0

275.0152 1.388e2

275.9025 1.149e2

276.8793 1.726e2

277.6830 4.756e1

278.4832 1.621e2

279.2119 7.914e1

279.9780 3.663e2

280.9592 1.715e2

281.6094 3.263e1

282.2472 1.469e2

283.0102 5.678e1

283.7425 1.601e2

284.6696 1.110e2

285.3000 2.487e1

285.9377 1.643e2

286.6854 6.392e1

287.4887 1.343e2

288.4980 1.346e2

289.1402 2.430e1

289.7288 1.262e2

290.2799 6.434e0

290.8253 1.255e2

291.4932 2.883e1

292.1624 1.283e2

293.1599 1.725e2

294.0991 1.012e2

295.0613 1.484e2

296.0339 1.051e2

296.6078 1.411e1

297.2197 1.465e2

298.0593 8.837e1

298.9094 1.639e2

299.5764 3.097e1

300.2262 1.483e2

301.2204 1.219e2

301.9990 5.914e1

302.8009 7.151e1

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305.6979 1.272e2

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306.9594 1.112e2

307.8810 8.769e1

308.5328 2.436e1

309.1921 2.200e2

310.0979 9.148e1

310.9980 1.291e2

311.8314 2.846e2

312.4860 6.779e1

313.1721 2.031e2

314.1105 6.373e1

315.0763 1.250e2

315.6838 2.142e1

316.3468 5.909e1

317.1635 1.127e2

317.8397 1.485e1

318.5068 9.714e1

319.2262 2.686e1

320.0374 8.159e1

320.5530 1.293e0

321.0659 1.075e2

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322.3076 1.053e2

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323.5901 1.195e2

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324.9668 1.421e2

325.5128 5.438e0

326.0789 8.798e1

327.0672 1.138e2

328.0485 5.922e1

328.9916 1.130e2

329.9028 9.761e1

330.6206 2.416e1

331.2876 7.502e1

332.0134 1.511e1

332.6888 7.192e1

333.4972 7.040e1

334.2247 8.365e0

334.8193 9.189e1

335.7108 7.417e1

336.2722 1.328e1

336.9227 1.371e2

337.5919 1.936e1

338.1946 6.286e1

339.1657 1.182e2

339.8086 2.651e1

340.4425 9.502e1

341.0039 4.876e0

341.5383 1.100e2

342.5189 9.887e1

343.5170 8.495e1

344.2651 4.489e1

345.1311 1.190e2

346.0071 2.605e1

346.7232 6.669e1

347.6823 7.977e1

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349.8887 7.992e1

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359.9950 1.040e2

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367.1071 1.118e0

367.6481 1.063e2

368.5229 7.490e1

369.4185 5.371e1

370.2196 8.932e1

370.8781 2.022e1

371.5558 1.012e2

372.4635 6.937e1

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383.7081 7.989e1

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386.0905 9.215e1

386.5941 4.051e0

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389.1091 1.147e2

390.0639 7.014e1

390.9203 5.121e1

391.7367 1.007e2

392.5880 4.299e1

393.3761 1.161e2

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394.7833 8.672e1

395.2964 4.996e0

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404.9993 1.146e2

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416.0632 5.287e2

417.0633 2.841e2

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420.9045 1.258e2

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477.2473 6.750e1

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537.9288 7.664e1

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542.6830 5.698e0

543.2422 7.584e1

543.8080 6.429e0

544.4035 5.946e1

545.3295 1.100e2

545.8564 3.544e0

546.4008 5.509e1

546.9183 2.025e0

547.4217 8.999e1

548.3613 4.547e1

549.1834 5.608e1

550.1263 6.896e1

551.0936 1.079e2

552.0226 6.672e1

552.5263 1.519e0

553.0273 9.028e1

553.8461 4.502e1

554.6555 1.922e1

555.4114 6.808e1