



Isotope model

Elemental composition

Formula RDB Error (ppm)

C19 H21 O4 S 9.5 -0.009

m/z Intensity Relative

112.9845 761865408.0 8.75

148.9516 181188176.0 2.08

197.0273 1483330944.0 17.04

267.1390 8704276480.0 100.00

268.1425 1748345344.0 20.09

269.1454 196629408.0 2.26

301.1239 834931008.0 9.59

302.1273 184664912.0 2.12

345.1166 6839691264.0 78.58

346.1198 1444897408.0 16.60

347.1158 449058144.0 5.16

379.1024 1126377088.0 12.94

380.1057 276882304.0 3.18

381.0947 382021728.0 4.39

691.2408 4719038976.0 54.22

692.2441 2056401152.0 23.63

693.2422 895950464.0 10.29

694.2420 275622432.0 3.17

725.2249 446233856.0 5.13

726.2283 212295184.0 2.44