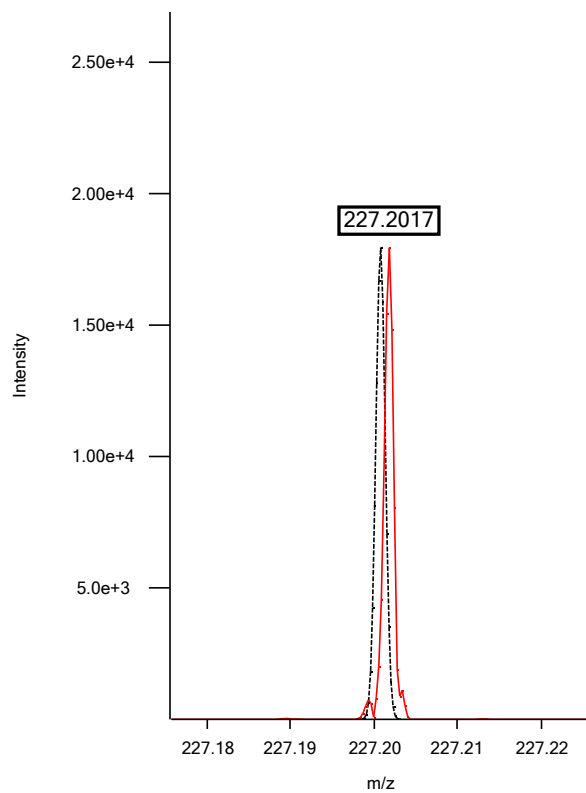


Comparison of theoretical (black, dashed line) and experimental (red, solid line) isotopic distributions

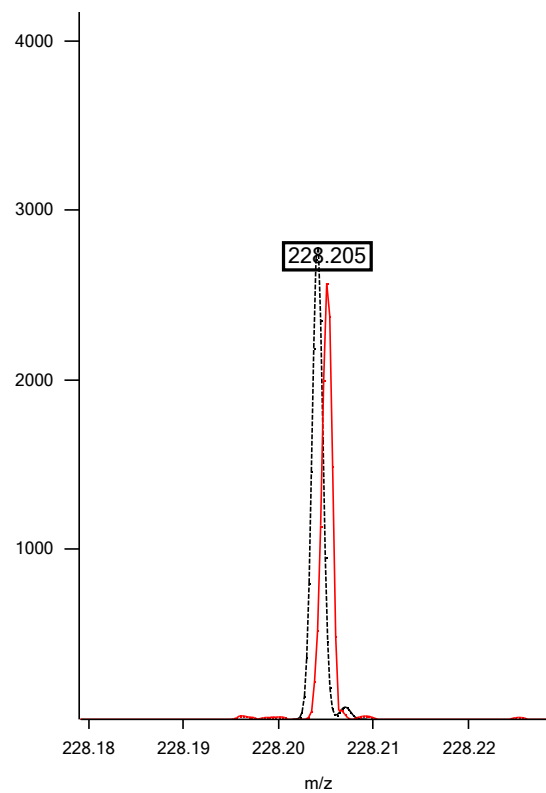
Fatty acids

Negative ESI: FA 14:0; C₁₄H₂₇O₂; theoretical *m/z* 227.2011, (M-H)⁻; isotopic fit 0.139

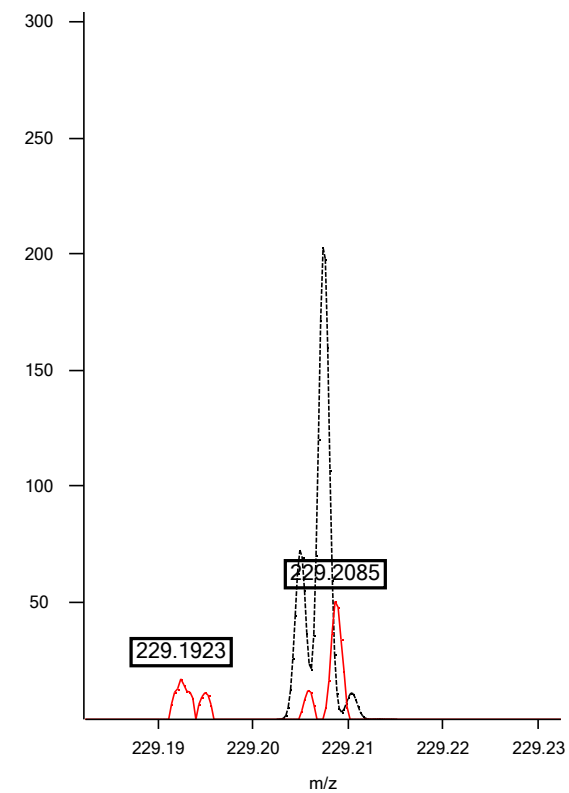
Isotope 1



Isotope 2

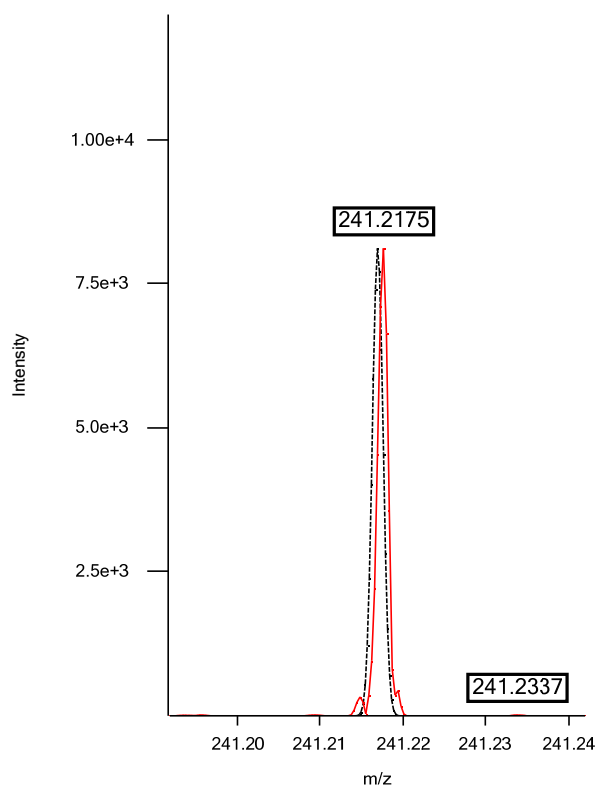


Isotope 3

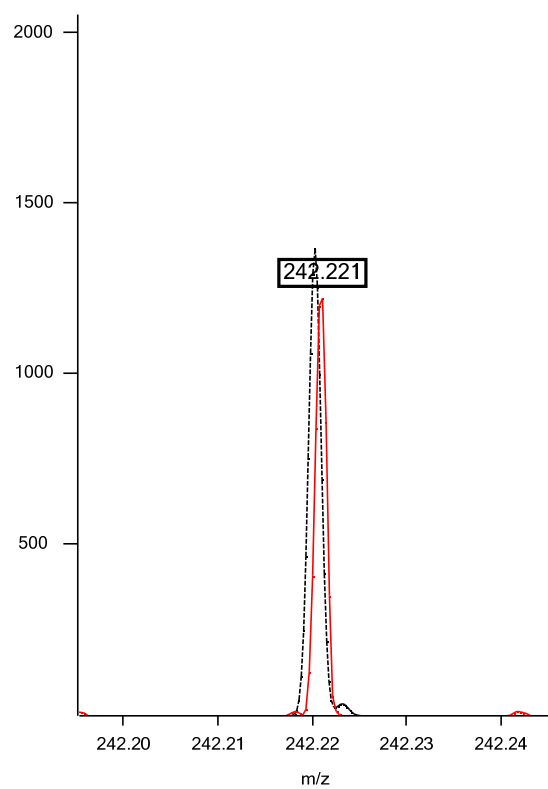


Negative ESI: FA 15:0; C₁₅H₂₉O₂; theoretical *m/z* 241.2167, (M-H)⁻; isotopic fit 0.000

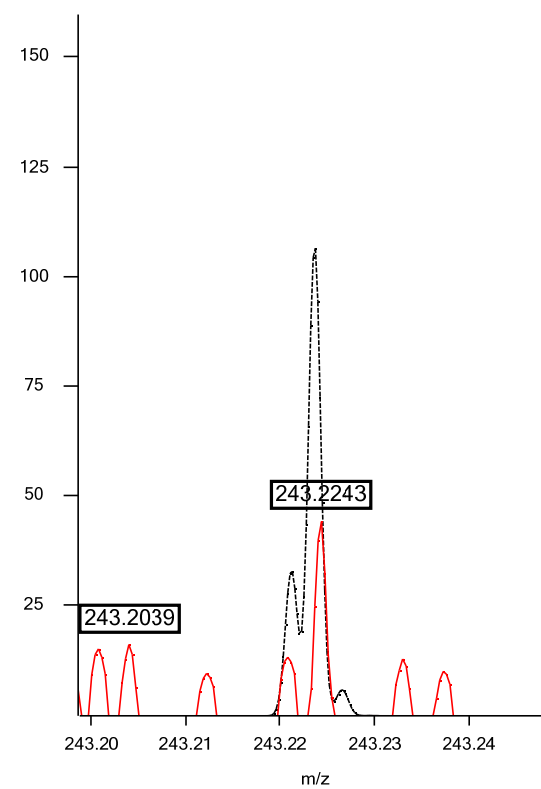
Isotope 1



Isotope 2

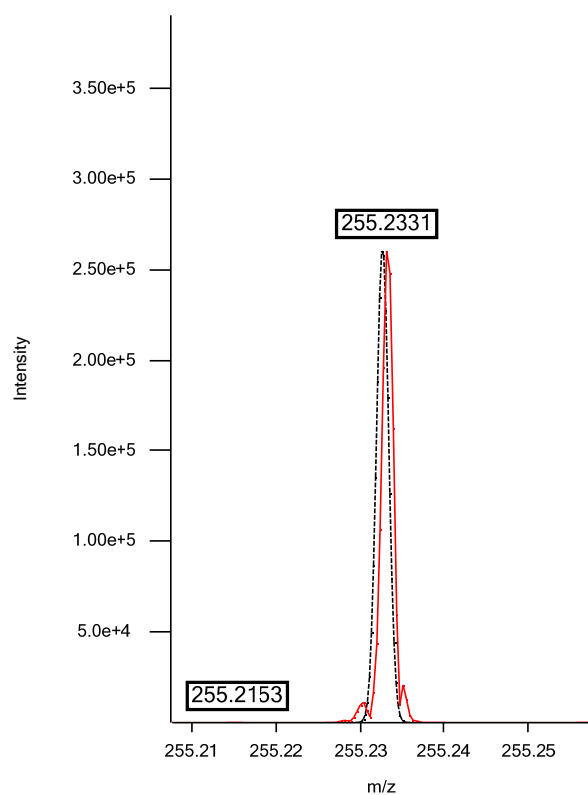


Isotope 3

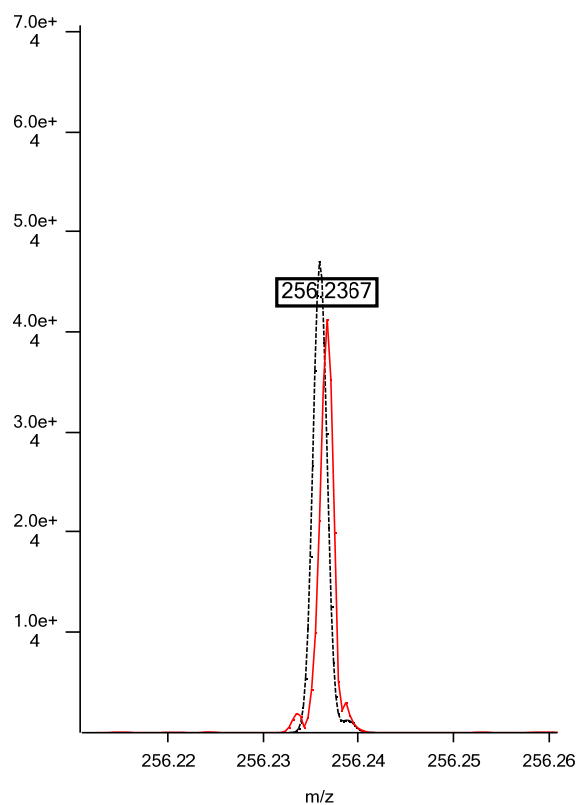


Negative ESI: FA 16:0; C₁₆H₃₁O₂; theoretical *m/z* 255.2324, (M-H)⁻; isotopic fit 0.000

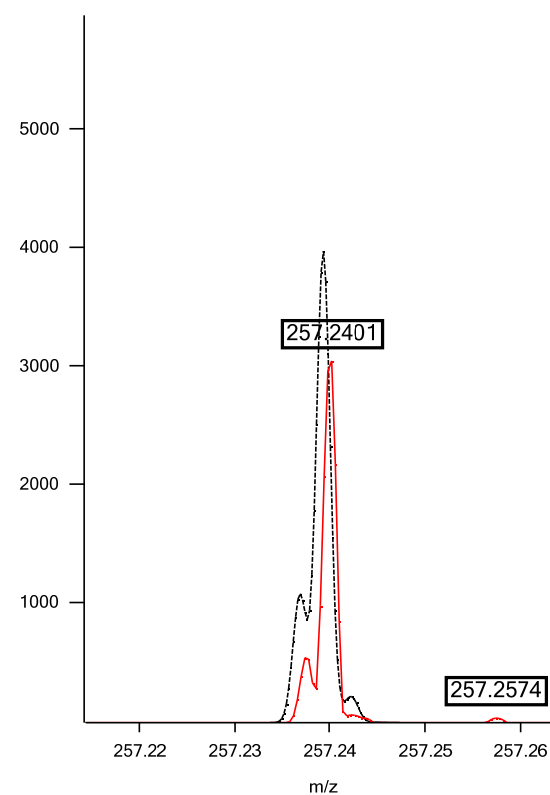
Isotope 1



Isotope 2

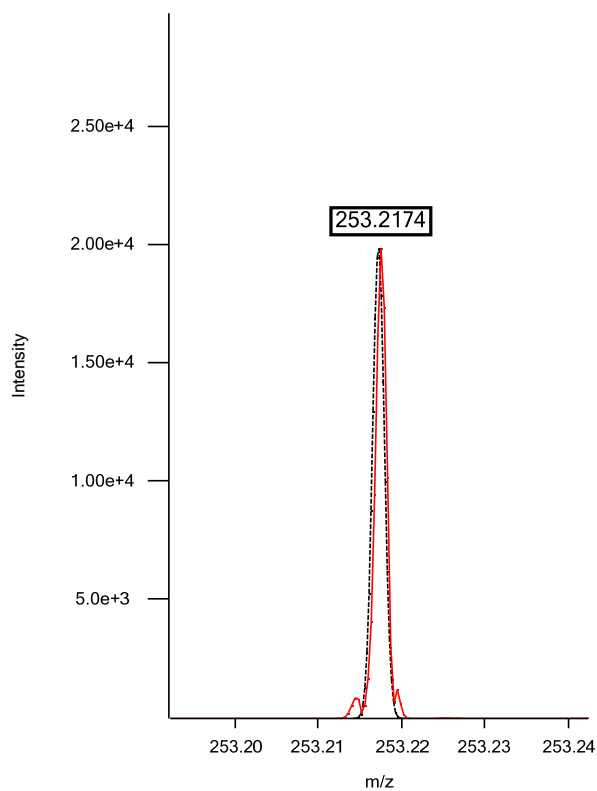


Isotope 3

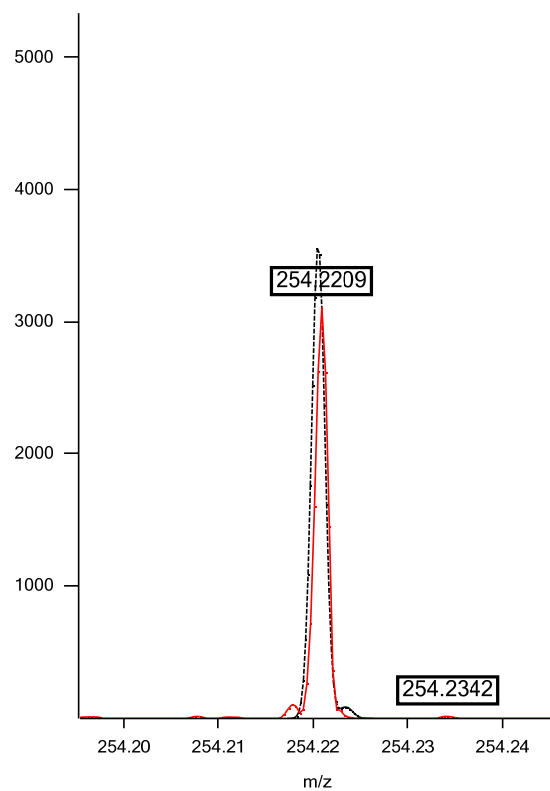


Negative ESI: FA 16:1; C₁₆H₂₉O₂; theoretical *m/z* 255.2324, (M-H)⁻; isotopic fit 0.0823

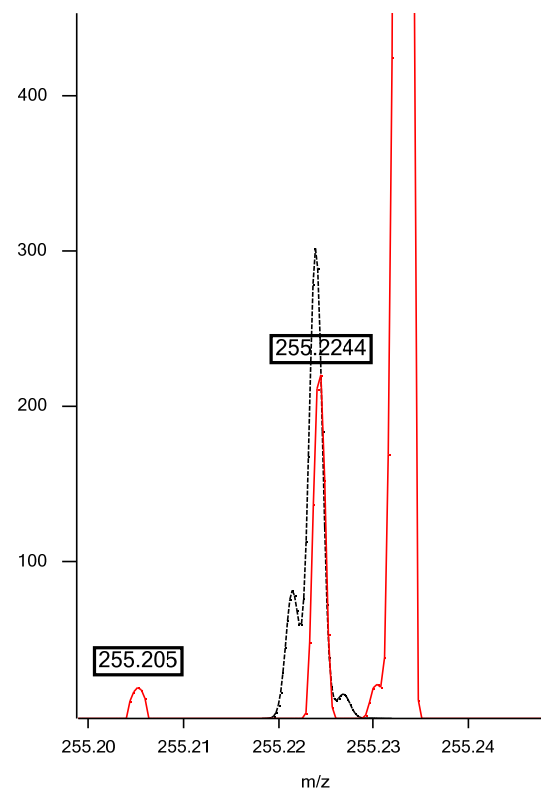
Isotope 1



Isotope 2

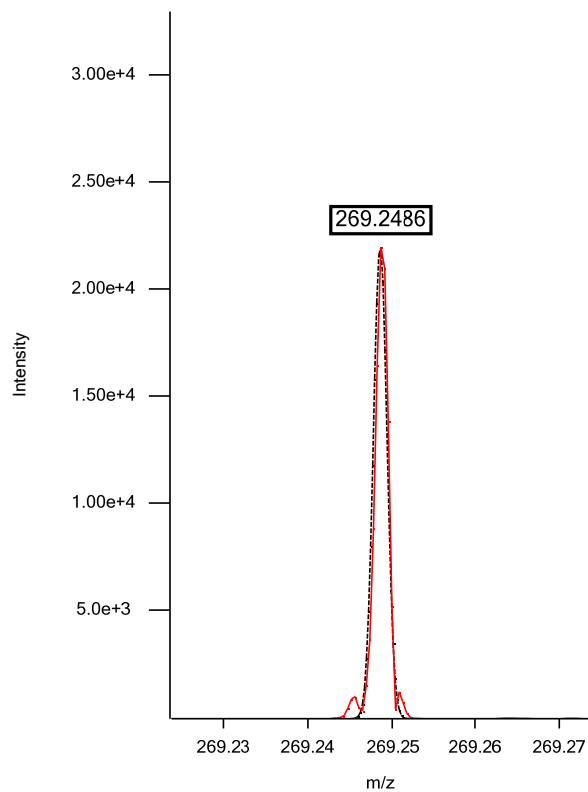


Isotope 3

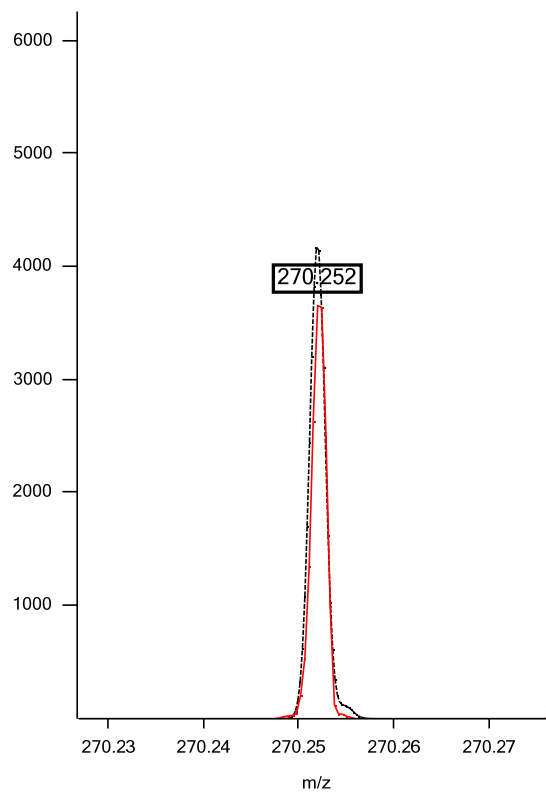


Negative ESI: FA 17:0; $C_{17}H_{33}O_2$; theoretical m/z 269.2481, (M-H)⁻; isotopic fit 0.1045

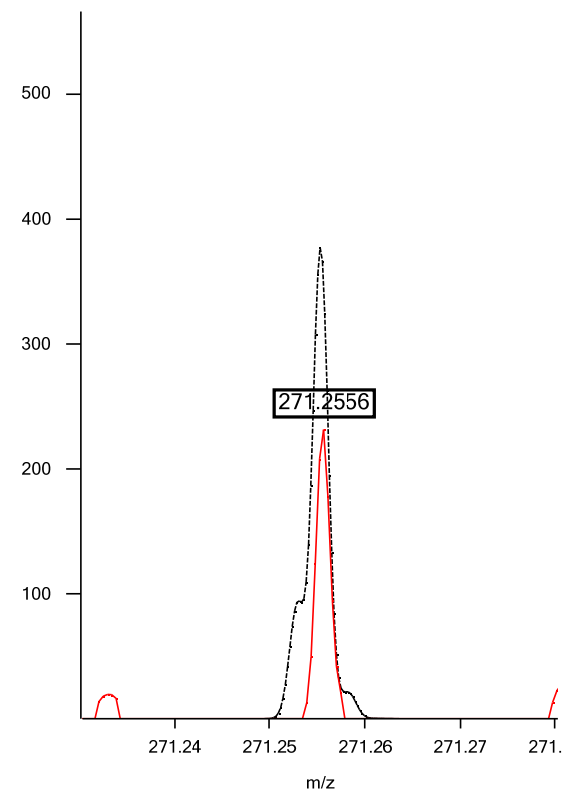
Isotope 1



Isotope 2

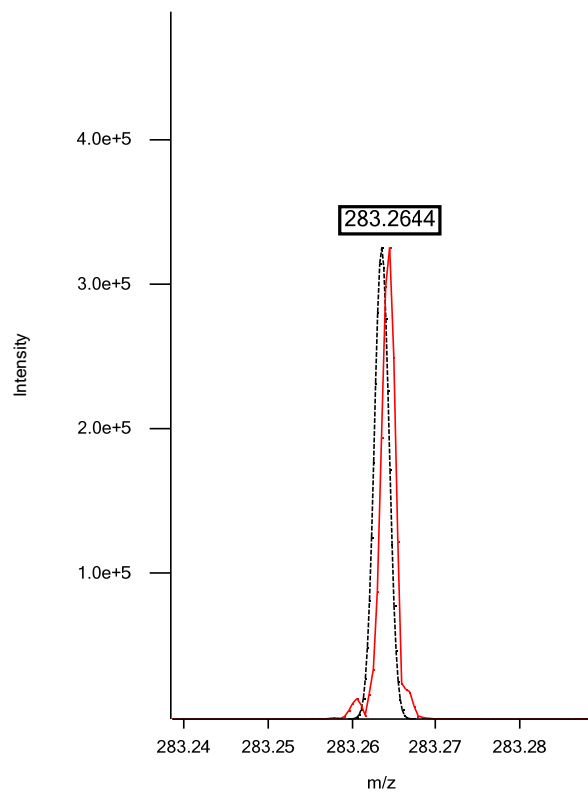


Isotope 3

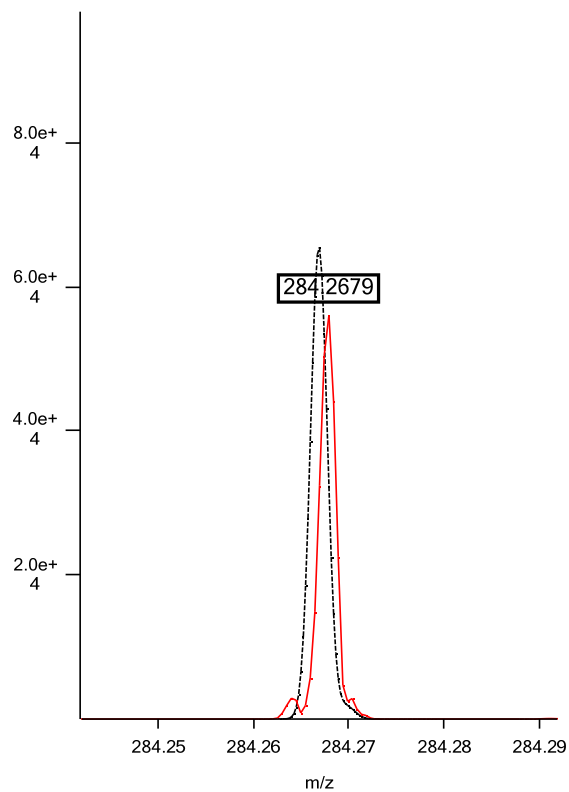


Negative ESI: FA 18:0; C₁₈H₃₅O₂; theoretical *m/z* 283.2637, (M-H)⁻; isotopic fit 0.1743

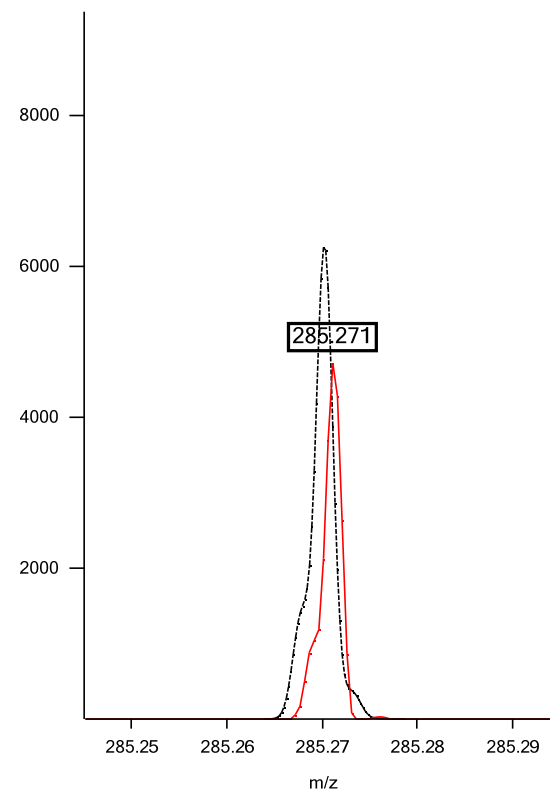
Isotope 1



Isotope 2

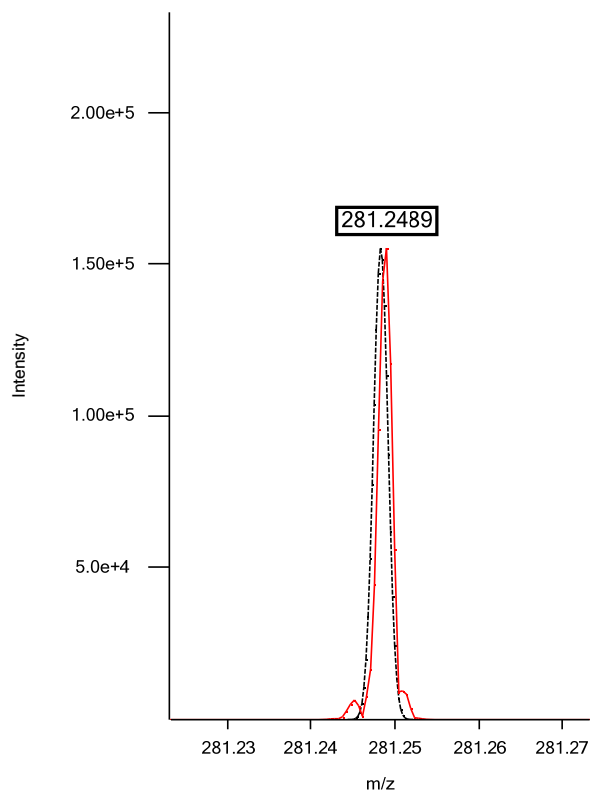


Isotope 3

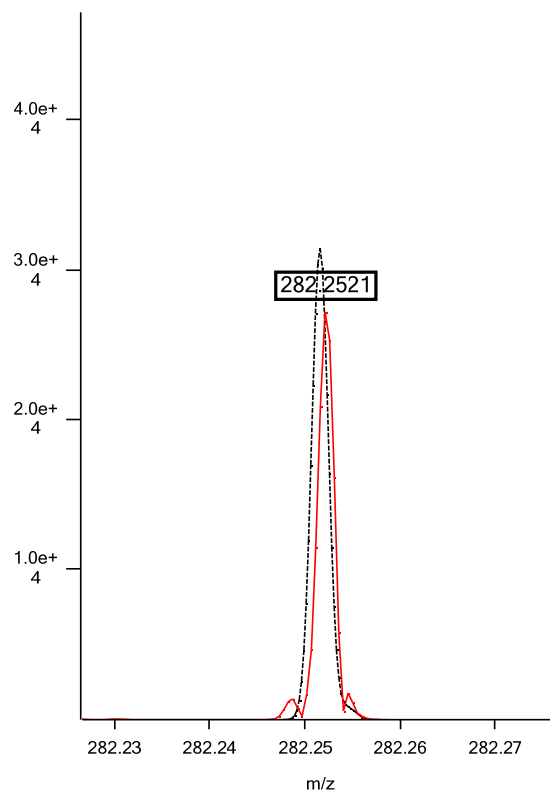


Negative ESI: FA 18:1; C₁₈H₃₃O₂; theoretical *m/z* 281.2481, (M-H)⁻; isotopic fit 0.2398

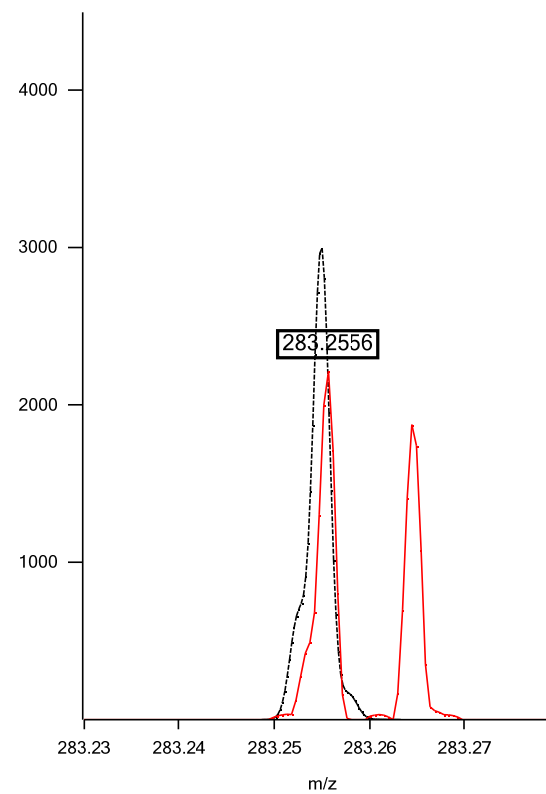
Isotope 1



Isotope 2

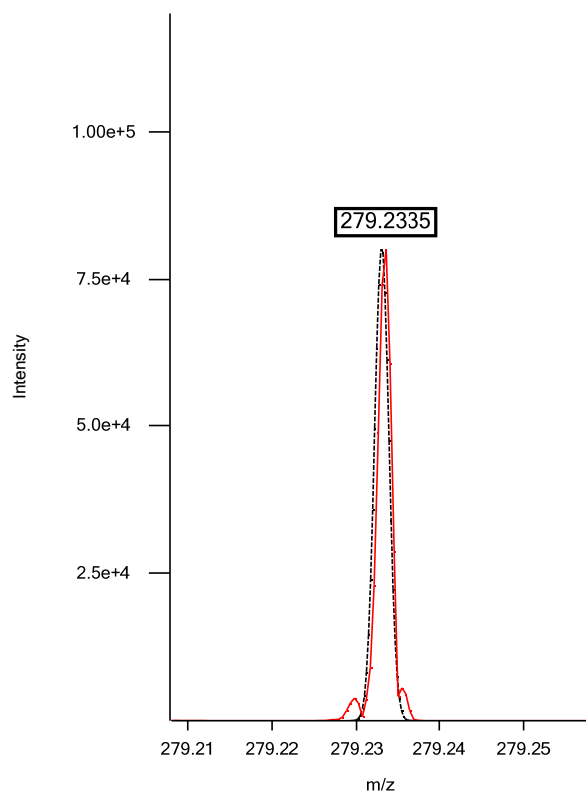


Isotope 3

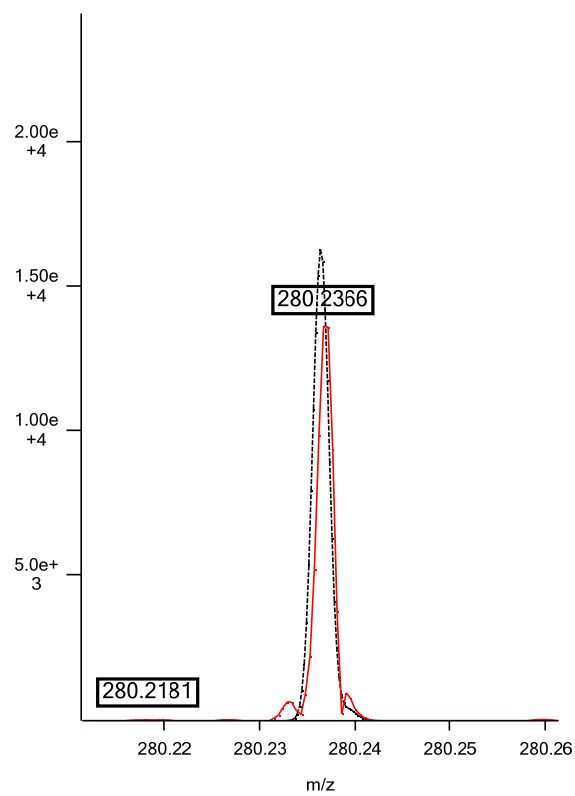


Negative ESI: FA 18:2; C₁₈H₃₁O₂; theoretical *m/z* 279.2324, (M-H)⁻; isotopic fit 0.1243

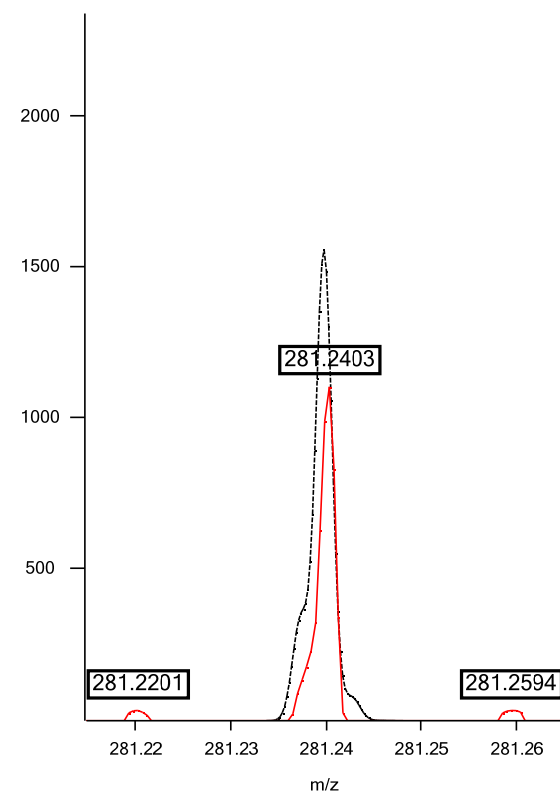
Isotope 1



Isotope 2

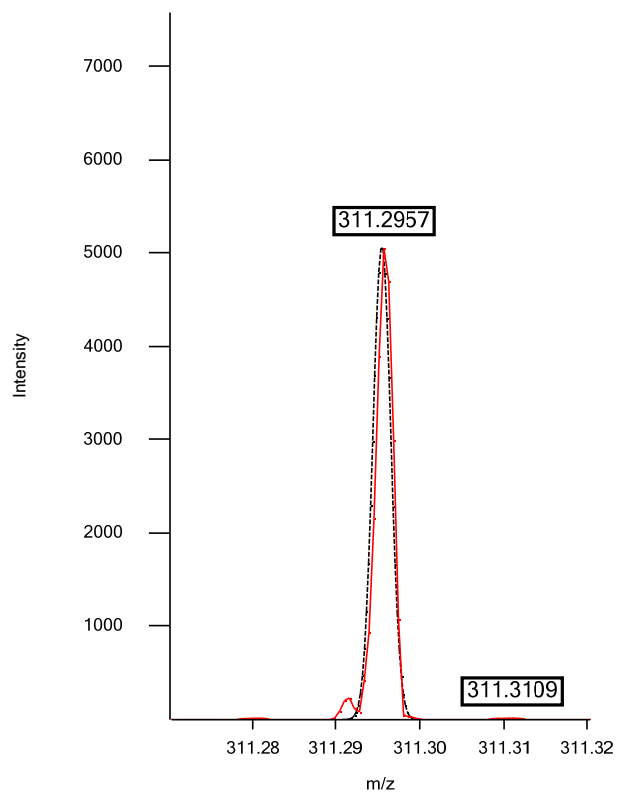


Isotope 3

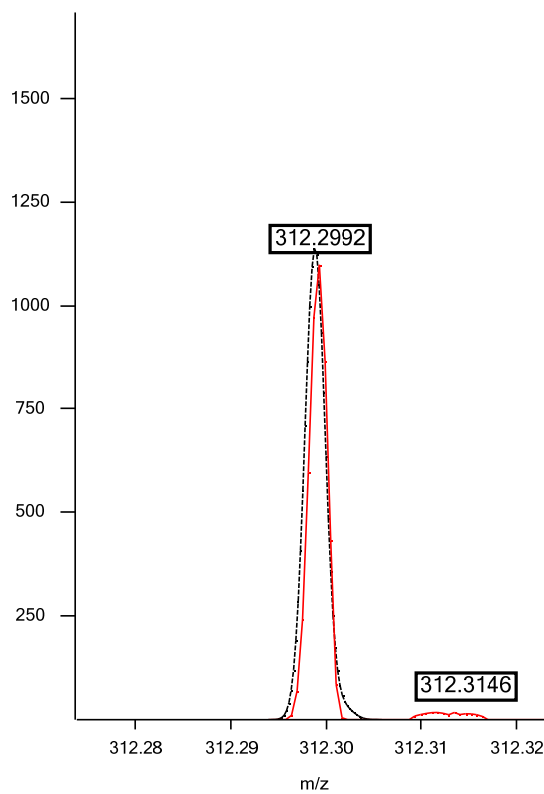


Negative ESI: FA 20:0; C₂₀H₃₉O₂; theoretical *m/z* 311.2950, (M-H)⁻; isotopic fit 0.0537

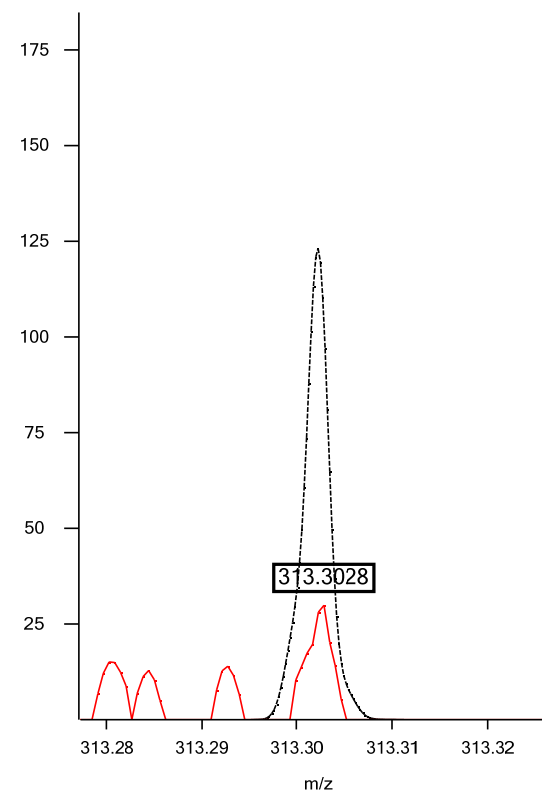
Isotope 1



Isotope 2

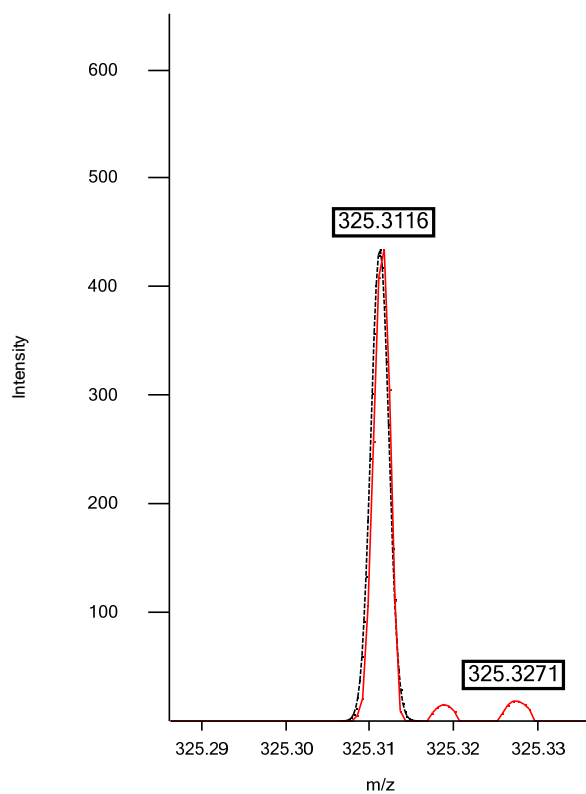


Isotope 3

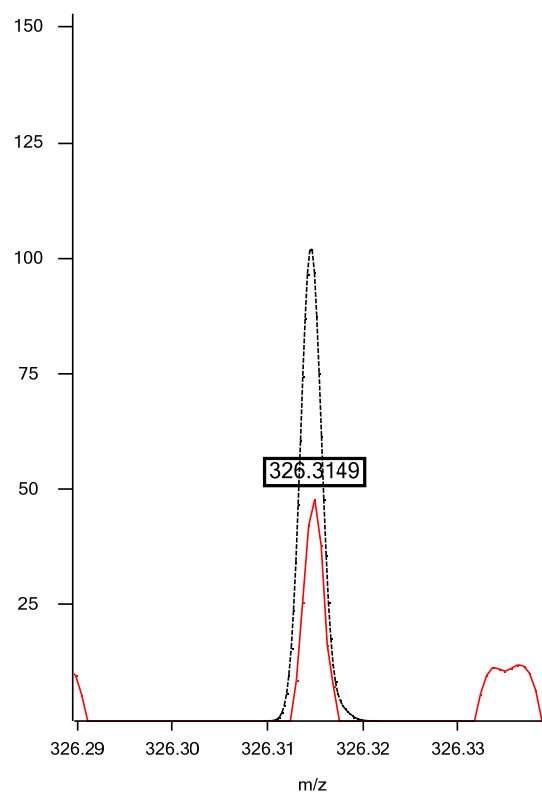


Negative ESI: FA 21:0; C₂₁H₄₁O₂; theoretical *m/z* 325.3107, (M-H)⁻; isotopic fit 0.0139

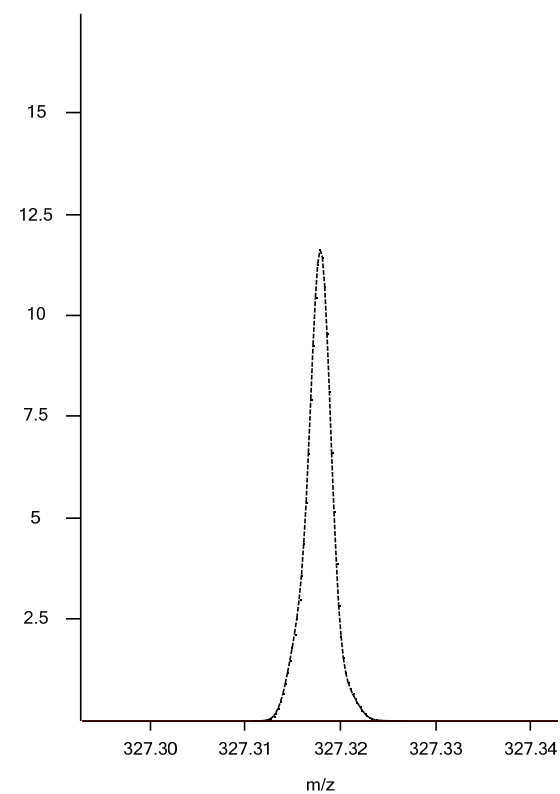
Isotope 1



Isotope 2

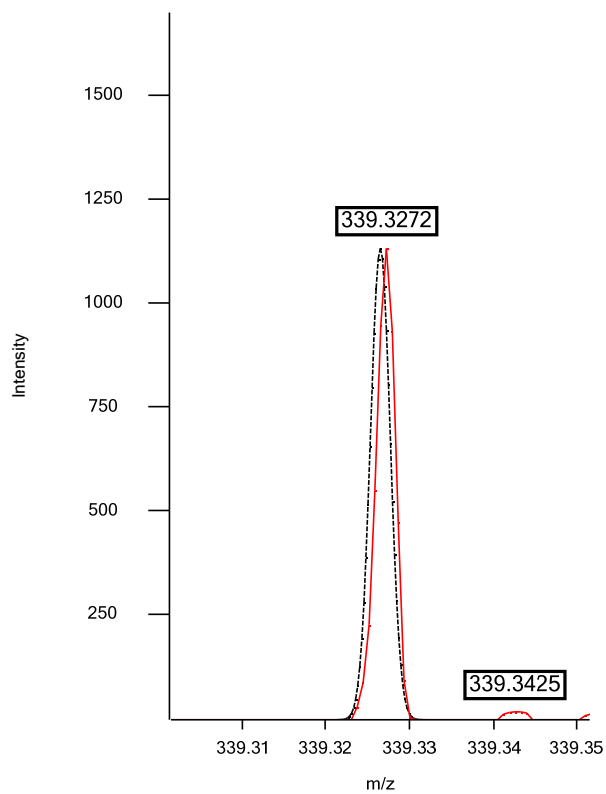


Isotope 3

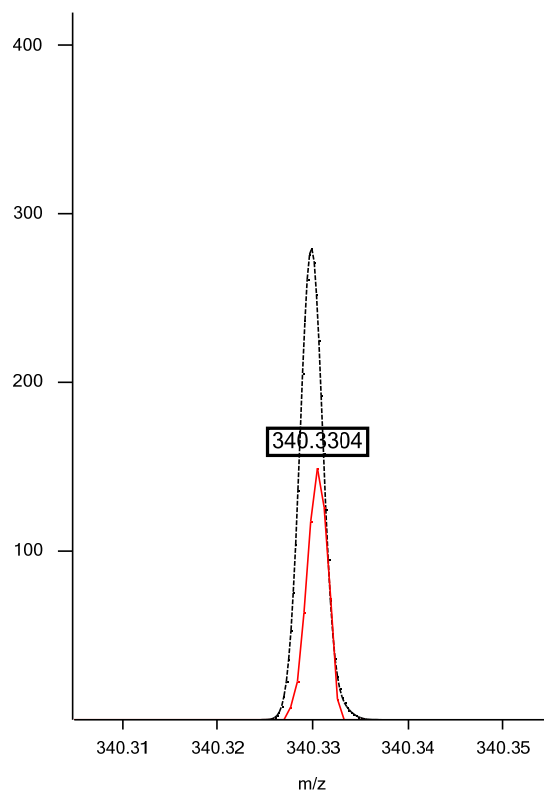


Negative ESI: FA 22:0; C₂₂H₄₃O₂; theoretical *m/z* 339.3263, (M-H)⁻; isotopic fit 0.0174

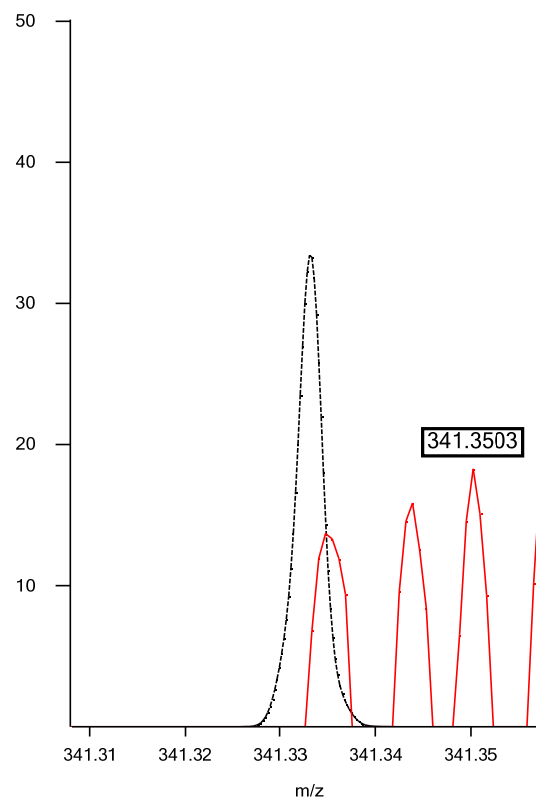
Isotope 1



Isotope 2

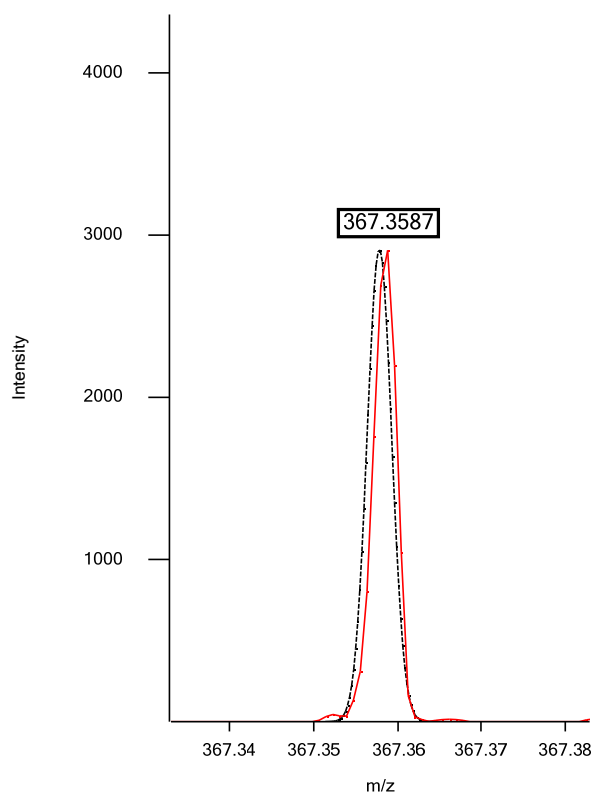


Isotope 3

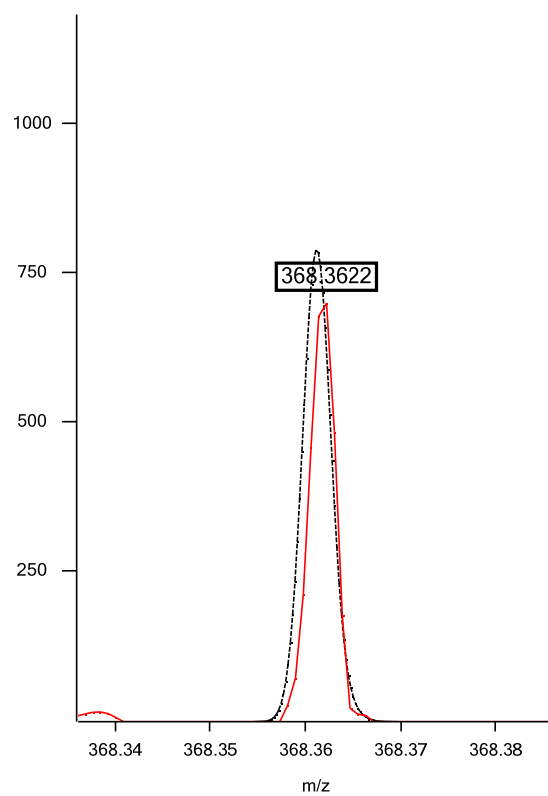


Negative ESI: FA 24:0; C₂₄H₄₇O₂; theoretical *m/z* 367.3576, (M-H)⁻; isotopic fit 0.0151

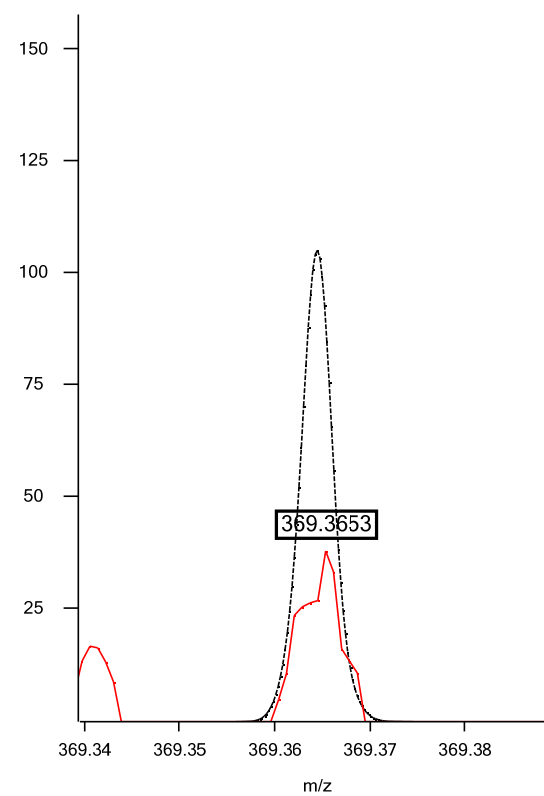
Isotope 1



Isotope 2

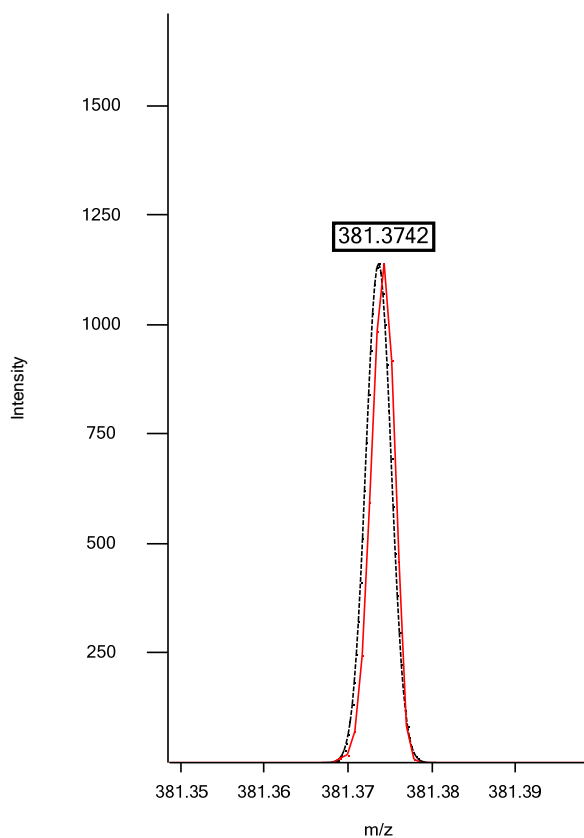


Isotope 3

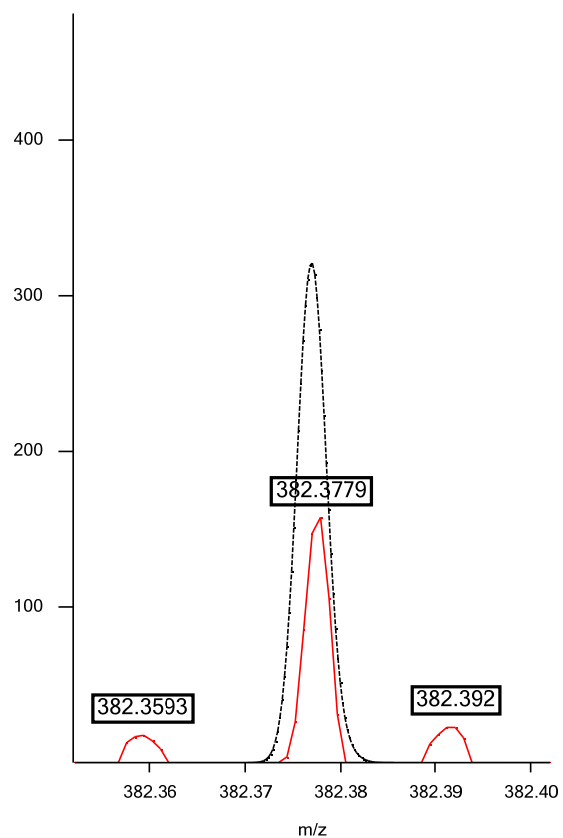


Negative ESI: FA 25:0; C₂₅H₄₉O₂; theoretical *m/z* 381.3733, (M-H)⁻; isotopic fit 0.0548

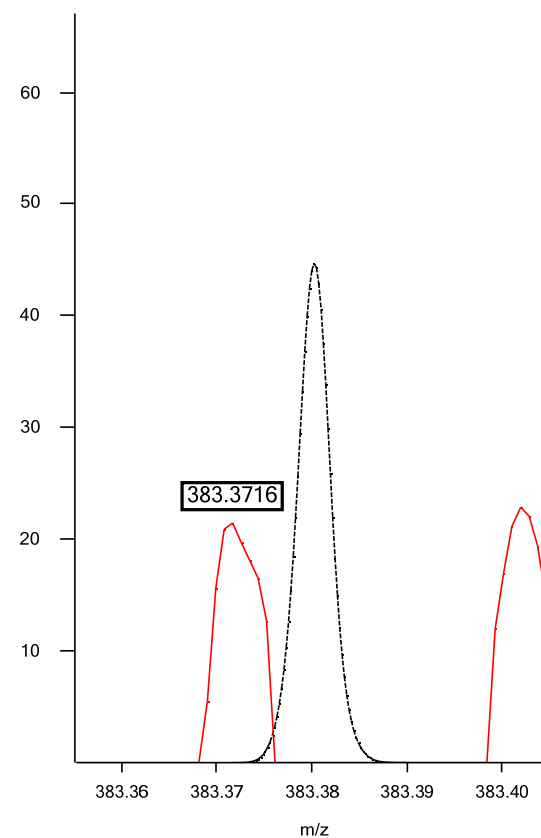
Isotope 1



Isotope 2



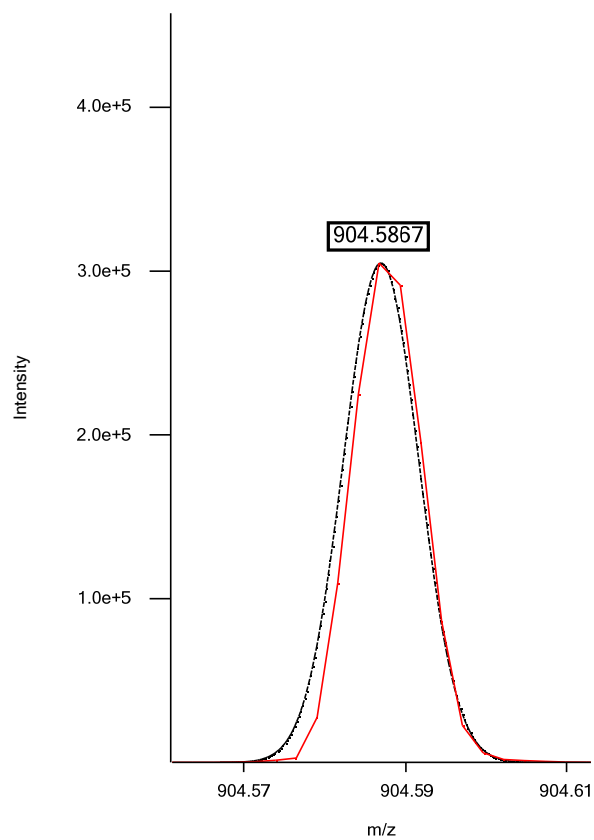
Isotope 3



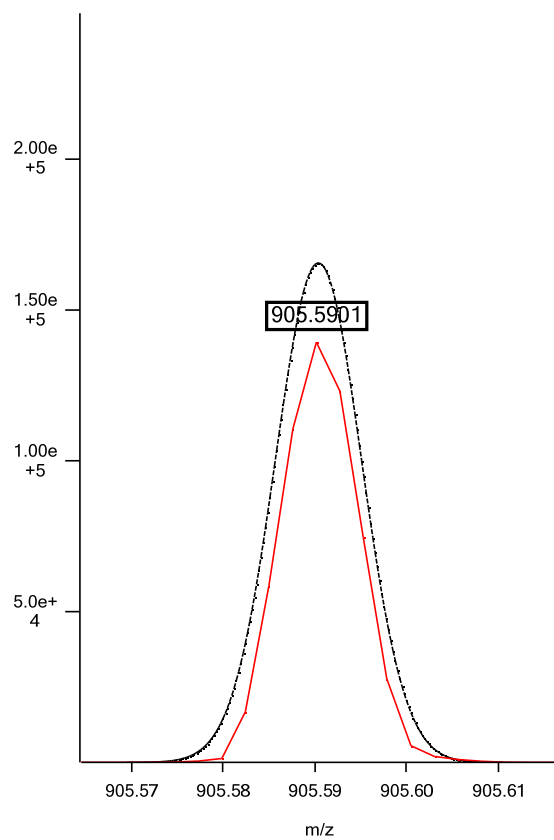
Glycerophosphoinositol

Positive ESI: PI 18:0/20:4; C₄₇H₈₇NO₁₃P; theoretical *m/z* 904.5915, (M+H)⁺; isotopic fit 0.0148

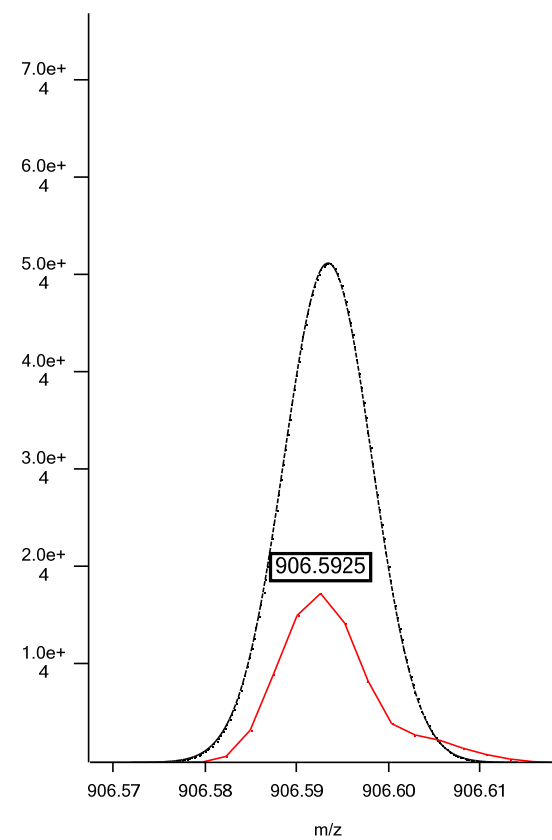
Isotope 1



Isotope 2



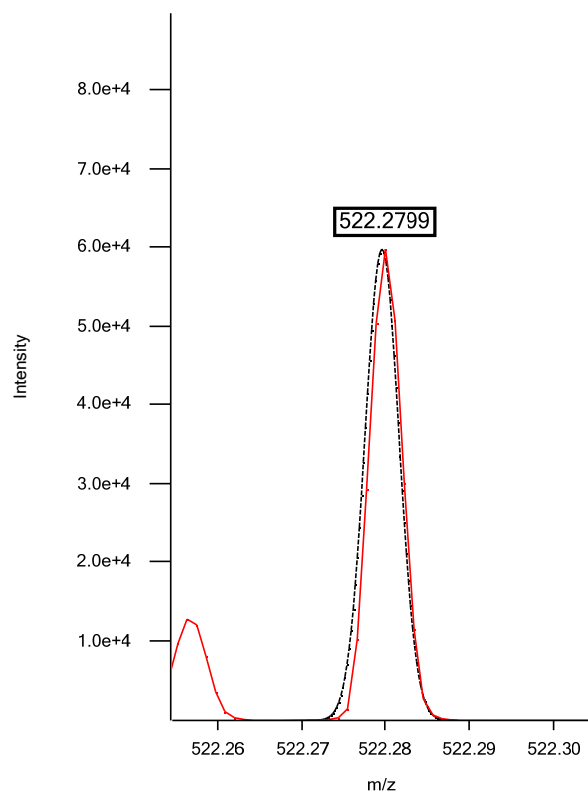
Isotope 3



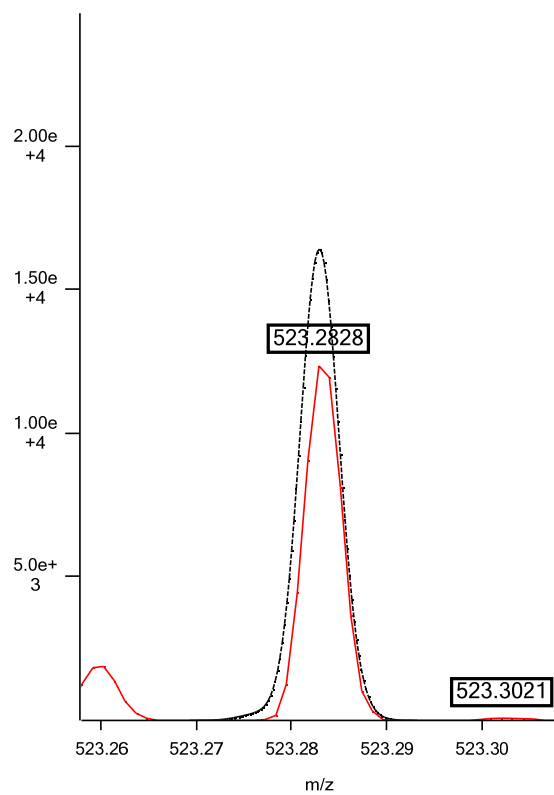
Glycerophosphoserines

Positive ESI: LPS 18:2; C₂₄H₄₅NO₉P; theoretical *m/z* 522.2832, (M+H)⁺; isotopic fit 0.0137

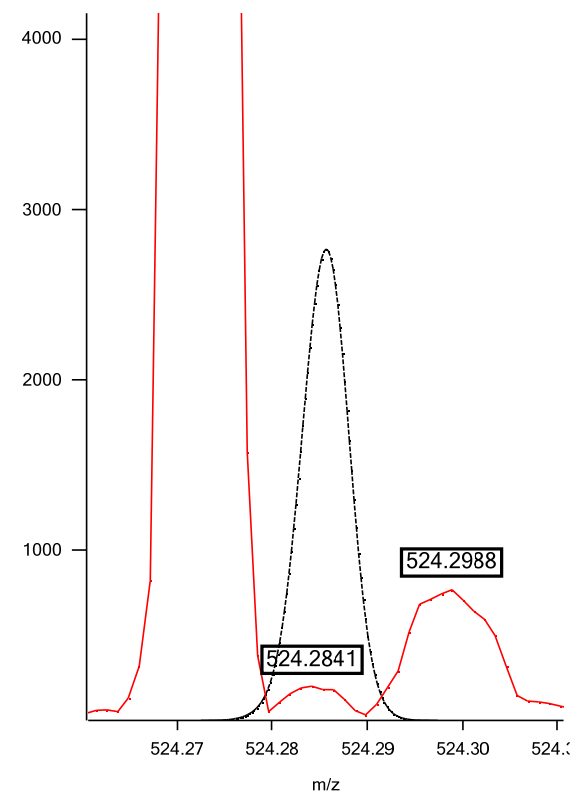
Isotope 1



Isotope 2

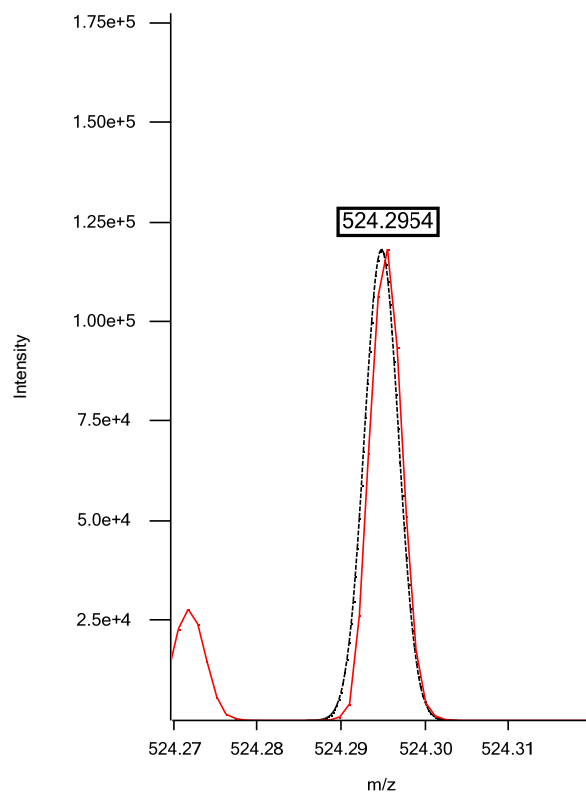


Isotope 3

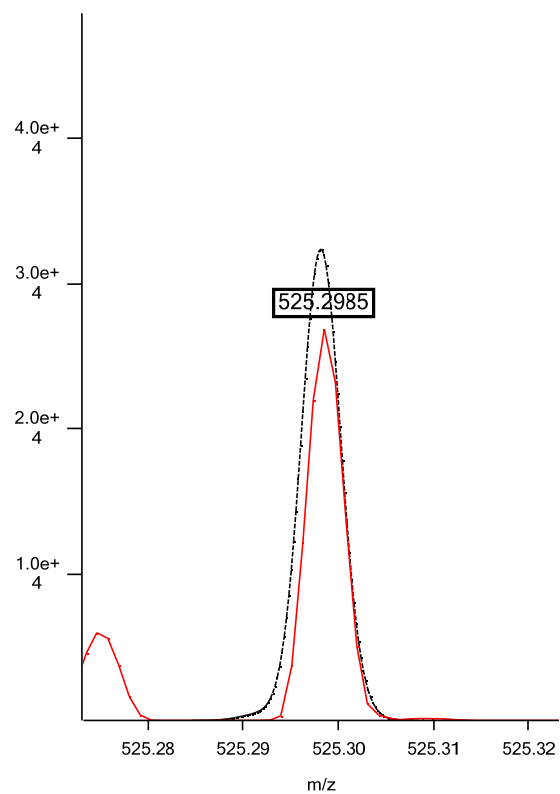


Positive ESI: LPS 18:1; $C_{24}H_{47}NO_9P$; theoretical m/z 524.2988, $(M+H)^+$; isotopic fit 0.0210

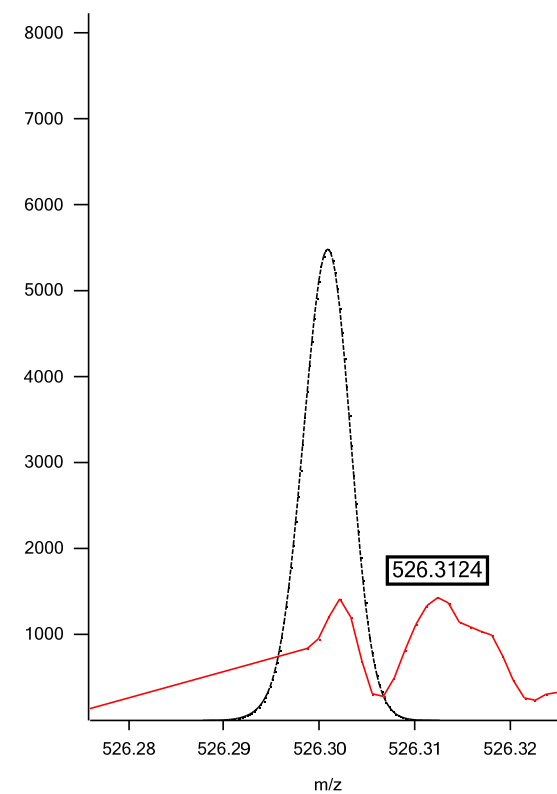
Isotope 1



Isotope 2

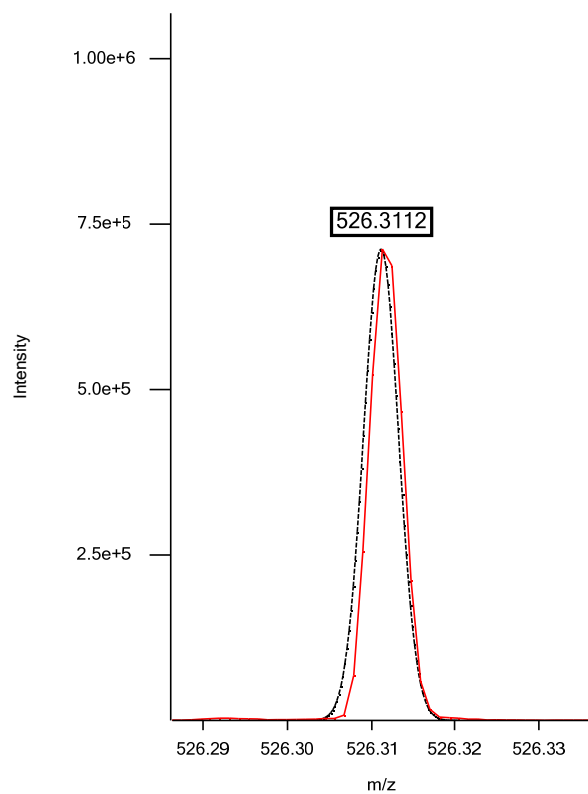


Isotope 3

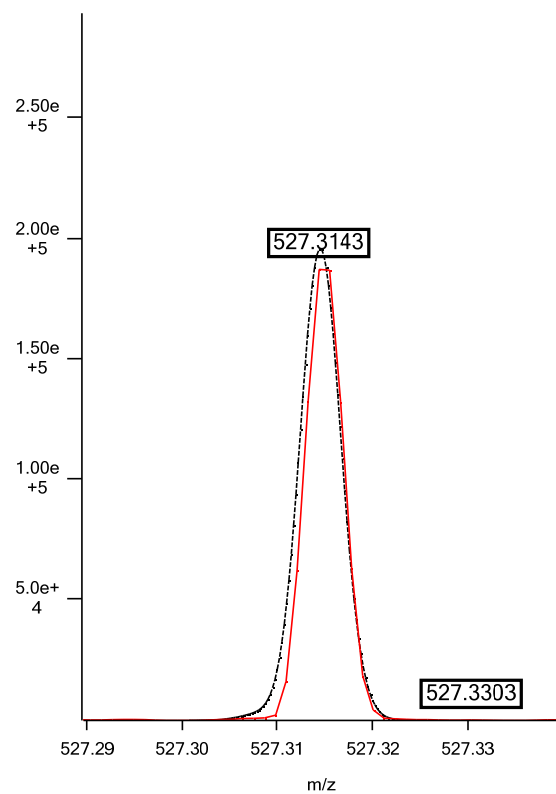


Positive ESI: LPS 18:0; C₂₄H₄₉NO₉P; theoretical m/z 526.3145, (M+H)⁺; isotopic fit 0.0075

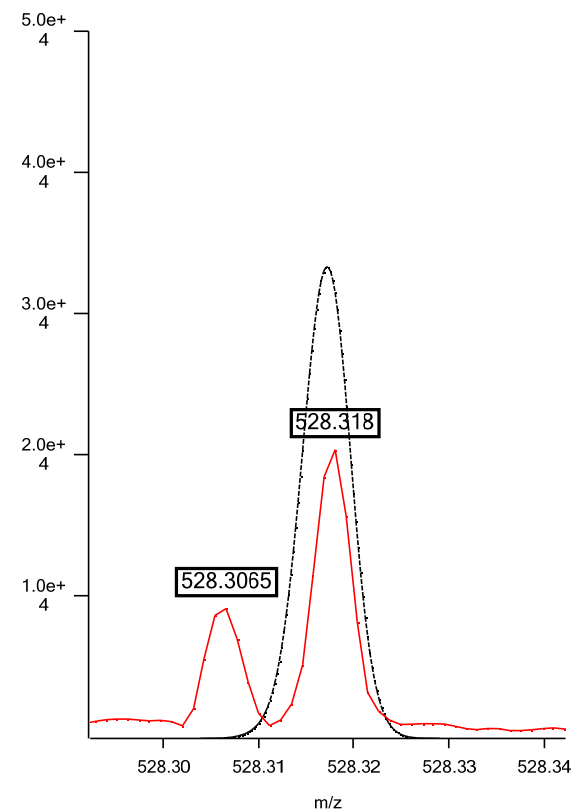
Isotope 1



Isotope 2

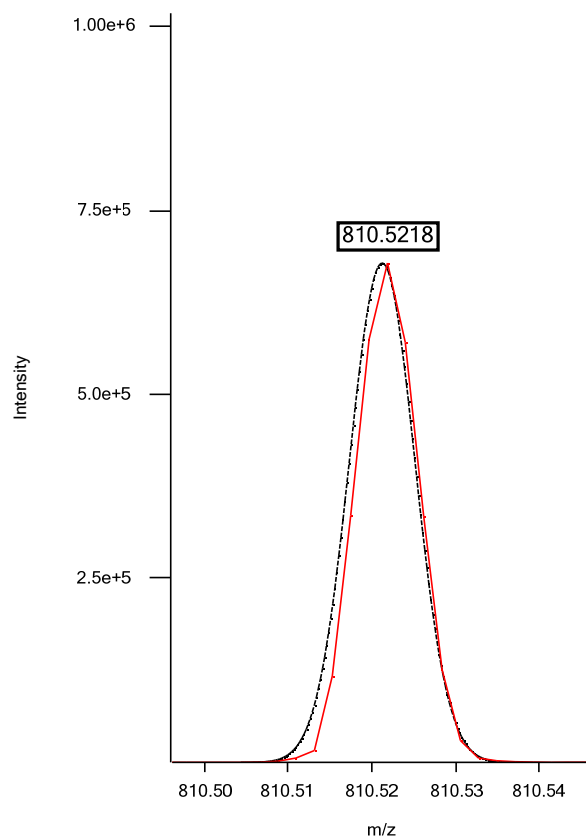


Isotope 3

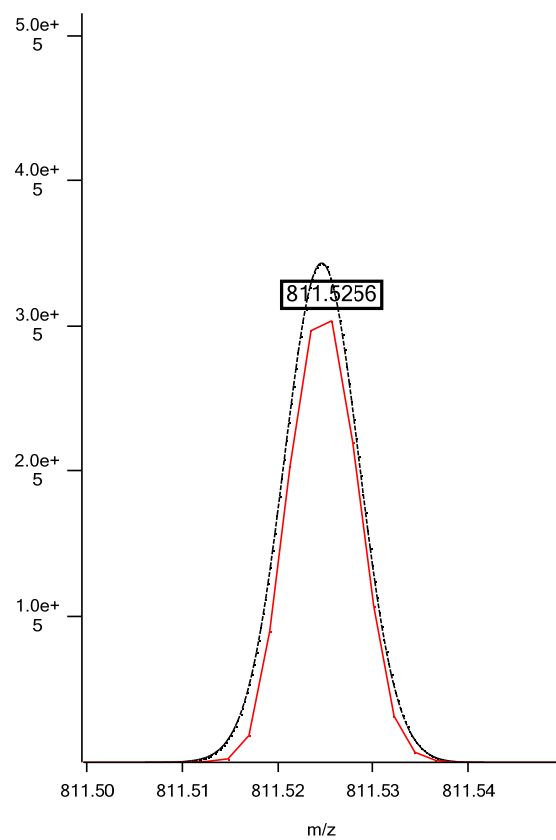


Positive ESI: PS 38:5; C₄₄H₇₇NO₁₀P; theoretical *m/z* 810.5285, (M+H)⁺; isotopic fit 0.0061

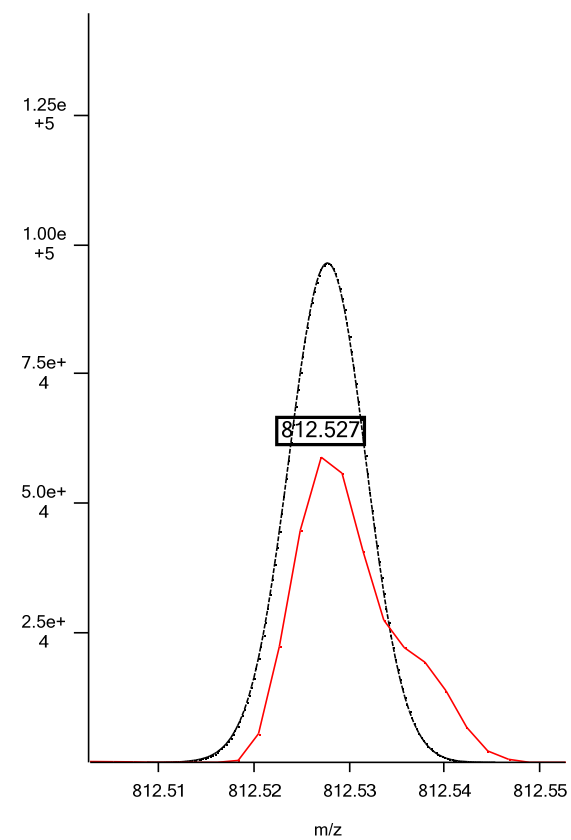
Isotope 1



Isotope 2

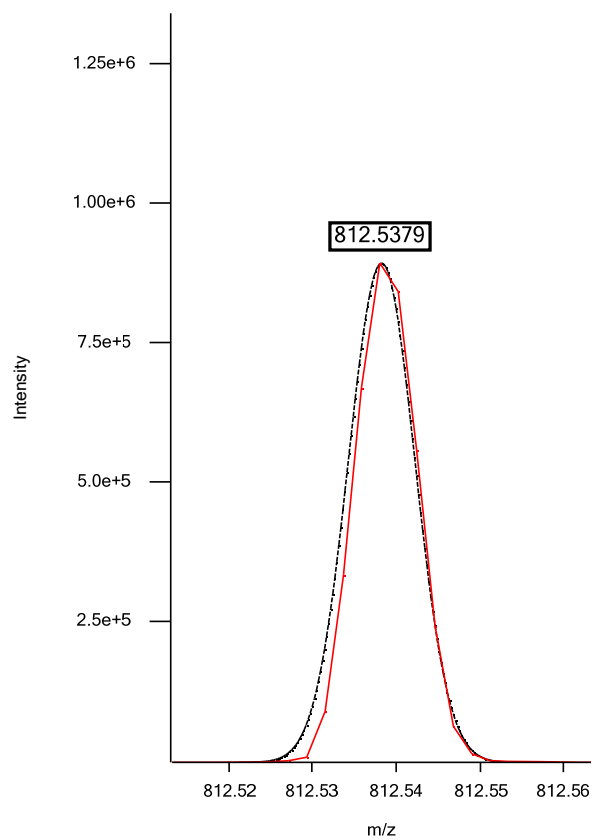


Isotope 3

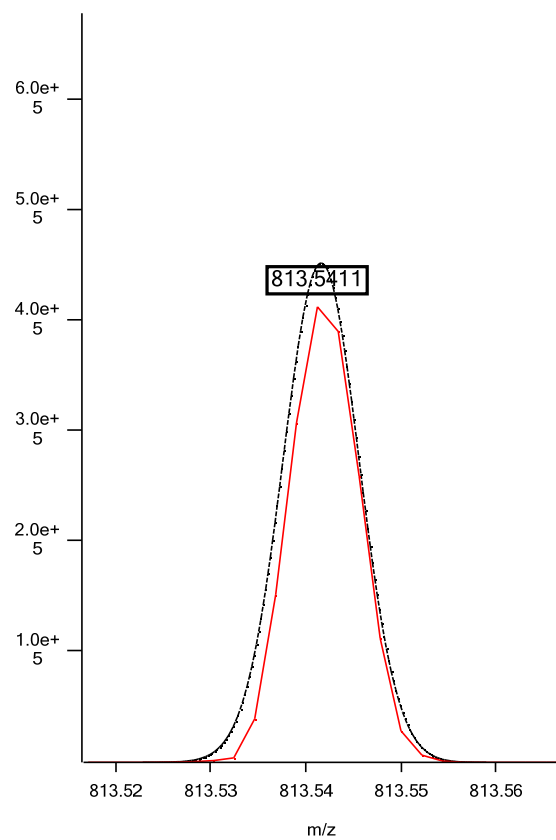


Positive ESI: PS 38:4; C₄₄H₇₉NO₁₀P; theoretical *m/z* 812.5441, (M+H)⁺; isotopic fit 0.0052

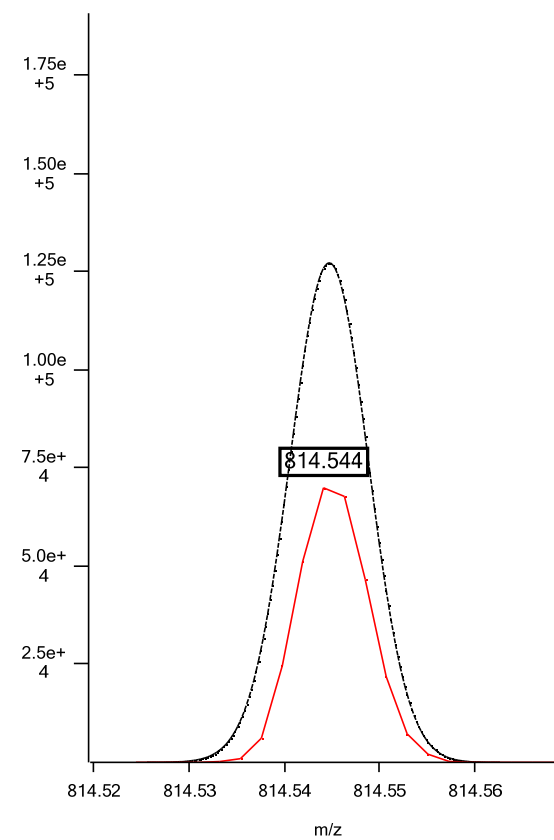
Isotope 1



Isotope 2

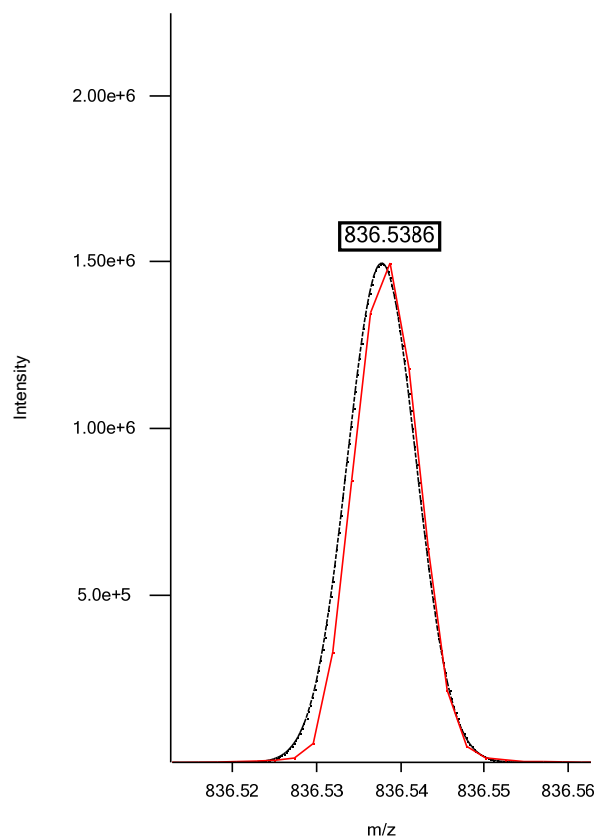


Isotope 3

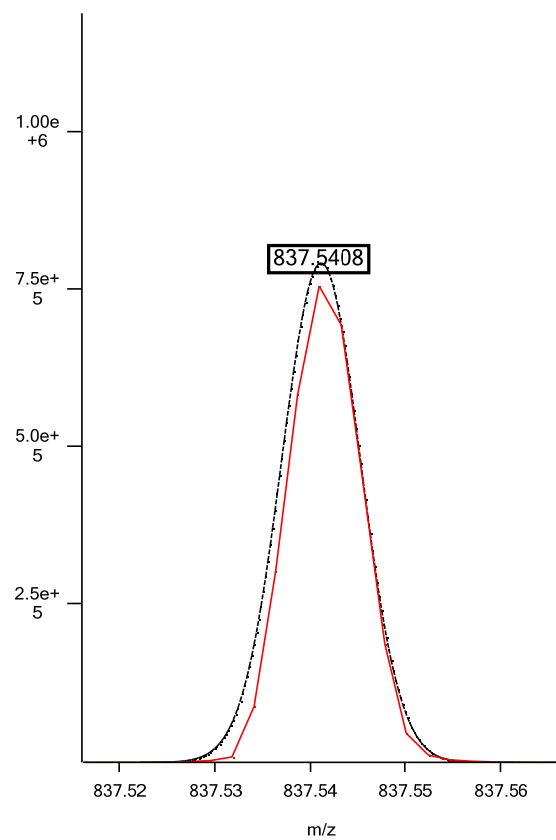


Positive ESI: PS 40:6; C₄₆H₇₉NO₁₀P; theoretical *m/z* 836.5441, (M+H)⁺; isotopic fit 0.0044

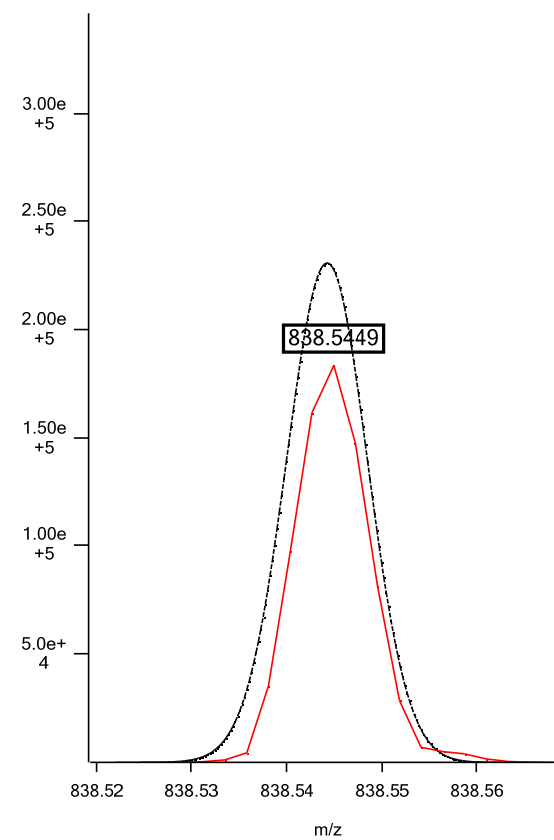
Isotope 1



Isotope 2

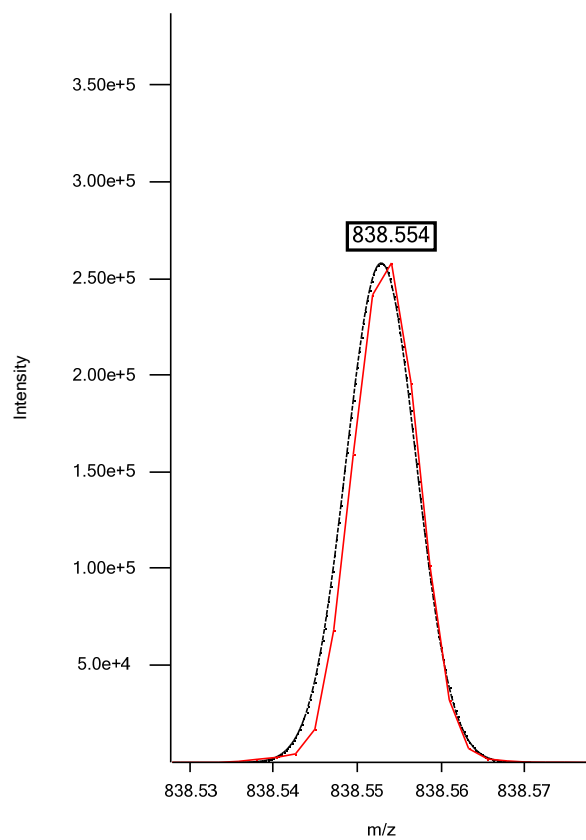


Isotope 3

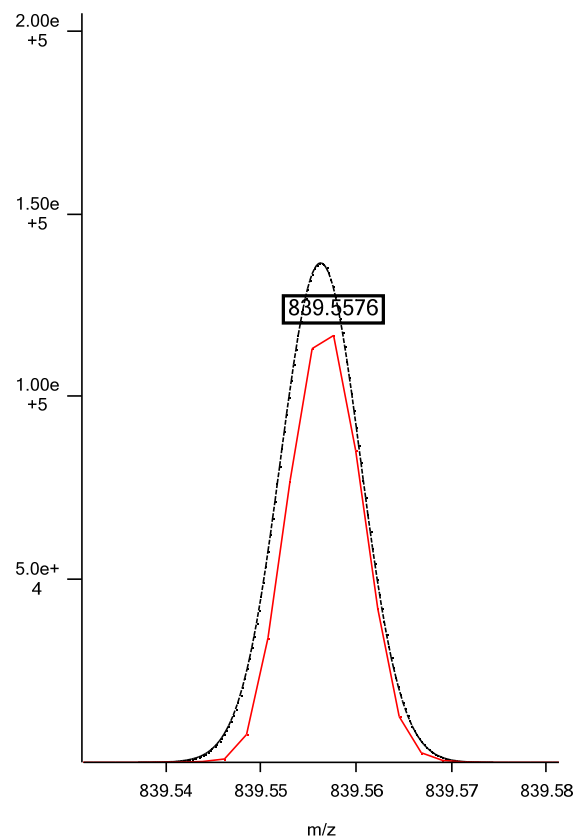


Positive ESI: PS 40:5; C₄₆H₈₁NO₁₀P; theoretical *m/z* 838.5598, (M+H)⁺; isotopic fit 0.0107

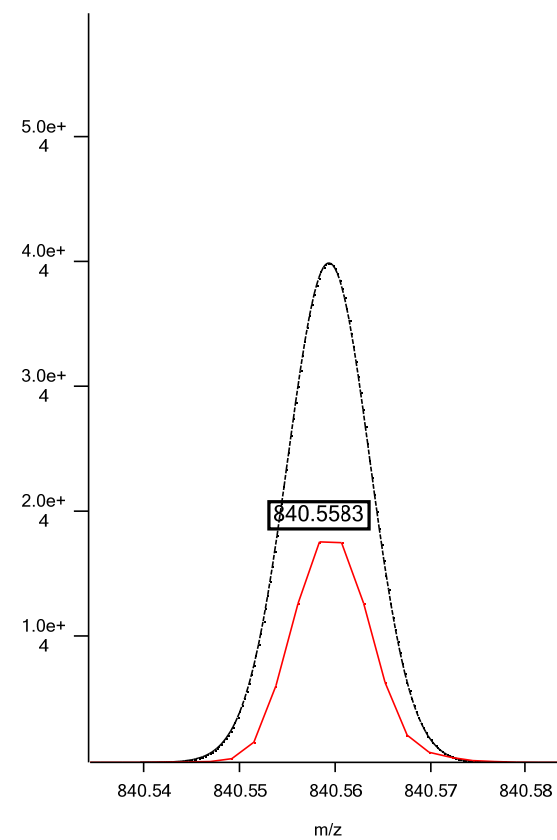
Isotope 1



Isotope 2

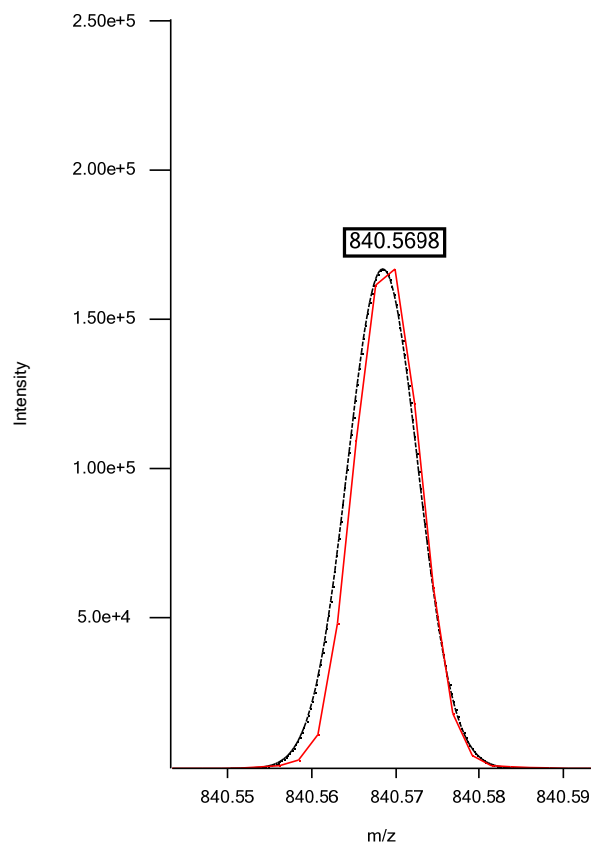


Isotope 3

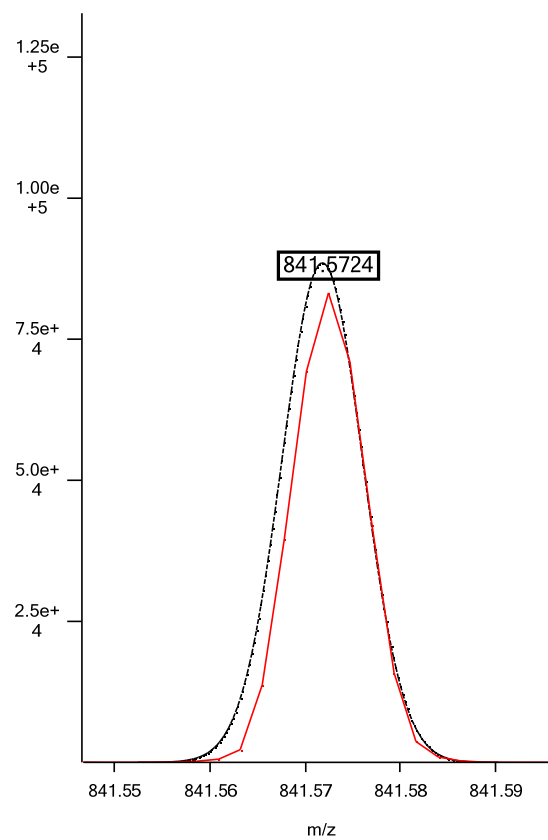


Positive ESI: PS 40:4; C₄₆H₈₃NO₁₀P; theoretical *m/z* 840.5754, (M+H)⁺; isotopic fit 0.0050

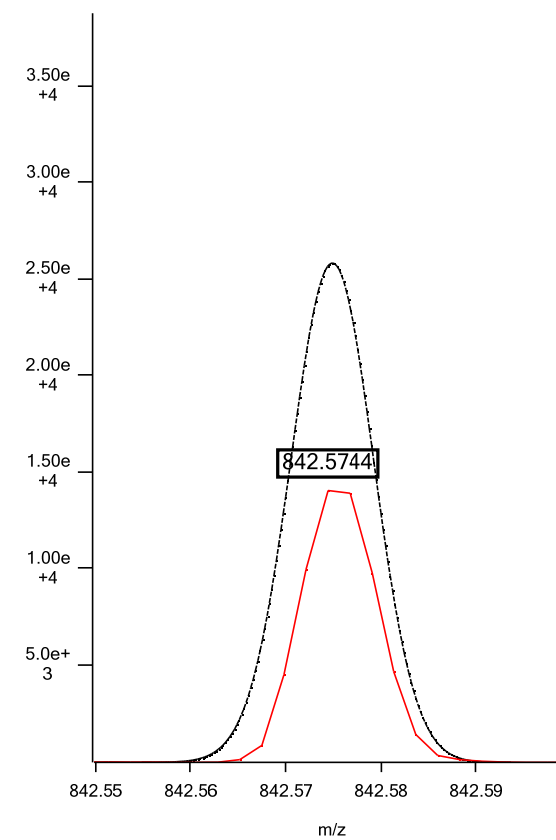
Isotope 1



Isotope 2



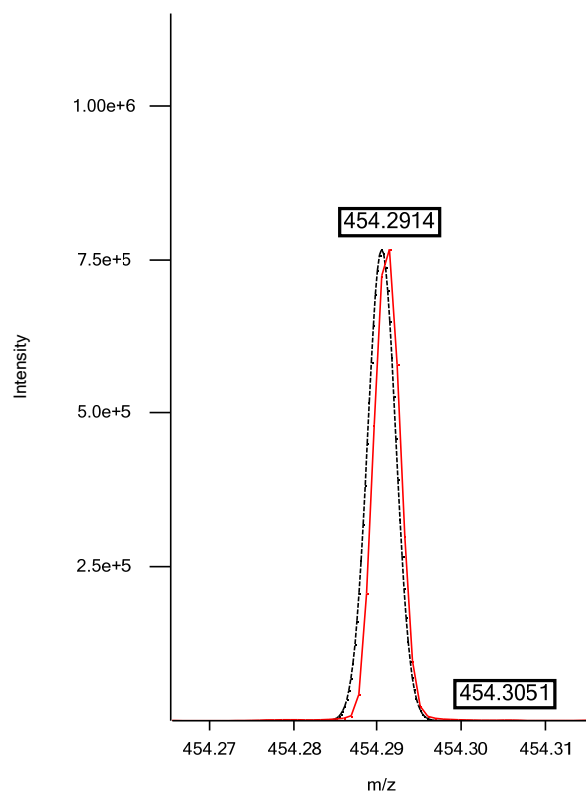
Isotope 3



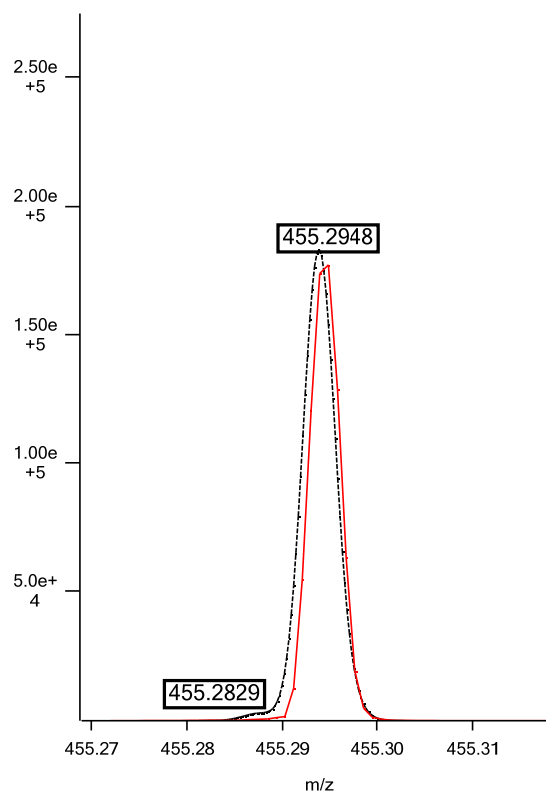
Glycerophosphoethanolamines

Positive ESI: LPE 16:0; C₂₁H₄₅NO₇P; theoretical *m/z* 454.2934, (M+H)⁺; isotopic fit 0.0091

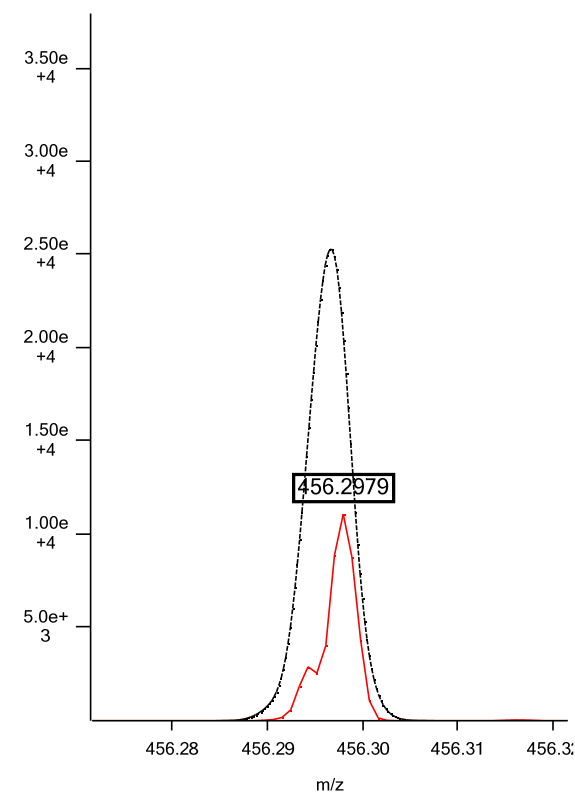
Isotope 1



Isotope 2

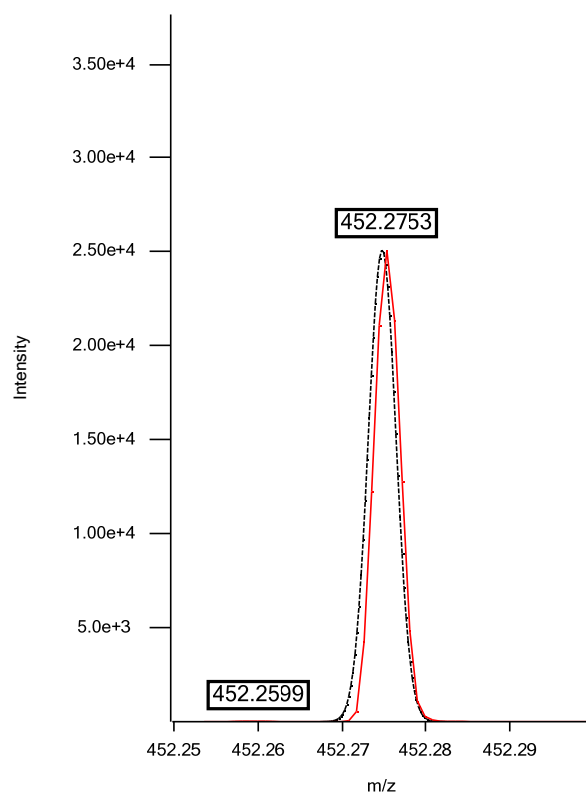


Isotope 3

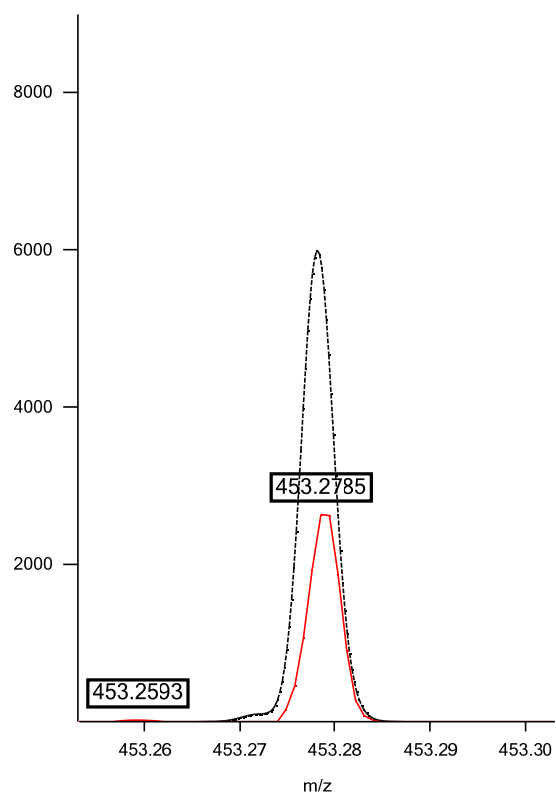


Positive ESI: LPE 16:1; C₂₁H₄₃NO₇P; theoretical *m/z* 452.2777, (M+H)⁺; isotopic fit 0.0379

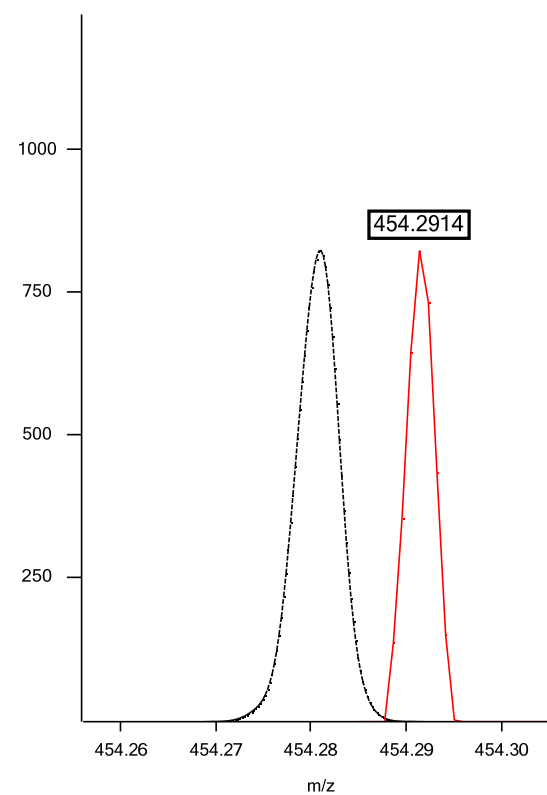
Isotope 1



Isotope 2

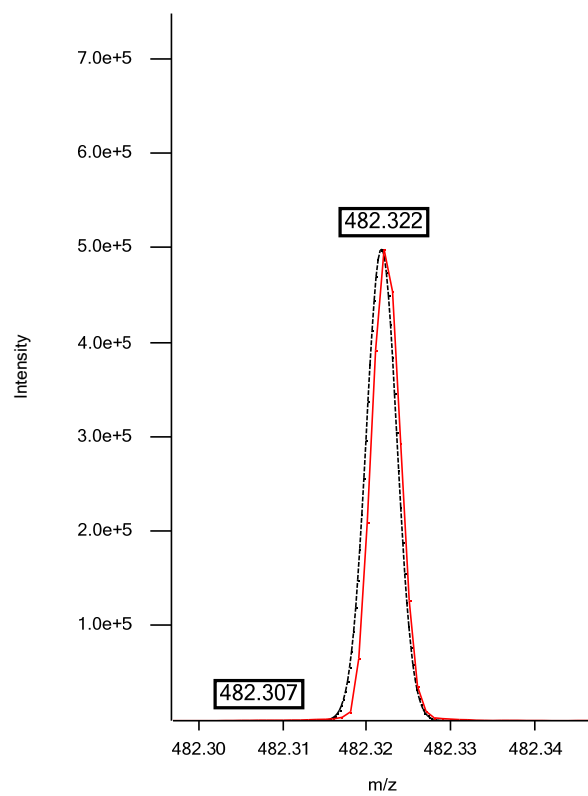


Isotope 3

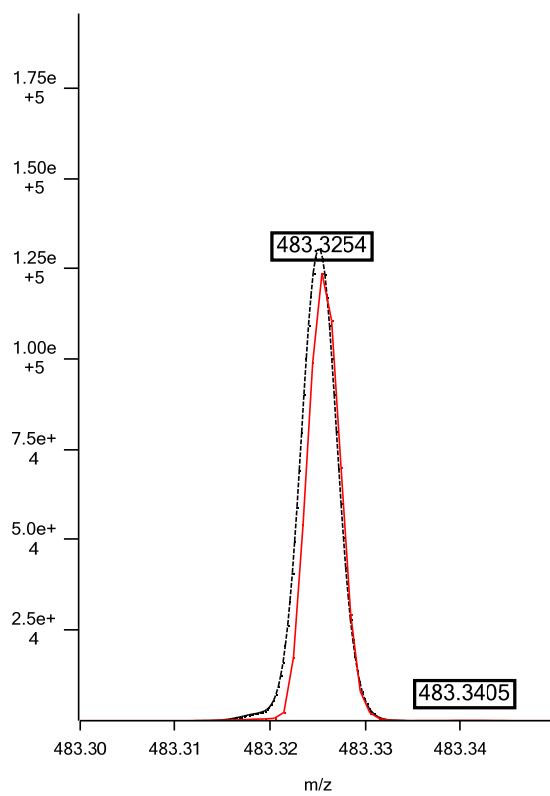


Positive ESI: LPE 18:0; C₂₃H₄₉NO₇P; theoretical *m/z* 482.3247, (M+H)⁺; isotopic fit 0.0193

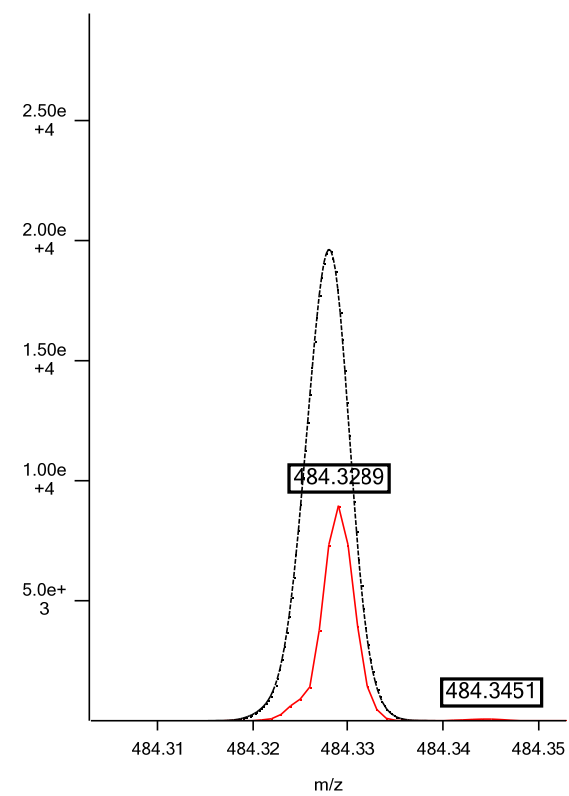
Isotope 1



Isotope 2

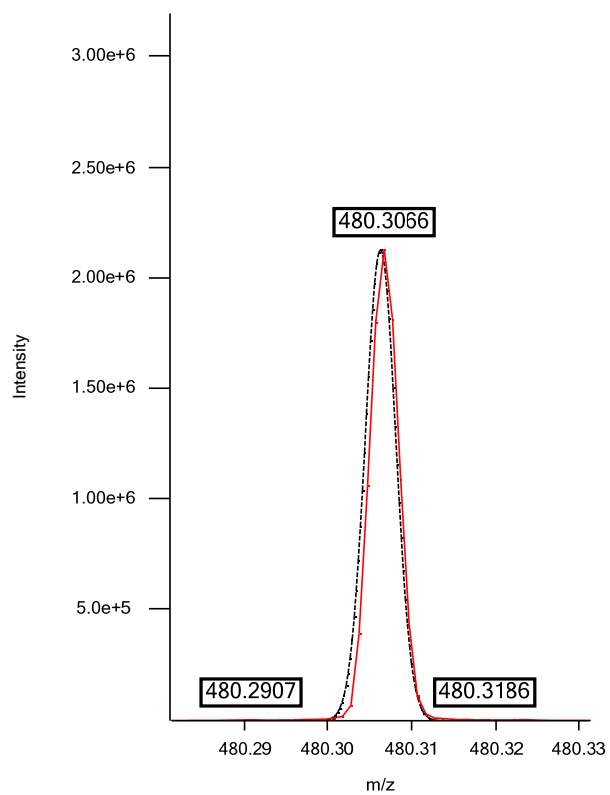


Isotope 3

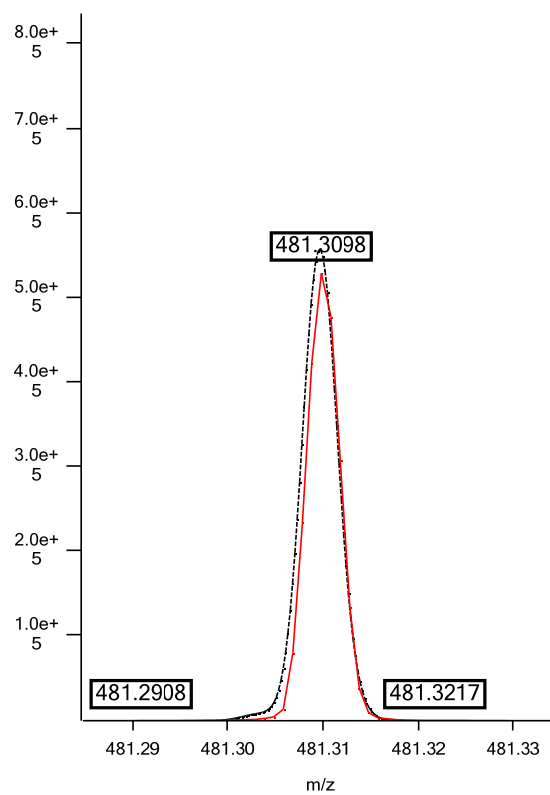


Positive ESI: LPE 18:1; $C_{23}H_{47}NO_7P$; theoretical m/z 480.3090, $(M+H)^+$; isotopic fit 0.0076

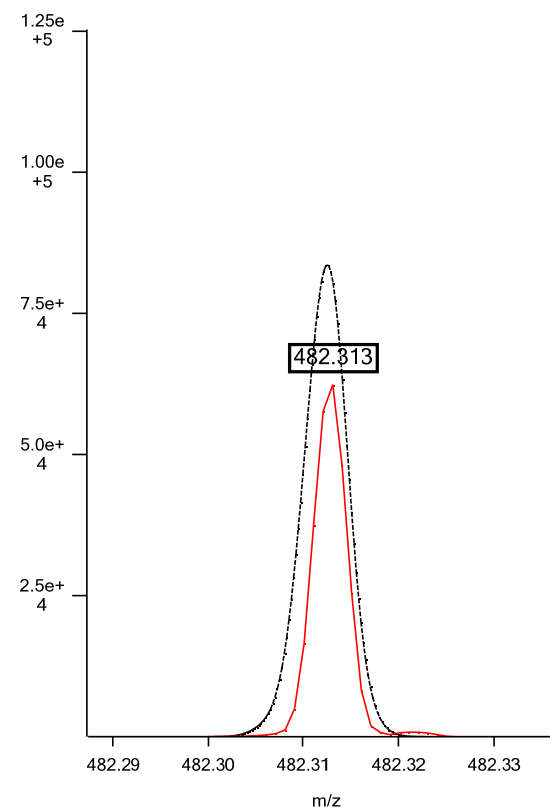
Isotope 1



Isotope 2

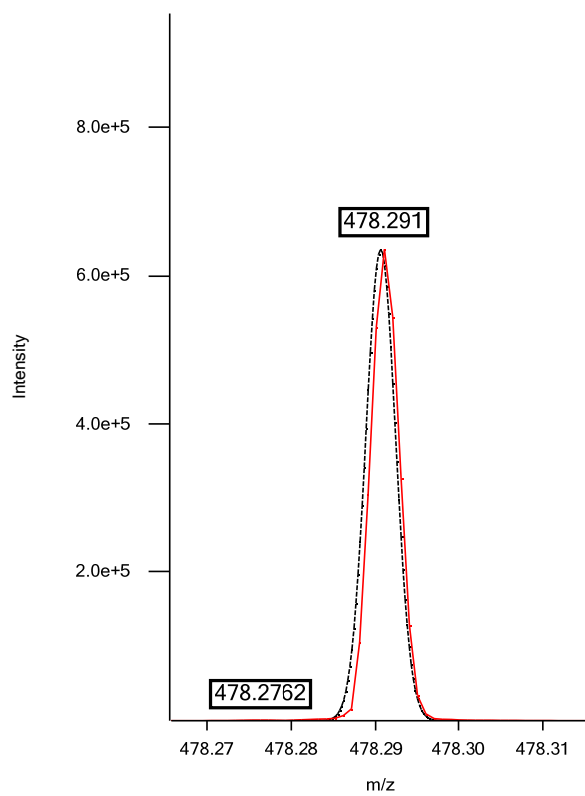


Isotope 3

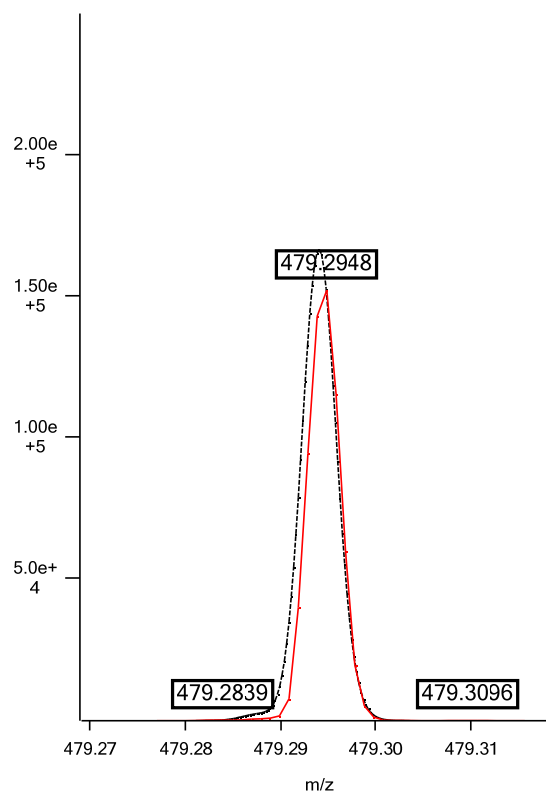


Positive ESI: LPE 18:2; C₂₃H₄₅NO₇P; theoretical *m/z* 478.2934, (M+H)⁺; isotopic fit 0.0036

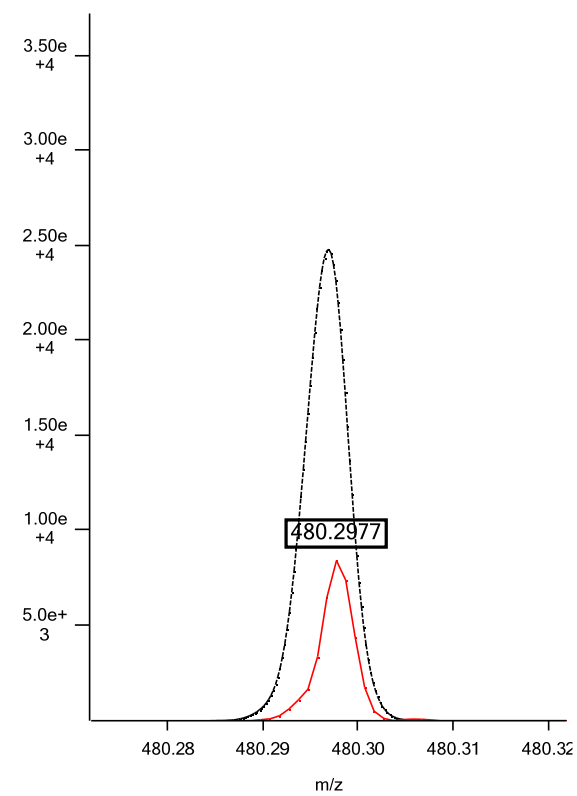
Isotope 1



Isotope 2

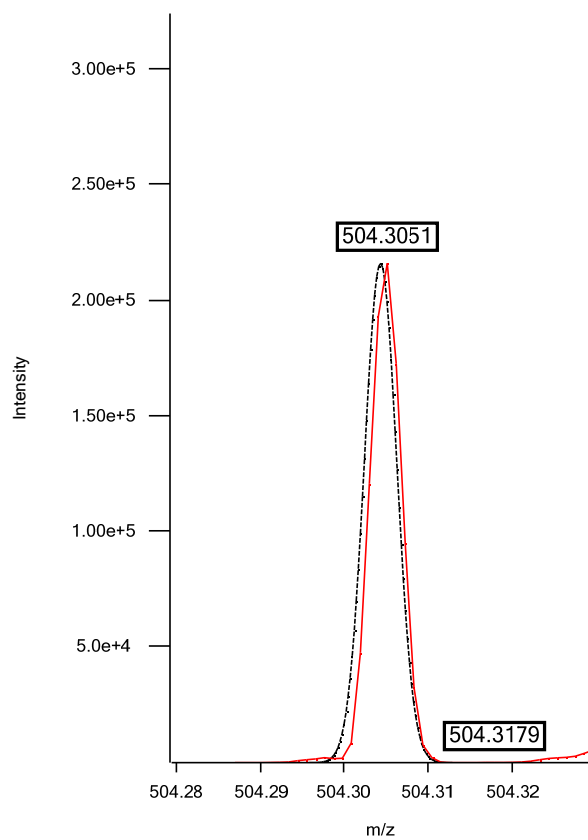


Isotope 3

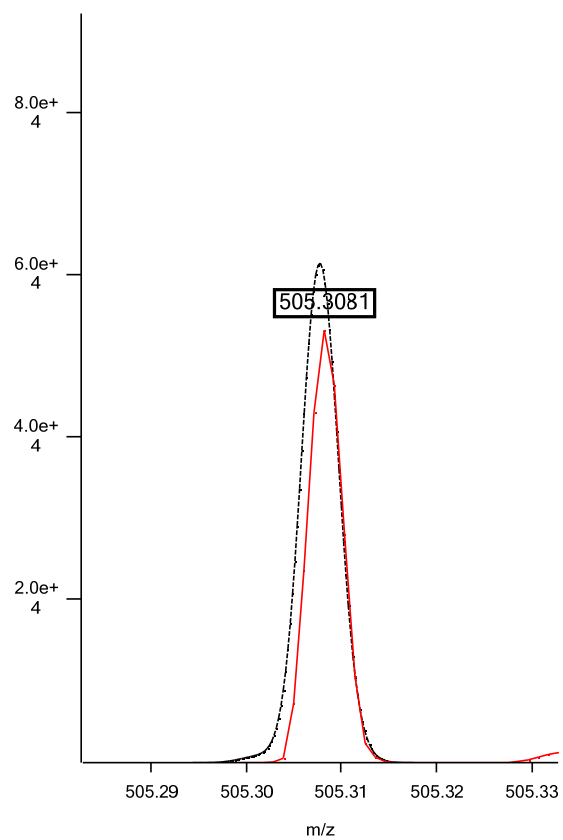


Positive ESI: LPE 20:3; C₂₅H₄₇NO₇P; theoretical m/z 504.3090, (M+H)⁺; isotopic fit 0.0125

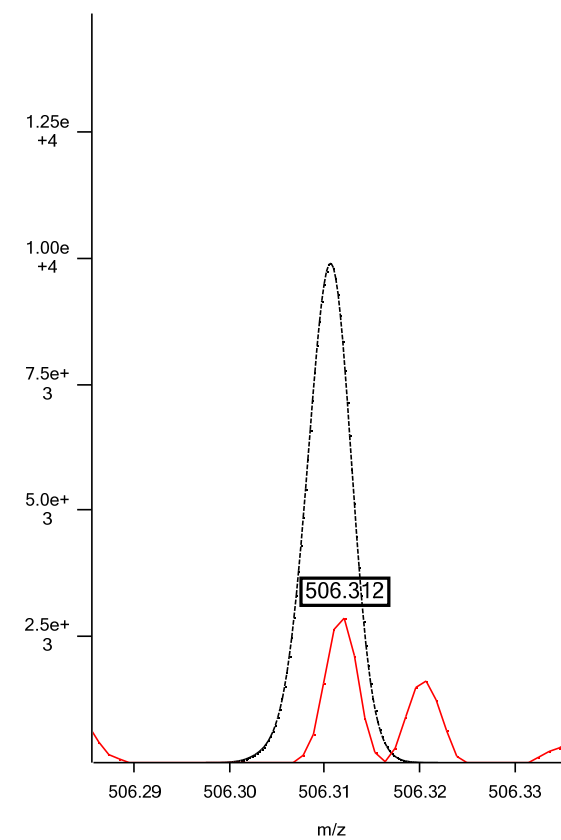
Isotope 1



Isotope 2

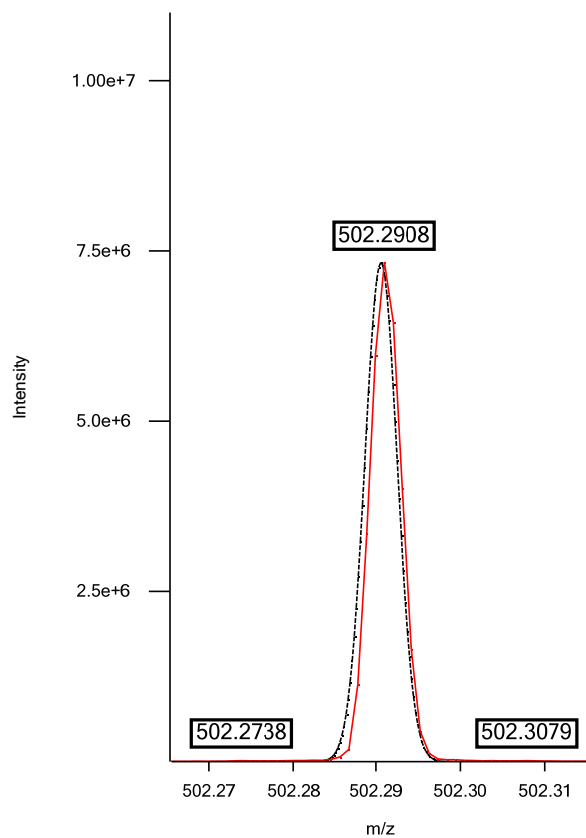


Isotope 3

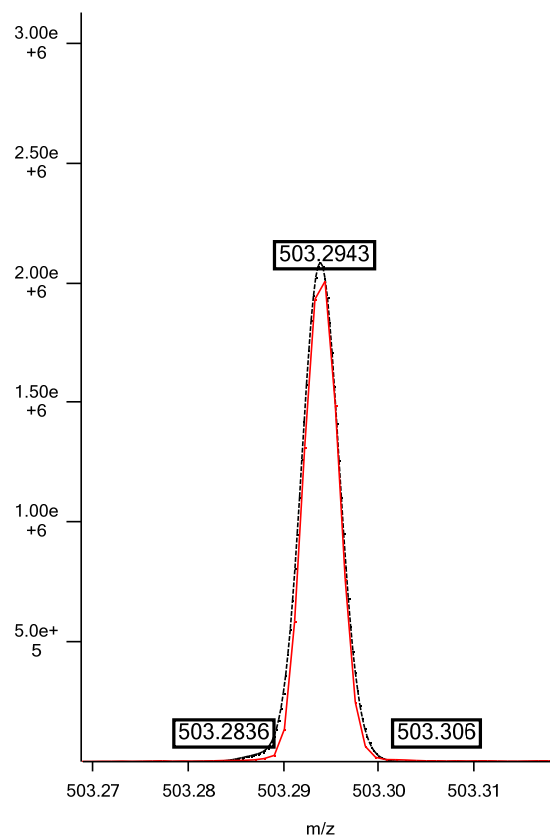


Positive ESI: LPE 20:4; C₂₅H₄₅NO₇P; theoretical *m/z* 502.2934, (M+H)⁺; isotopic fit 0.0226

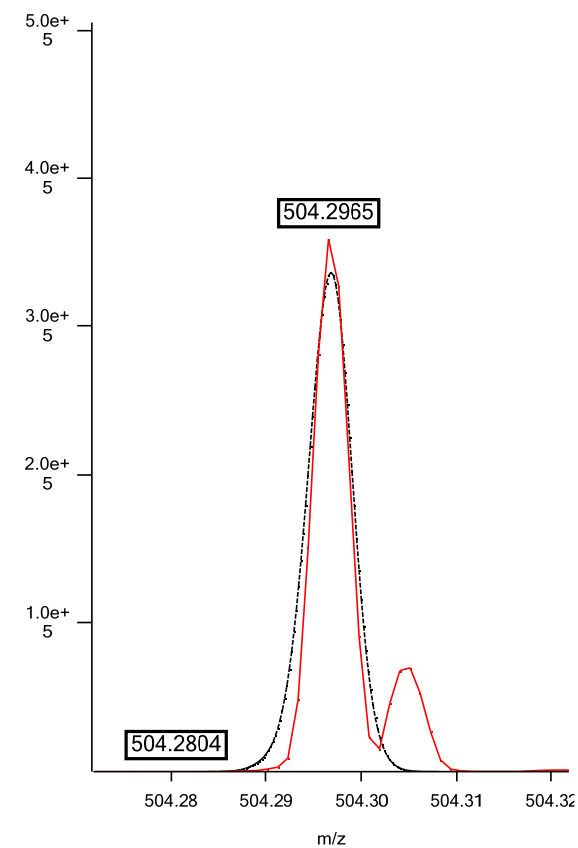
Isotope 1



Isotope 2

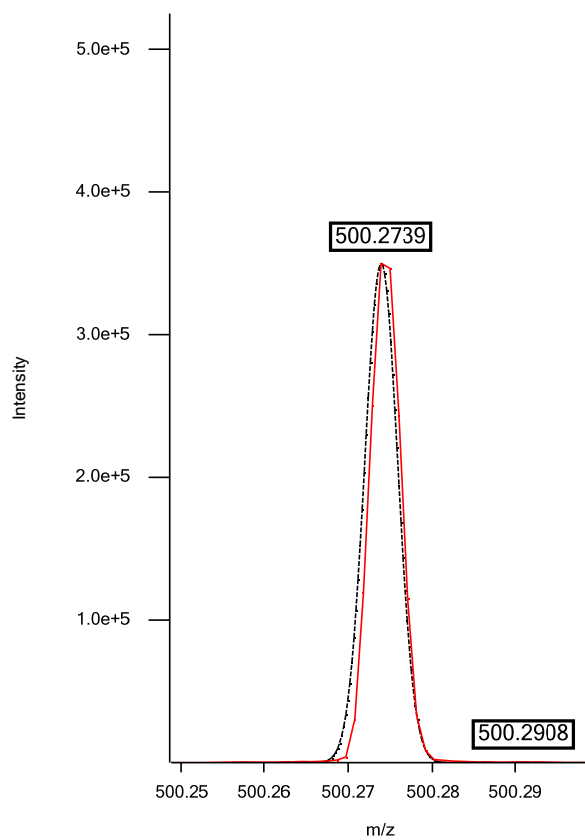


Isotope 3

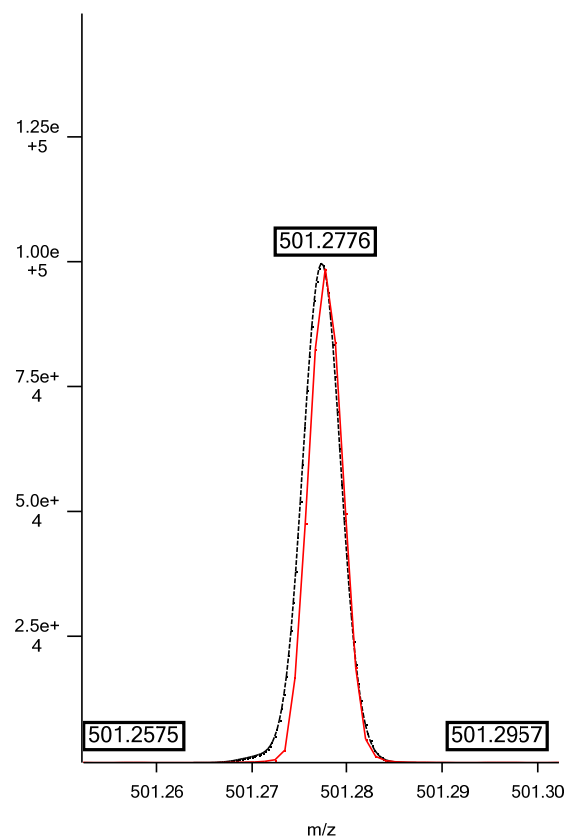


Positive ESI: LPE 20:5; C₂₅H₄₃NO₇P; theoretical *m/z* 500.2777, (M+H)⁺; isotopic fit 0.0099

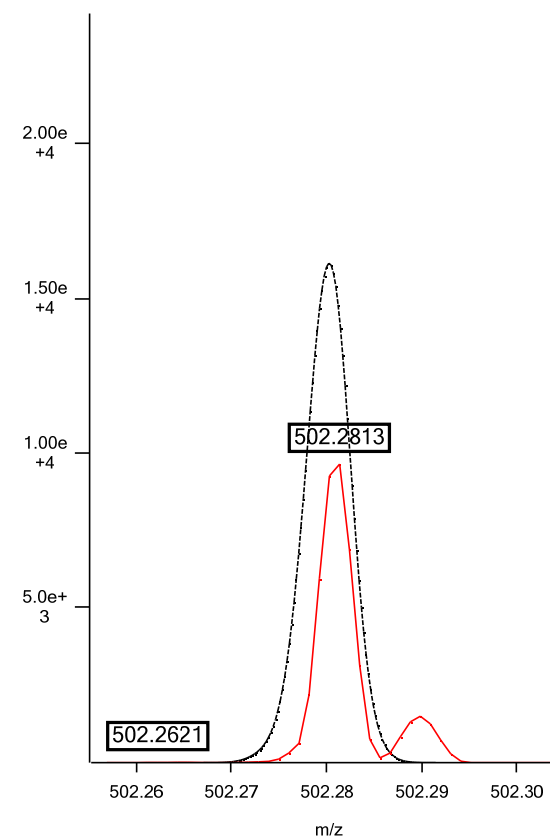
Isotope 1



Isotope 2

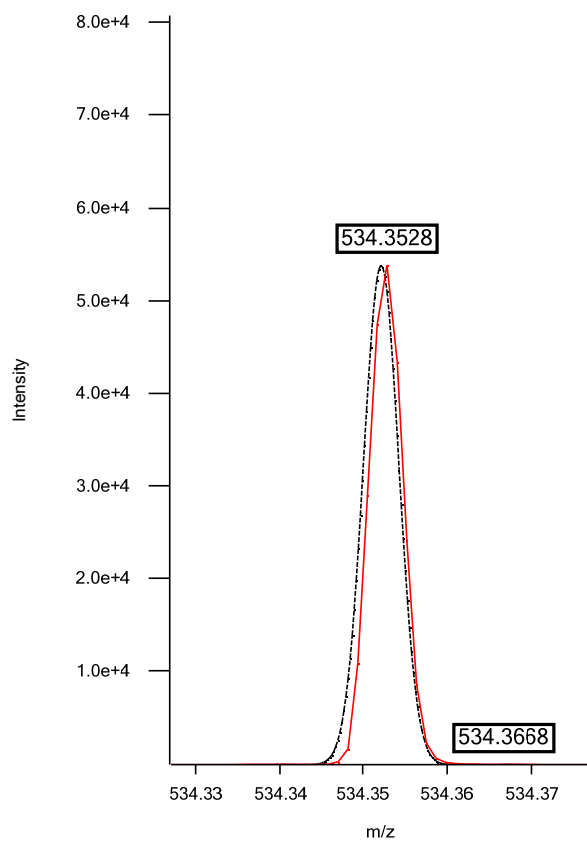


Isotope 3

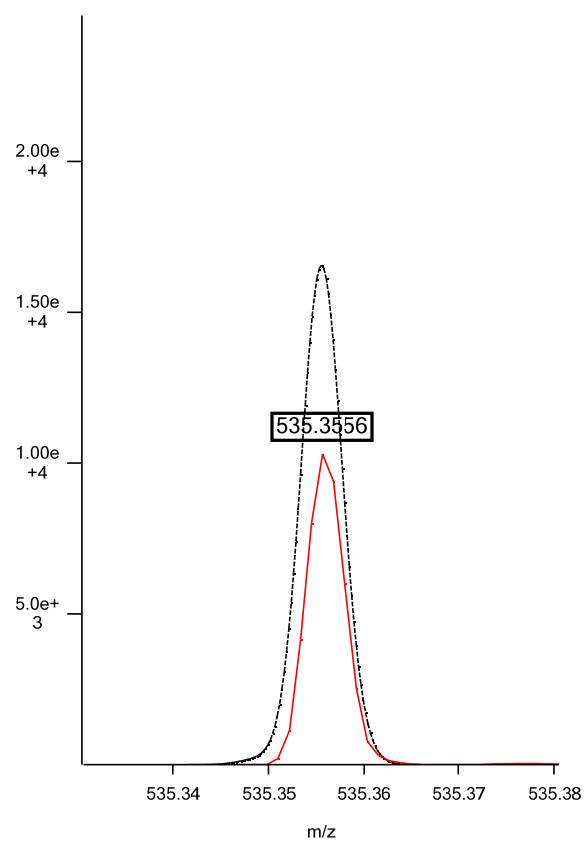


Positive ESI: LPE 22:2; C₂₇H₅₃NO₇P; theoretical *m/z* 534.3560, (M+H)⁺; isotopic fit 0.0316

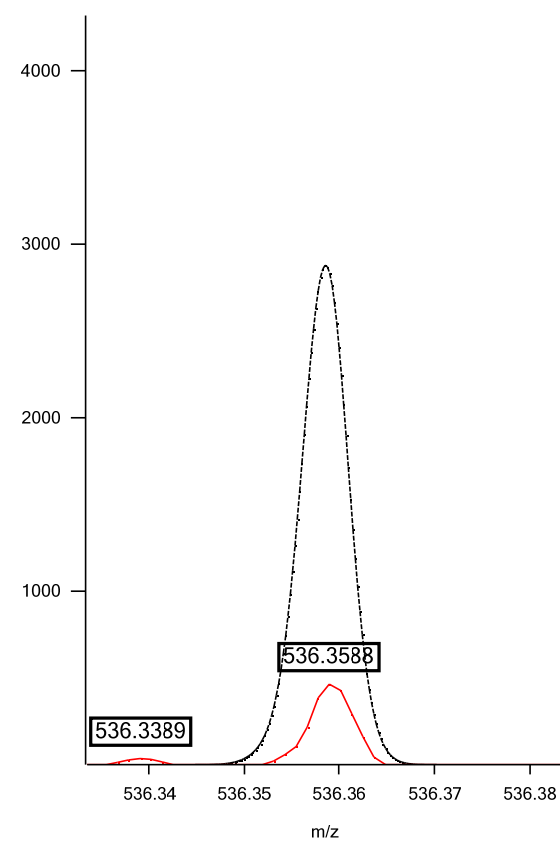
Isotope 1



Isotope 2

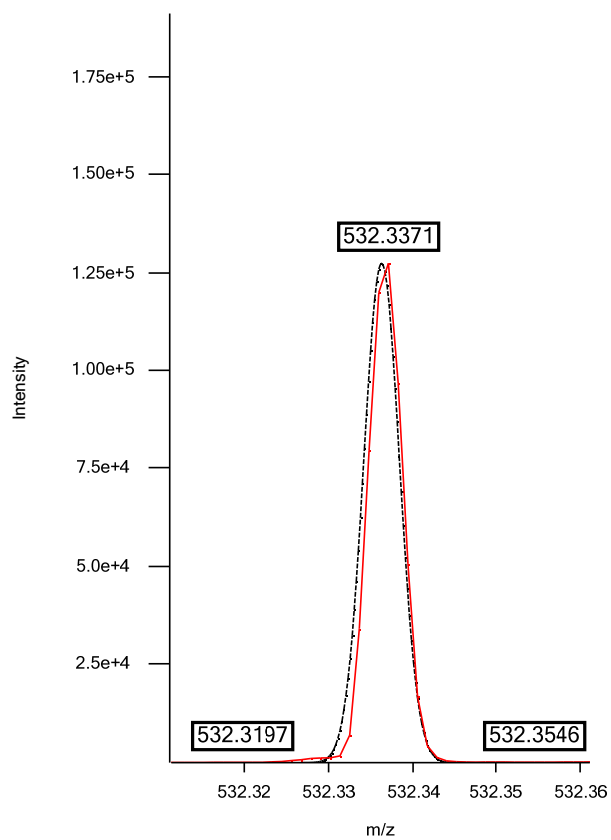


Isotope 3

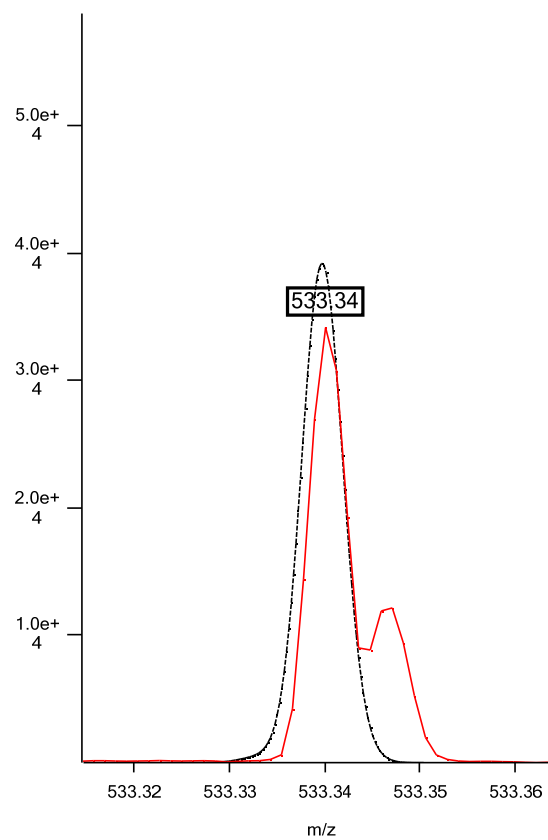


Positive ESI: LPE 22:3; C₂₇H₅₁NO₇P; theoretical m/z 532.3403, (M+H)⁺; isotopic fit 0.0111

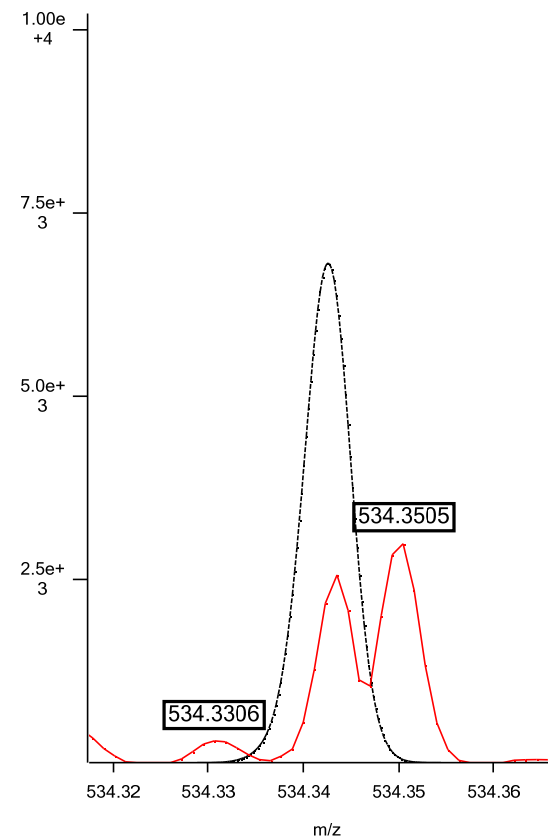
Isotope 1



Isotope 2

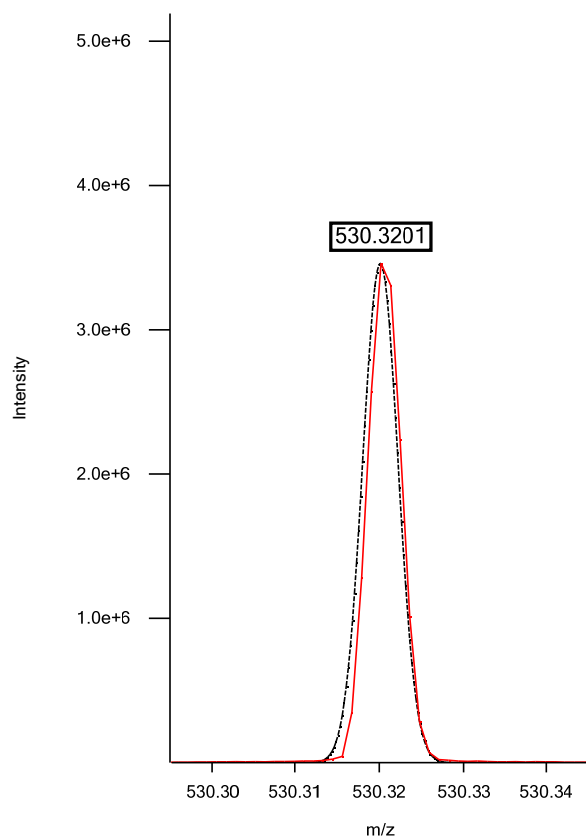


Isotope 3

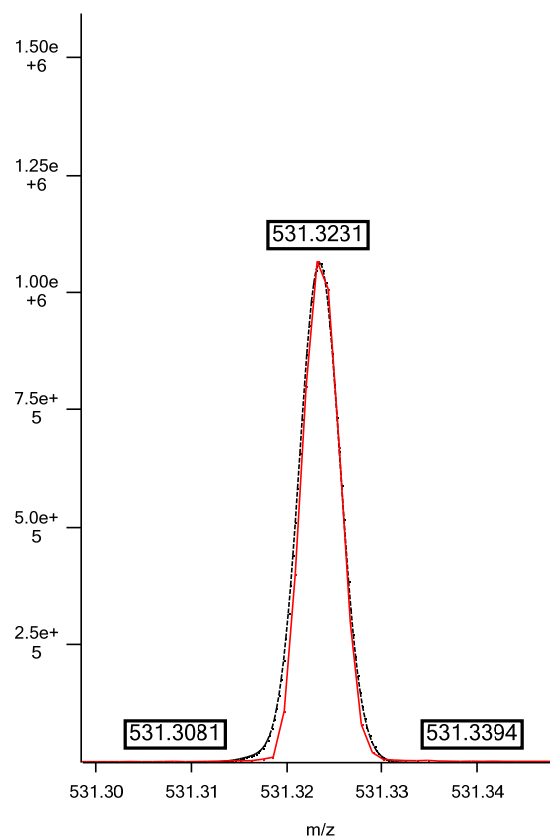


Positive ESI: LPE 22:4; C₂₇H₄₉NO₇P; theoretical *m/z* 530.3247, (M+H)⁺; isotopic fit 0.0023

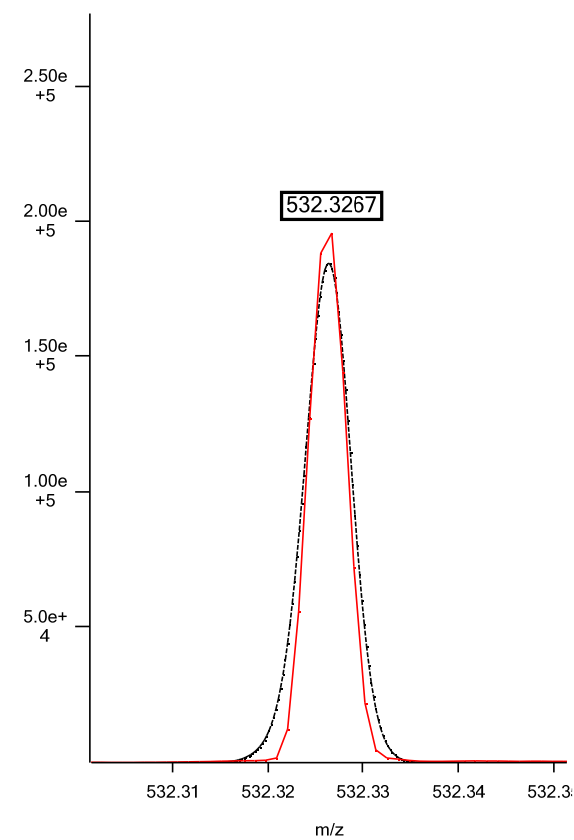
Isotope 1



Isotope 2

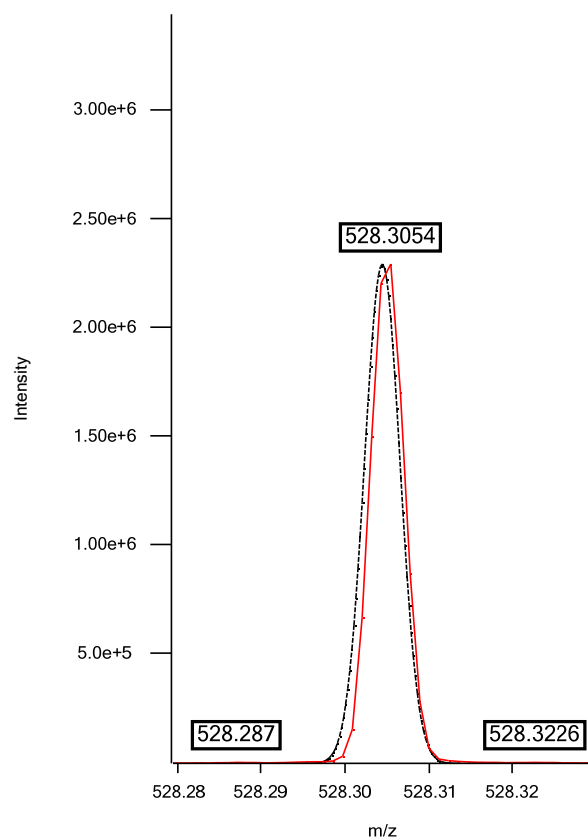


Isotope 3

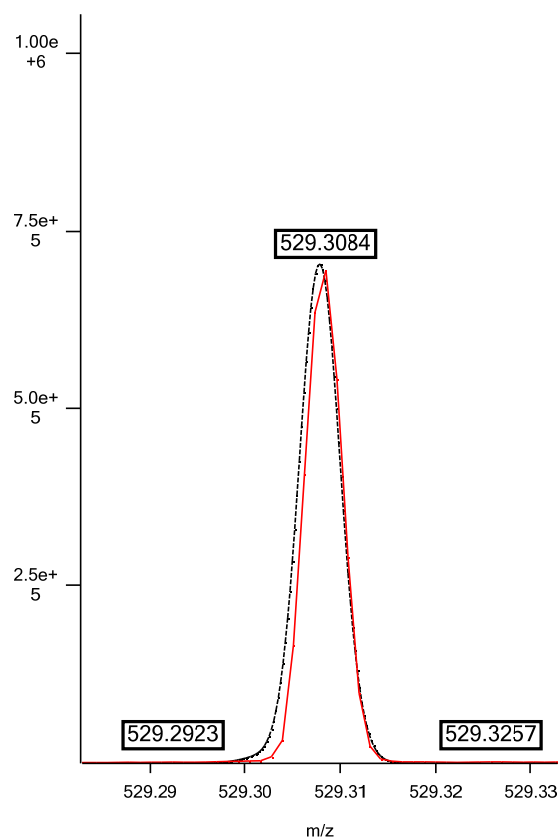


Positive ESI: LPE 22:5; C₂₇H₄₇NO₇P; theoretical *m/z* 528.3090, (M+H)⁺; isotopic fit 0.0013

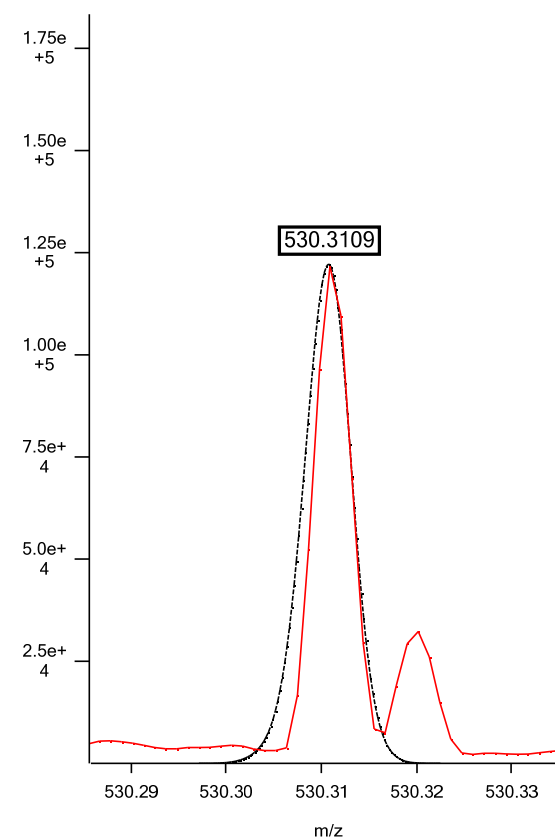
Isotope 1



Isotope 2

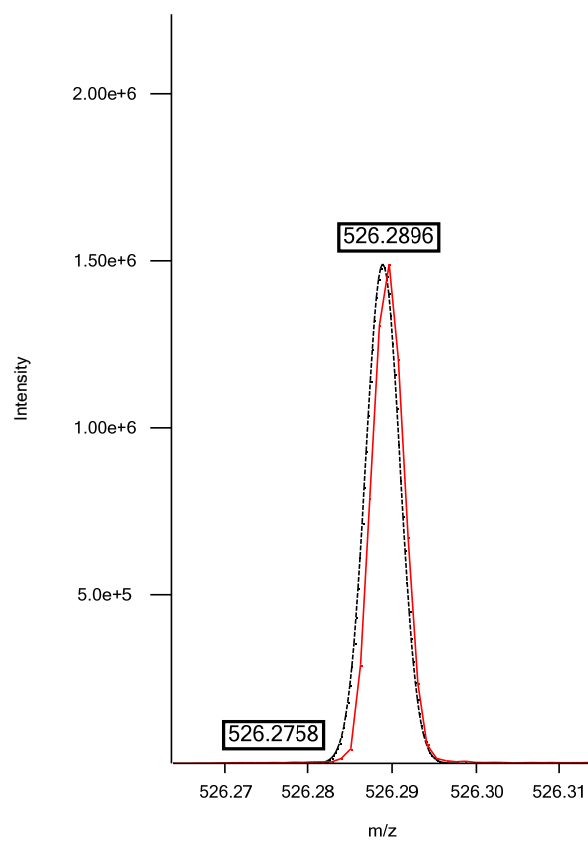


Isotope 3

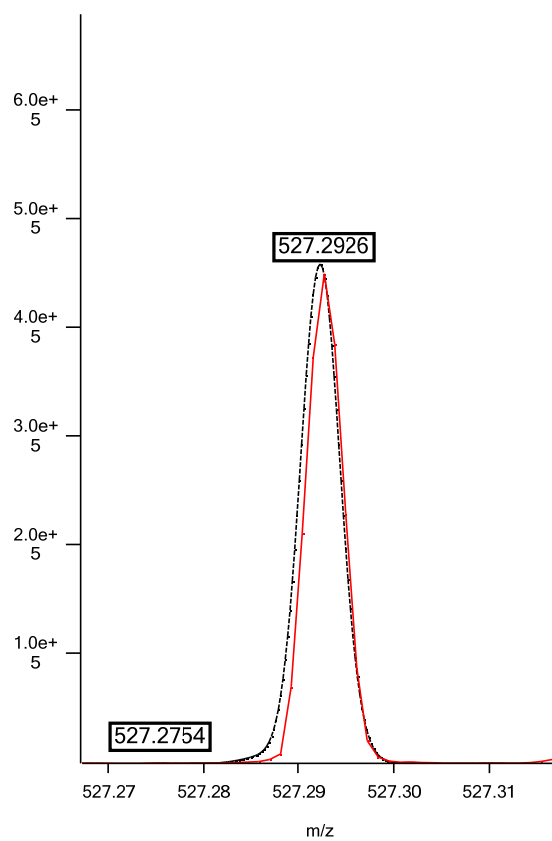


Positive ESI: LPE 22:6; C₂₇H₄₅NO₇P; theoretical *m/z* 526.2934, (M+H)⁺; isotopic fit 0.0032

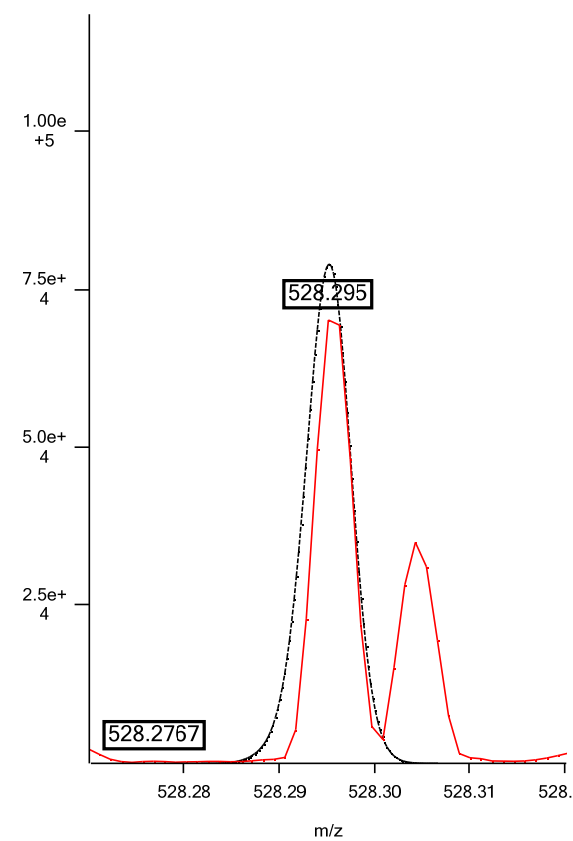
Isotope 1



Isotope 2

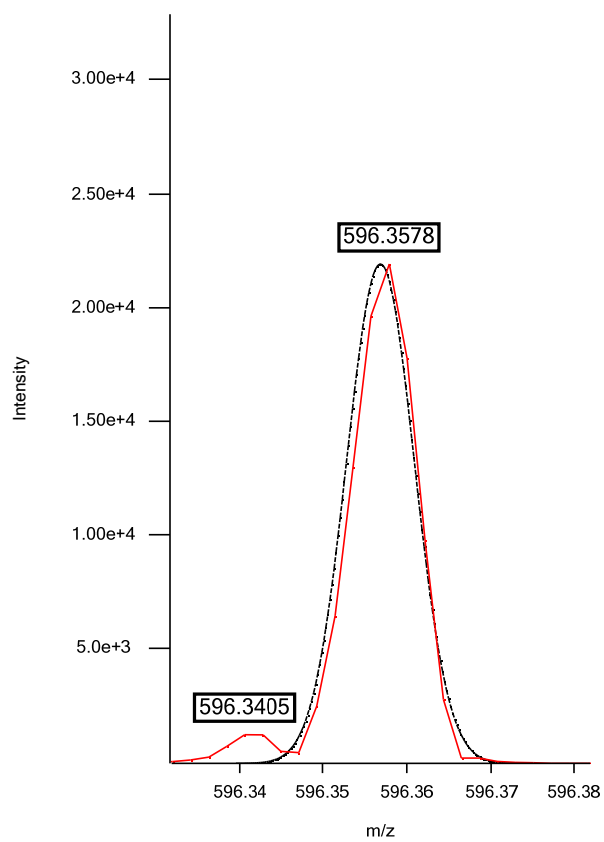


Isotope 3

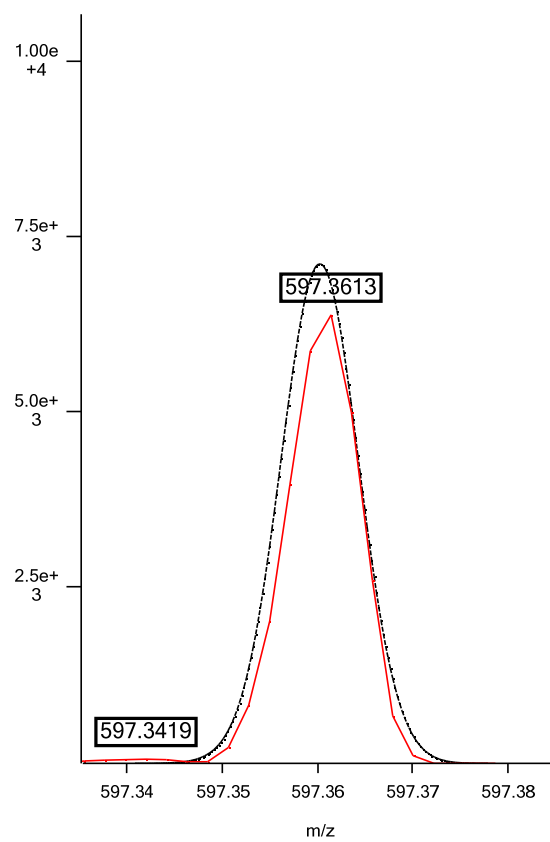


Negative ESI: Oxidized PE 18:0/Dihydroxy-5:0 or 18:0/Hydroperoxy-5:0; $C_{28}H_{55}NO_{10}P$; theoretical m/z 596.3563, (M-H)⁻; isotopic fit 0.0036

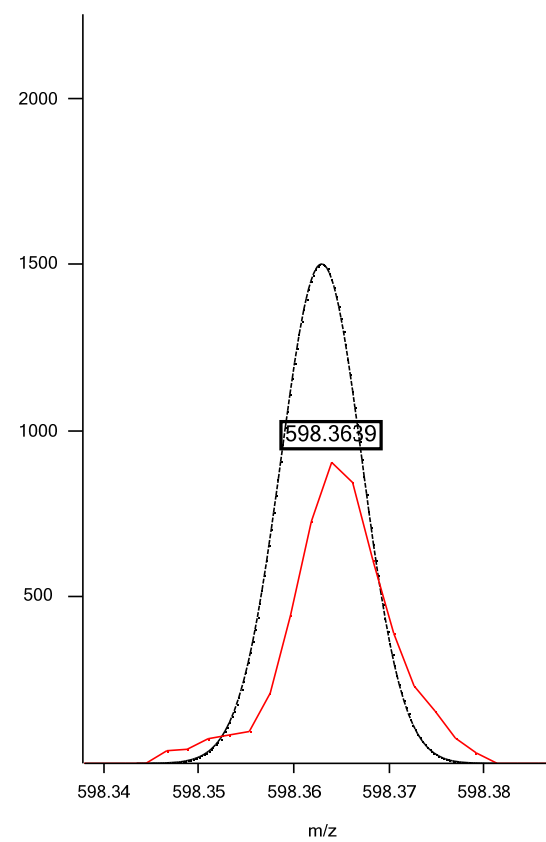
Isotope 1



Isotope 2

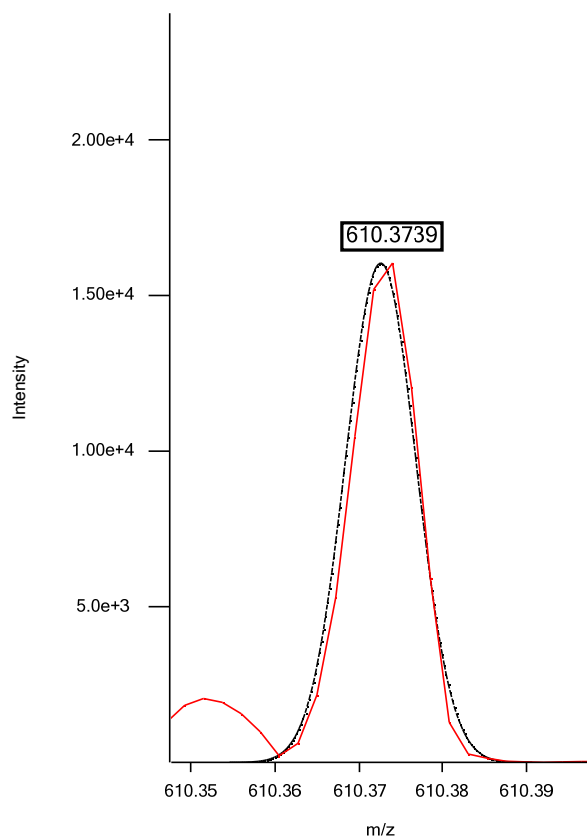


Isotope 3

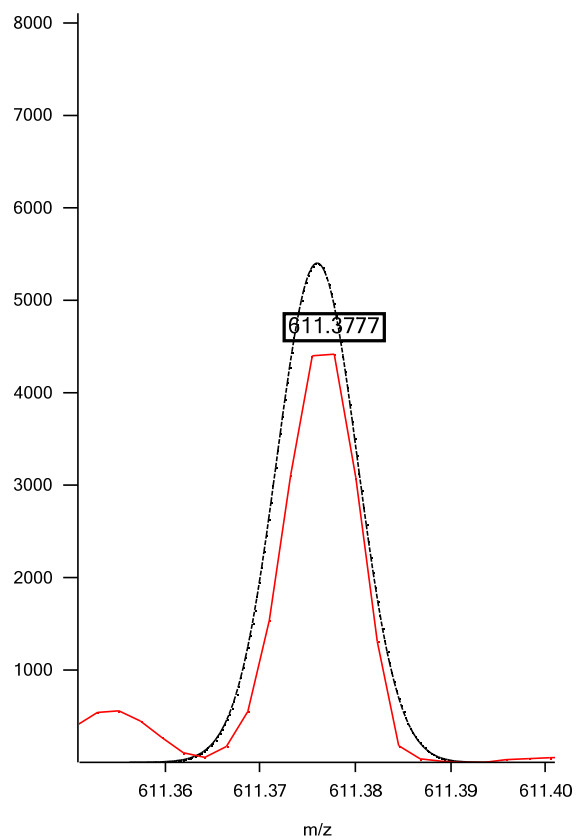


Negative ESI: Oxidized PE 18:0/Dihydroxy-6:0; $C_{29}H_{57}NO_{10}P$; theoretical m/z 610.3720, (M-H)⁻; isotopic fit 0.0048

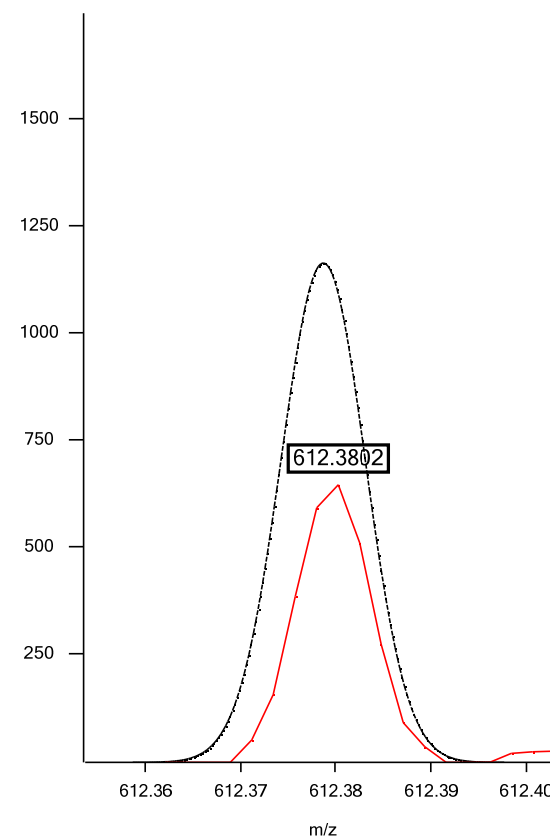
Isotope 1



Isotope 2

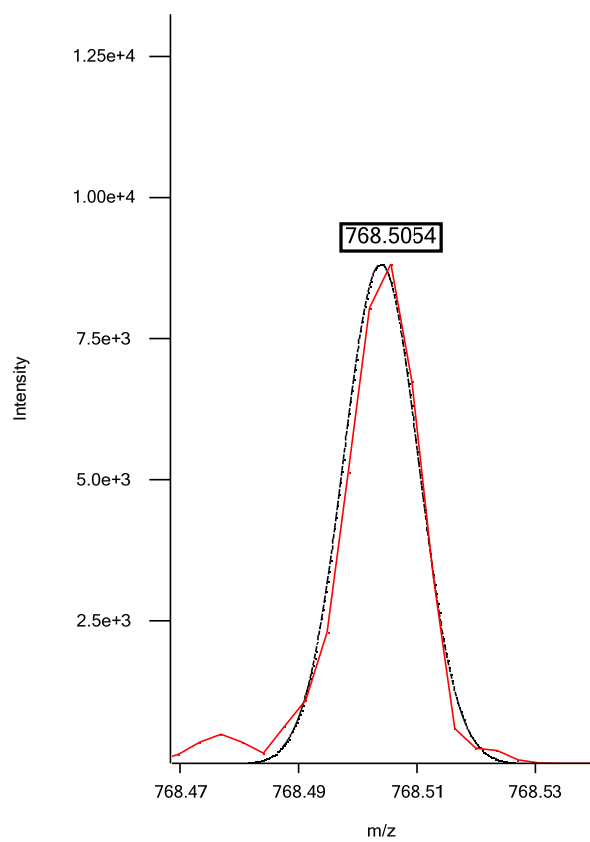


Isotope 3

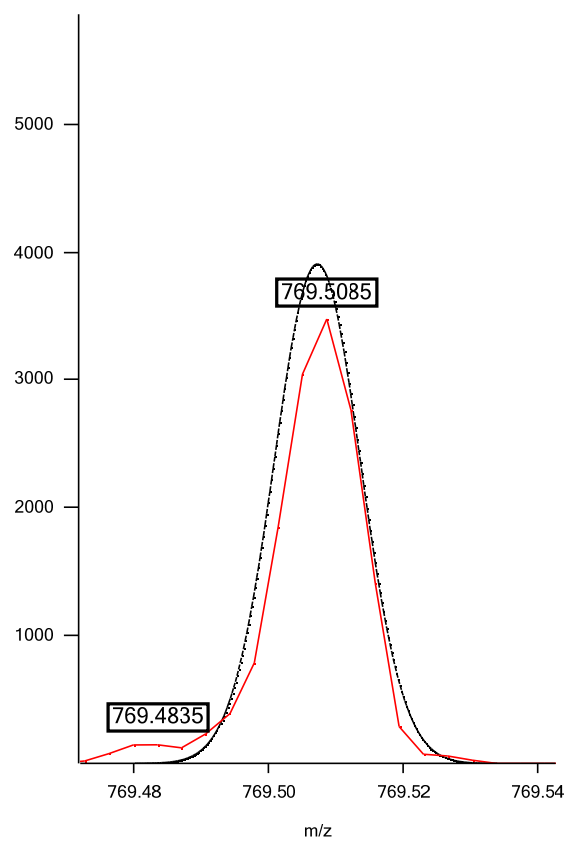


Negative ESI: Oxidized PE 16:0/ Tetrahydroxy-17:1; $C_{38}H_{75}NO_{12}P$; theoretical m/z 768.5027, (M-H)⁻; isotopic fit 0.0057

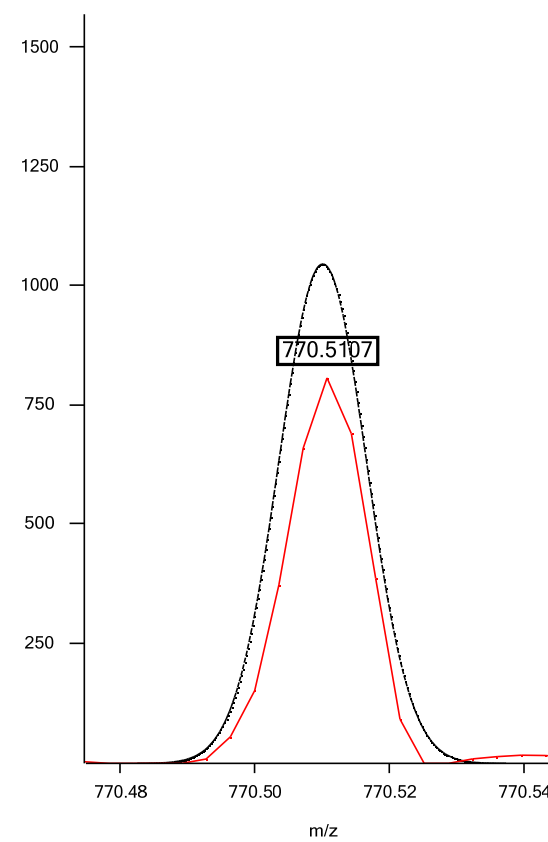
Isotope 1



Isotope 2

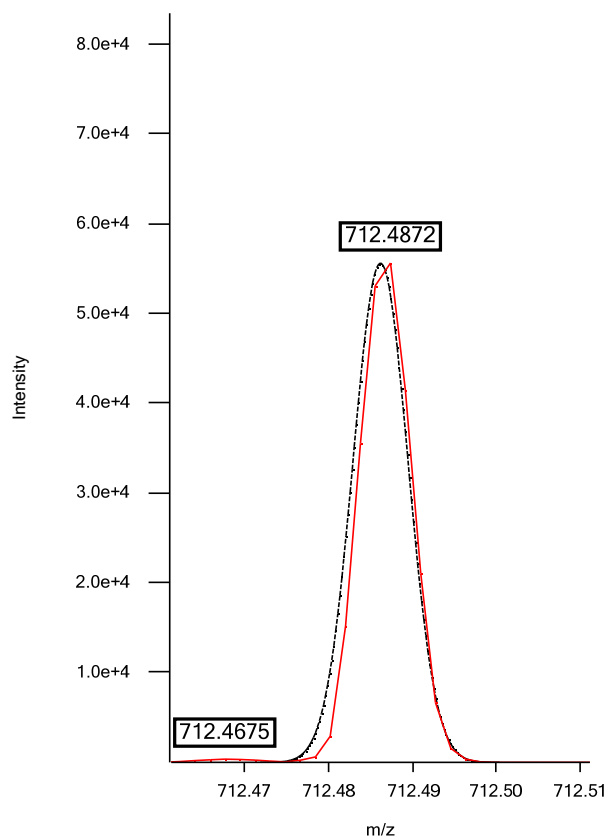


Isotope 3

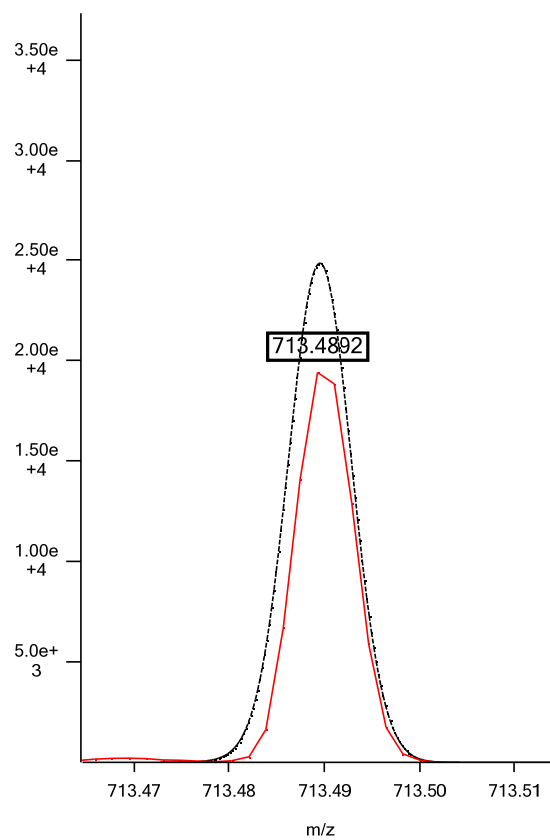


Positive ESI: PE 34:4; C₃₉H₇₁NO₈P; theoretical m/z 712.4917, (M+H)⁺; isotopic fit 0.0132

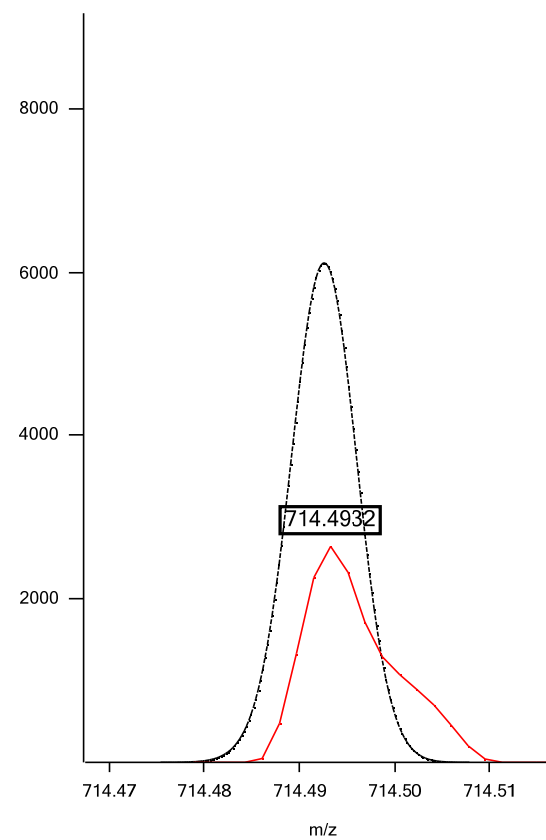
Isotope 1



Isotope 2

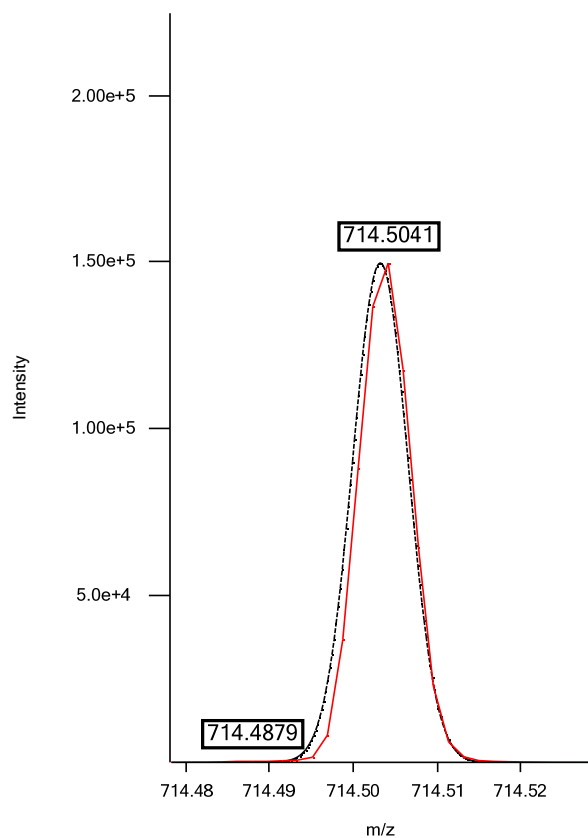


Isotope 3

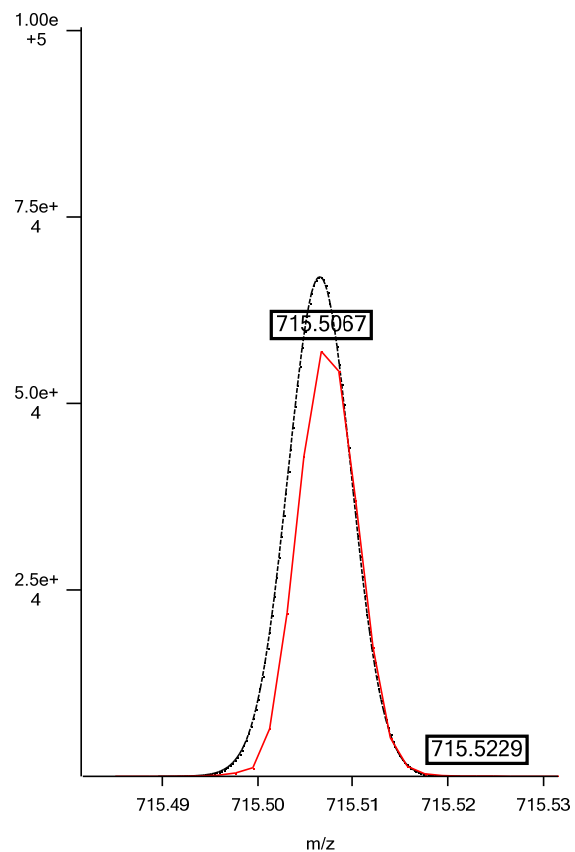


Positive ESI: PE 34:3; C₃₉H₇₃NO₈P; theoretical m/z 714.5074, (M+H)⁺; isotopic fit 0.0110

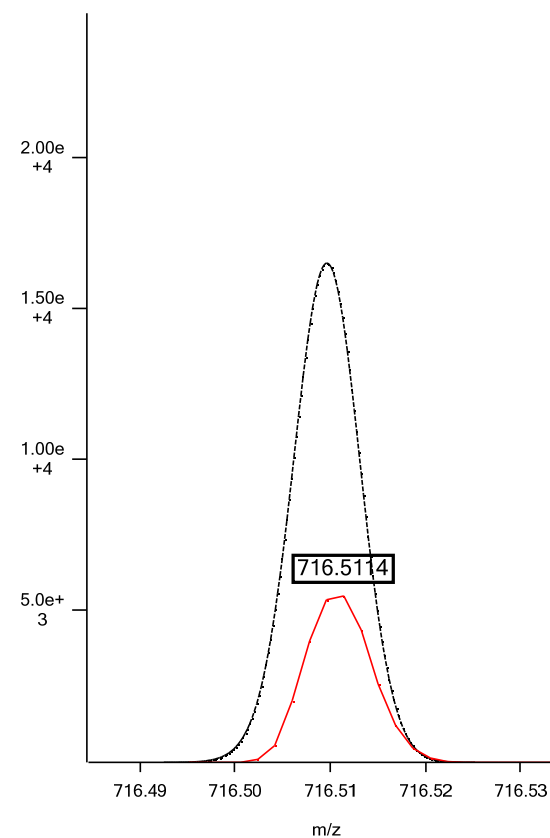
Isotope 1



Isotope 2

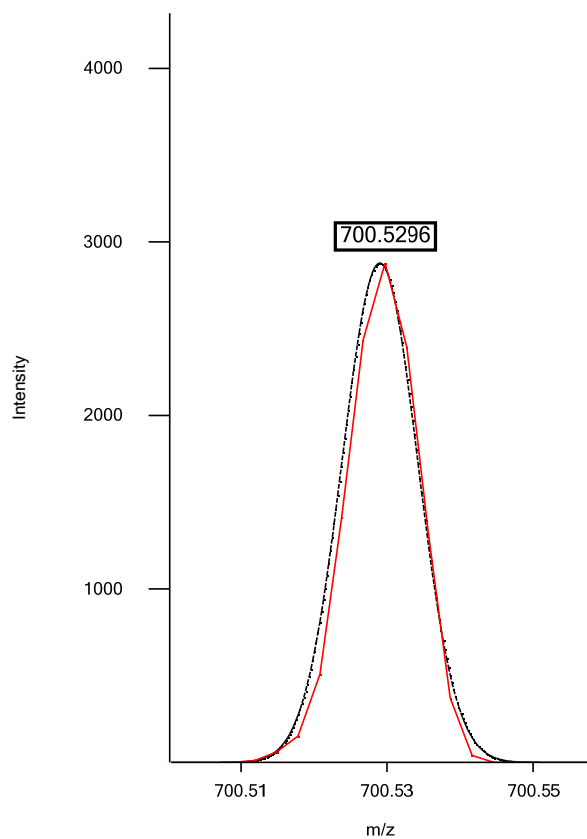


Isotope 3

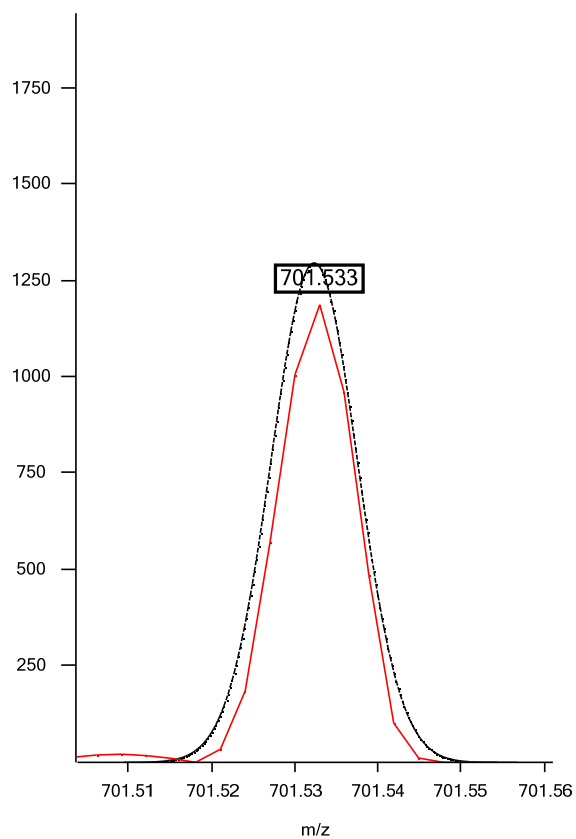


Negative ESI: PE 18:0p/16:1 or 16:0p/18:1; $C_{39}H_{75}NO_7P$; theoretical m/z 700.5281, (M-H)⁻; isotopic fit 0.0056

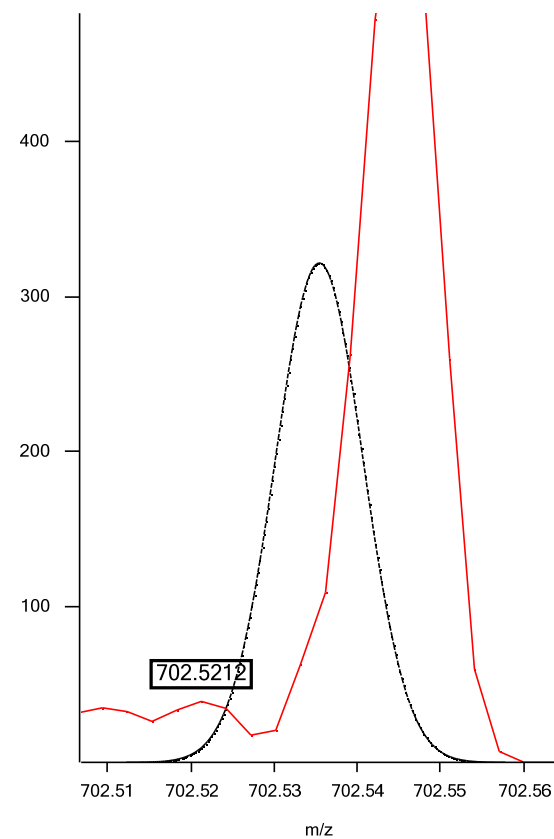
Isotope 1



Isotope 2

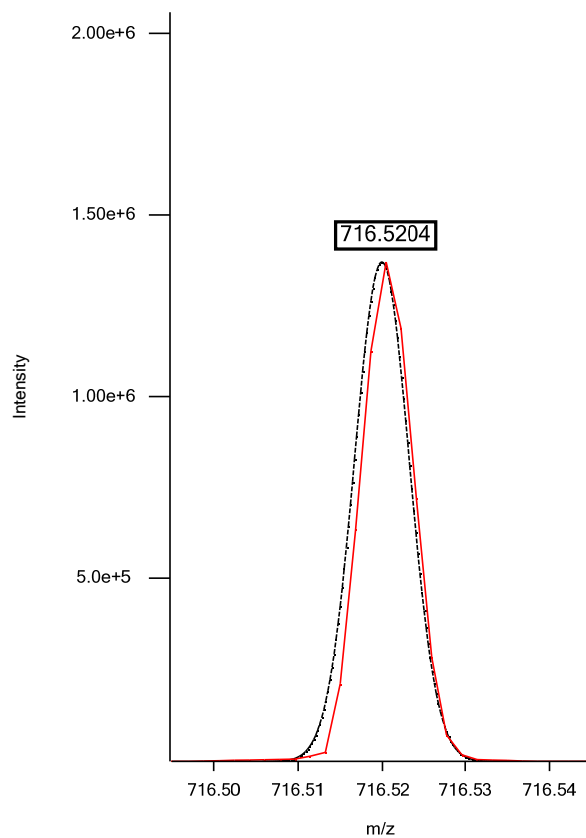


Isotope 3

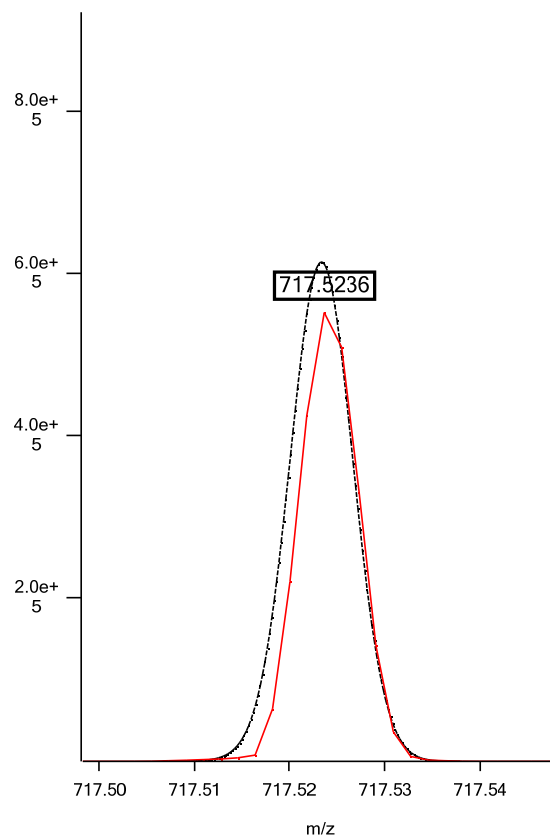


Positive ESI: PE 34:2; C₃₉H₇₅NO₈P; theoretical m/z 716.5230, (M+H)⁺; isotopic fit 0.0062

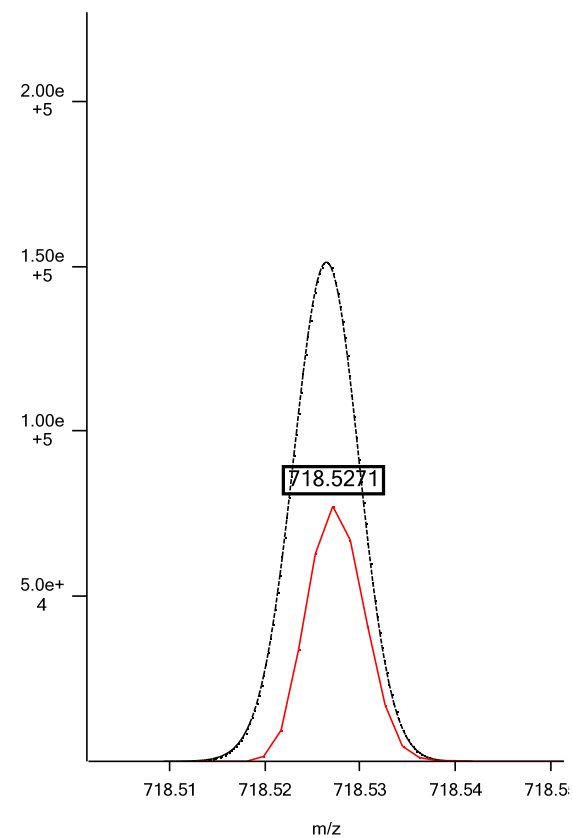
Isotope 1



Isotope 2

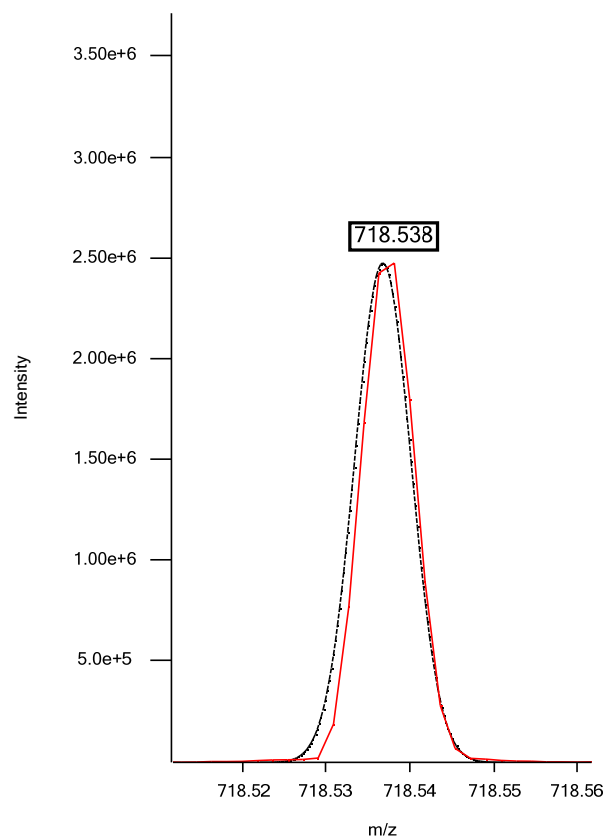


Isotope 3

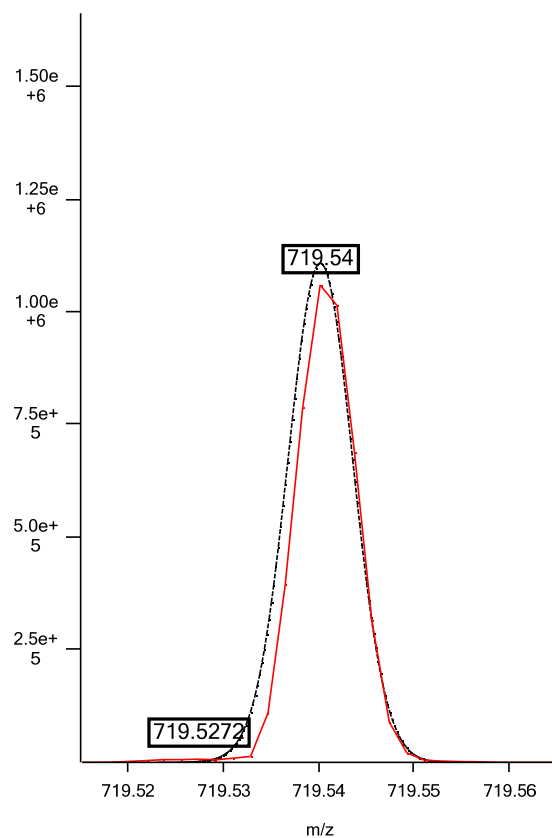


Positive ESI: PE 34:1; C₃₉H₇₇NO₈P; theoretical m/z 718.5387, (M+H)⁺; isotopic fit 0.0033

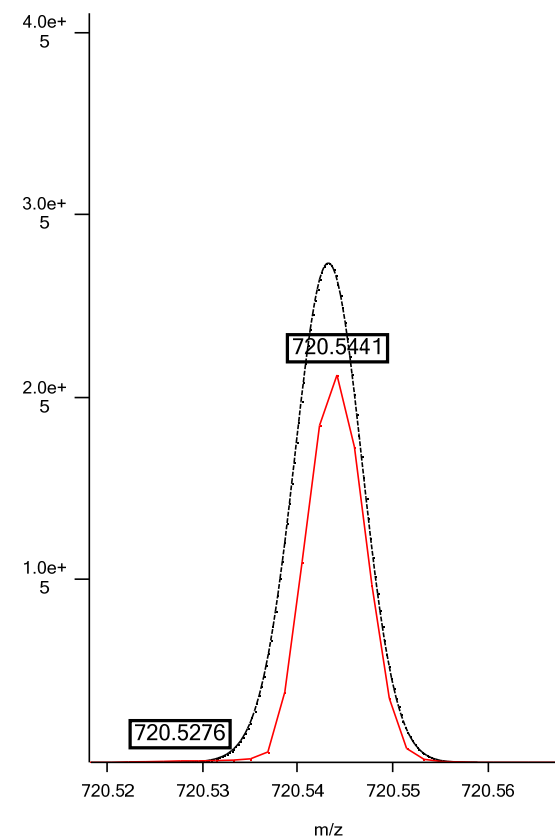
Isotope 1



Isotope 2

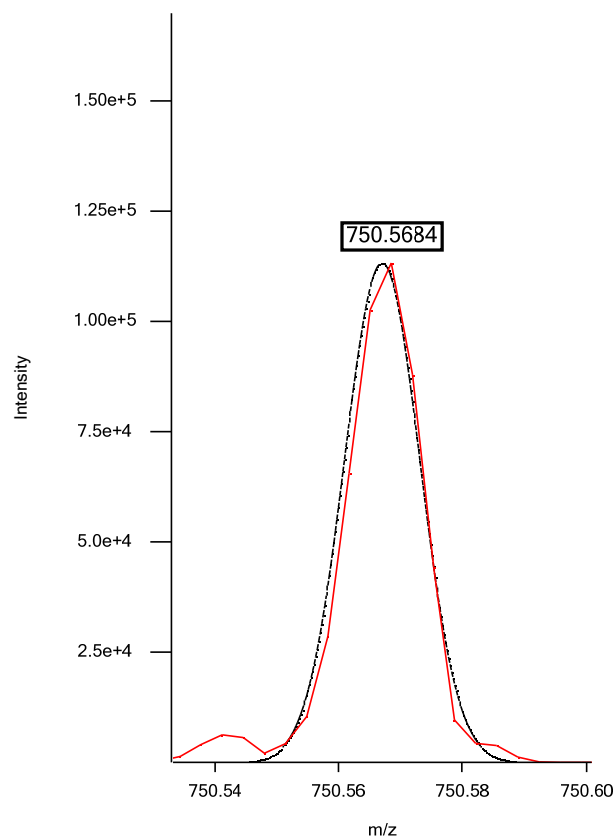


Isotope 3

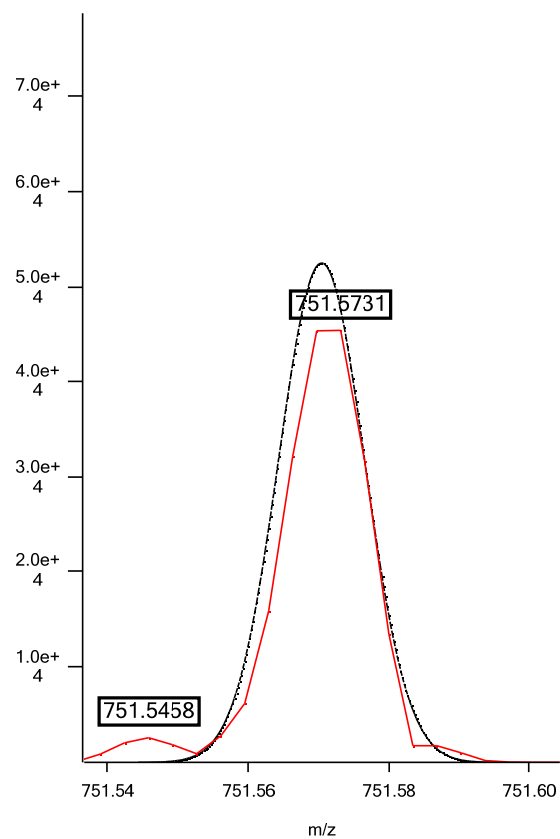


Negative ESI: Oxidized PE 16:0/Hydroperoxy-19:0; C₄₀H₈₁NO₉P; theoretical *m/z* 750.5649, (M-H)⁻; isotopic fit 0.0059

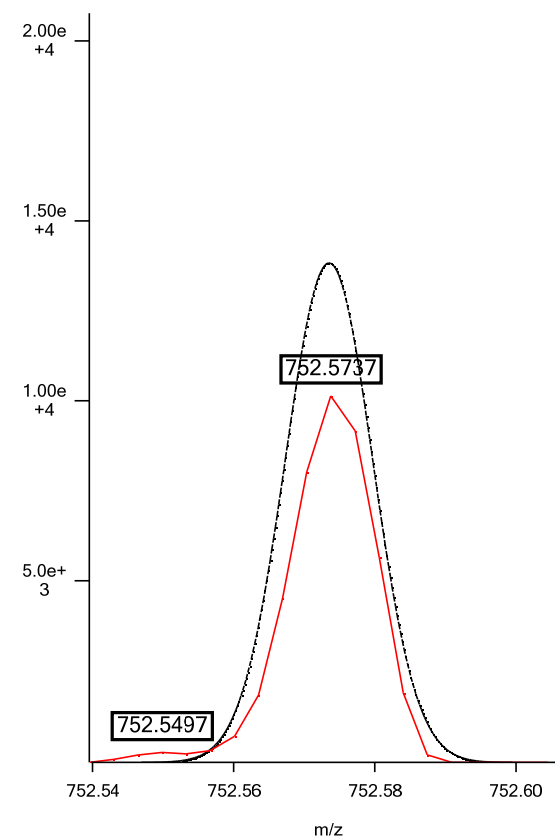
Isotope 1



Isotope 2

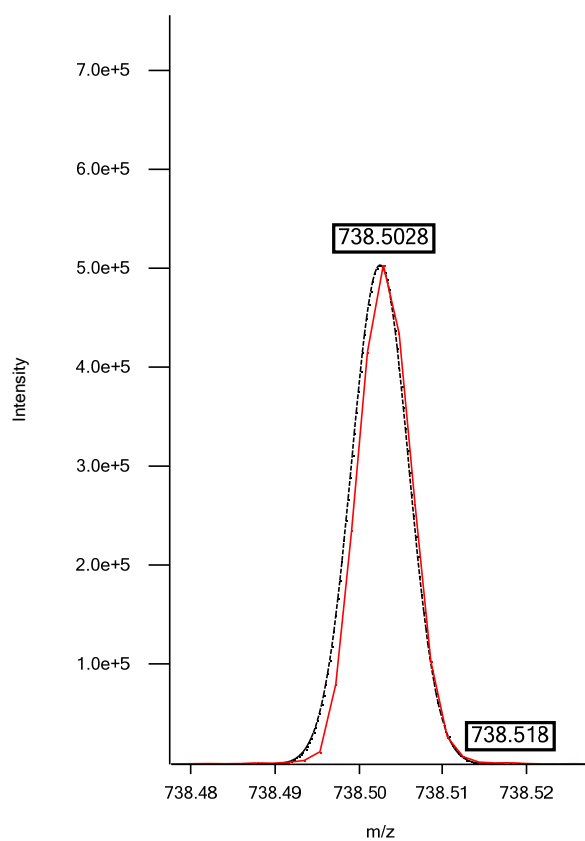


Isotope 3

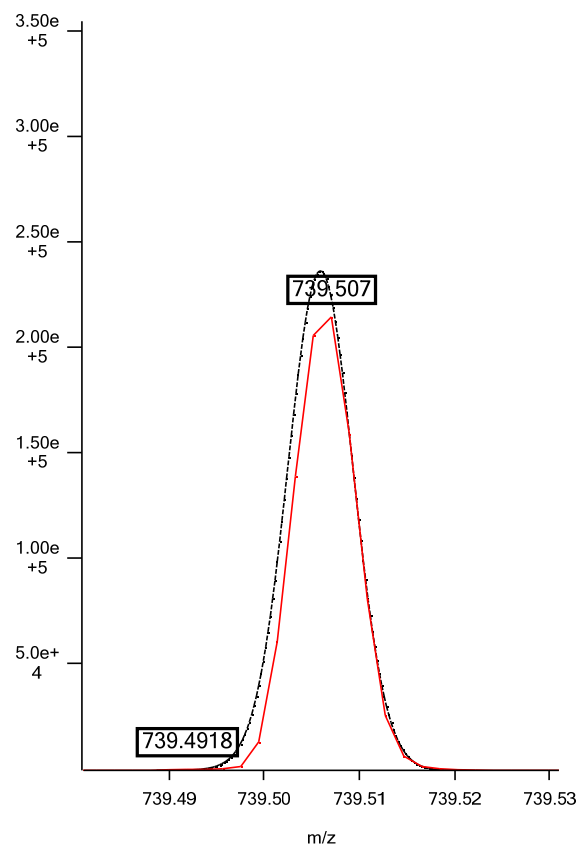


Positive ESI: PE 36:5; C₄₁H₇₃NO₈P; theoretical m/z 738.5074, (M+H)⁺; isotopic fit 0.0027

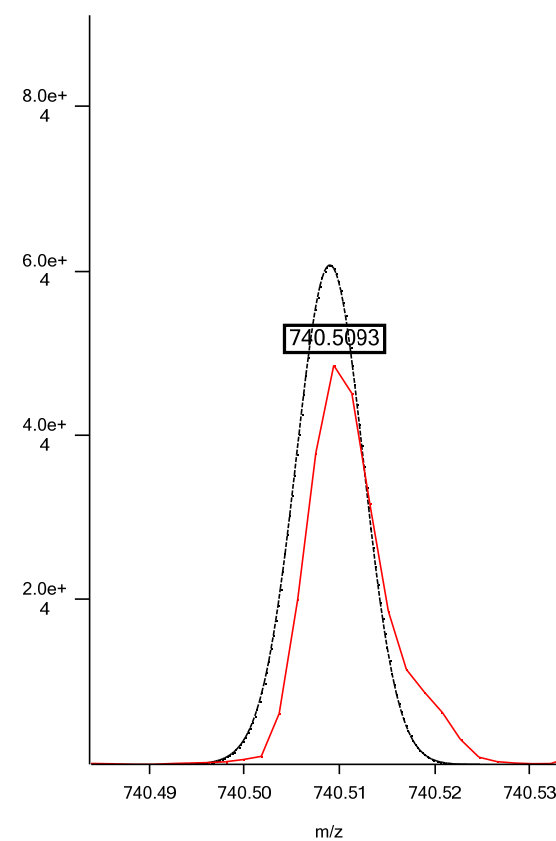
Isotope 1



Isotope 2

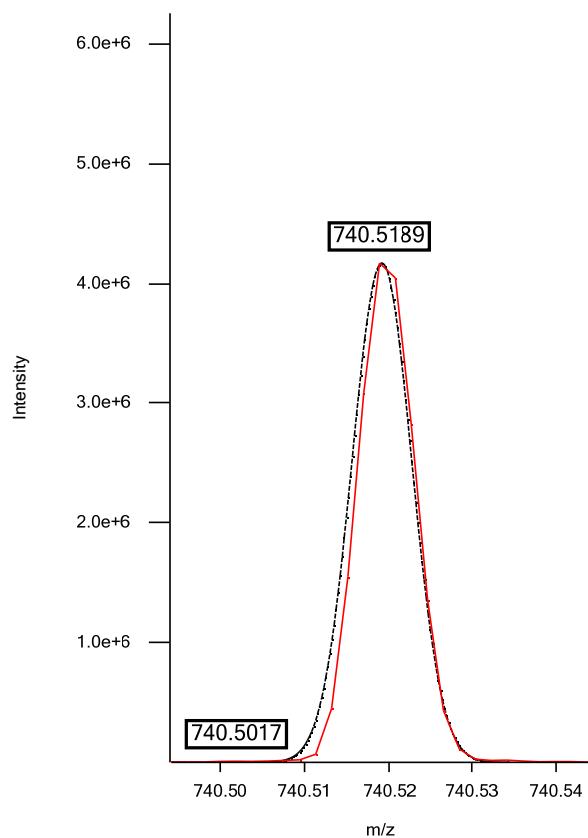


Isotope 3

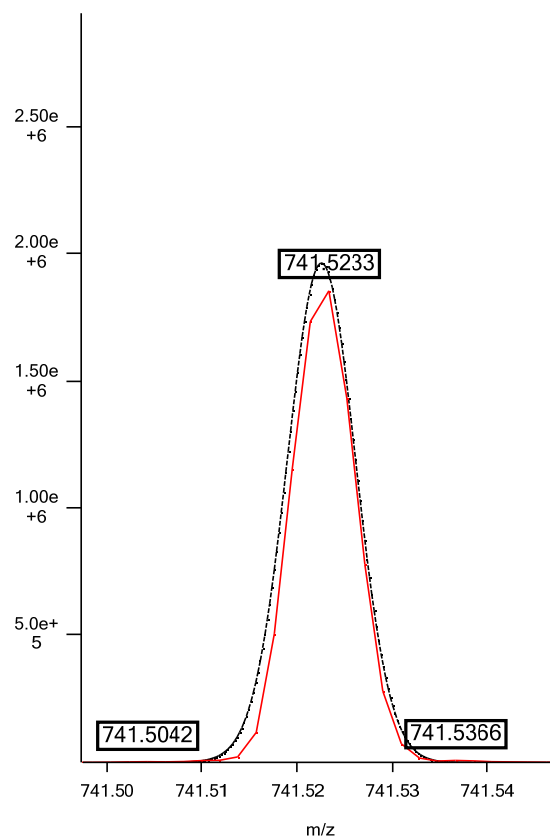


Positive ESI: PE 36:4; C₄₁H₇₅NO₈P; theoretical *m/z* 740.5230, (M+H)⁺; isotopic fit 0.0033

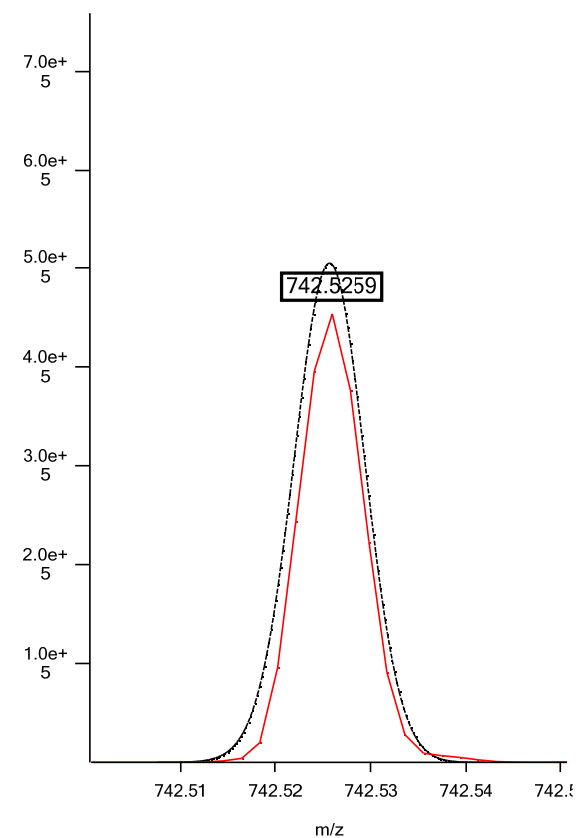
Isotope 1



Isotope 2

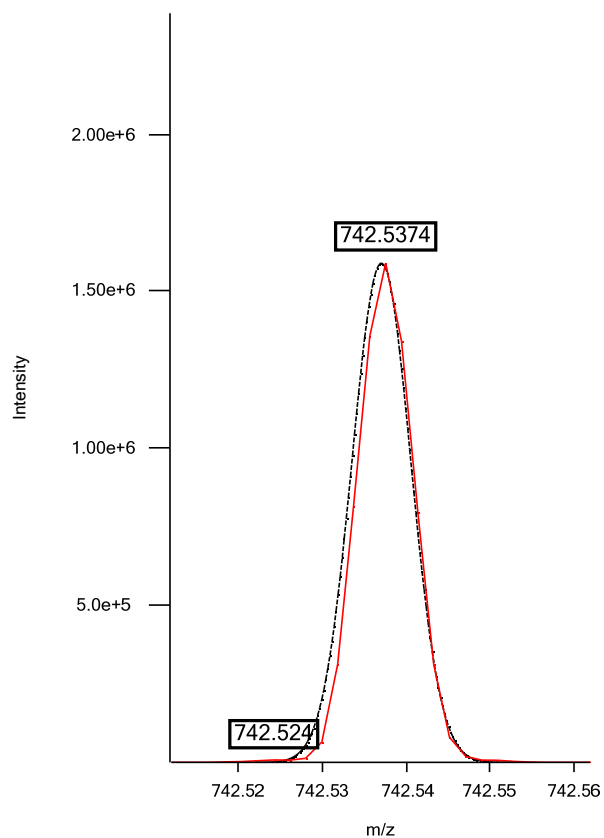


Isotope 3

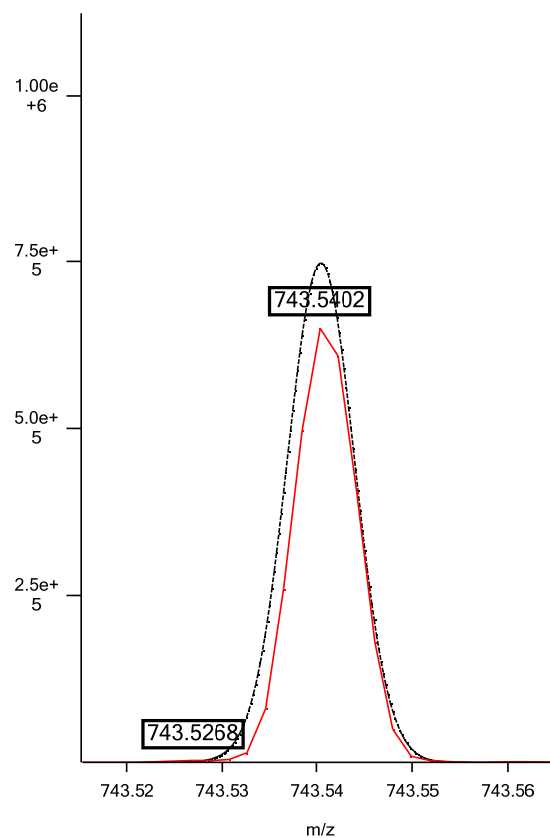


Positive ESI: PE 36:3; C₄₁H₇₇NO₈P; theoretical *m/z* 742.5387, (M+H)⁺; isotopic fit 0.0072

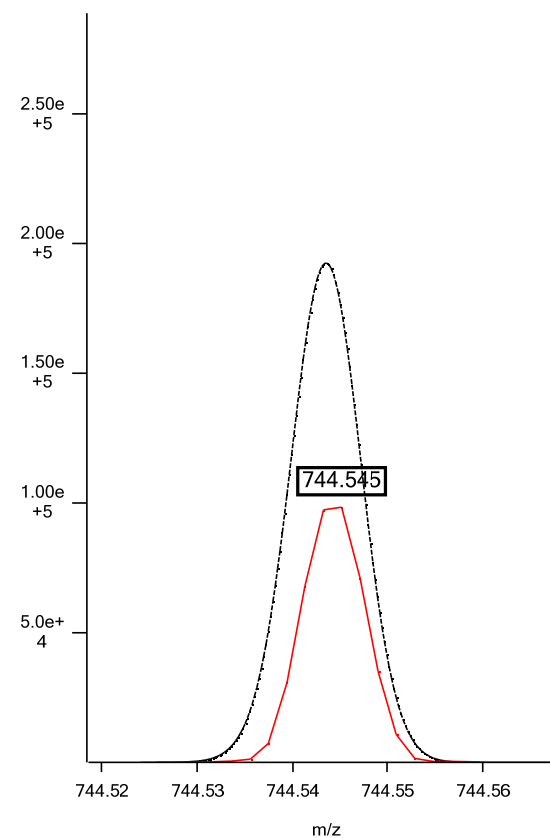
Isotope 1



Isotope 2

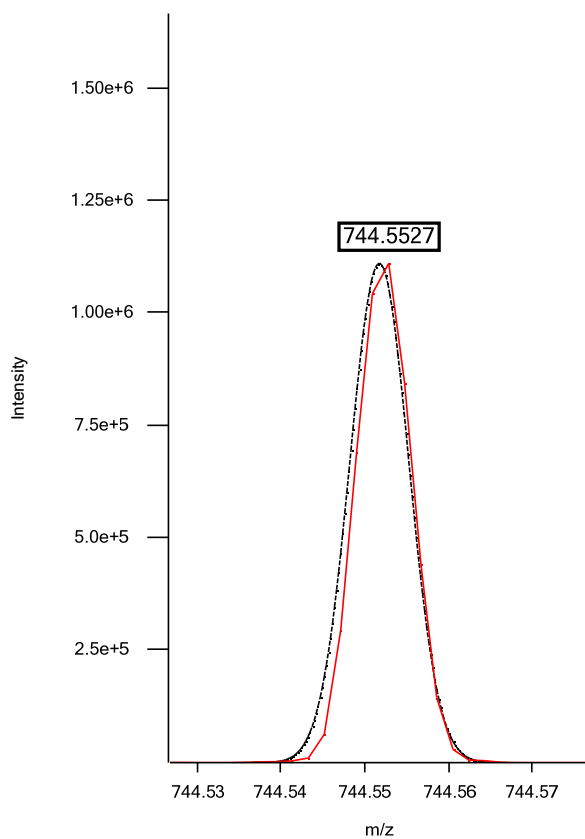


Isotope 3

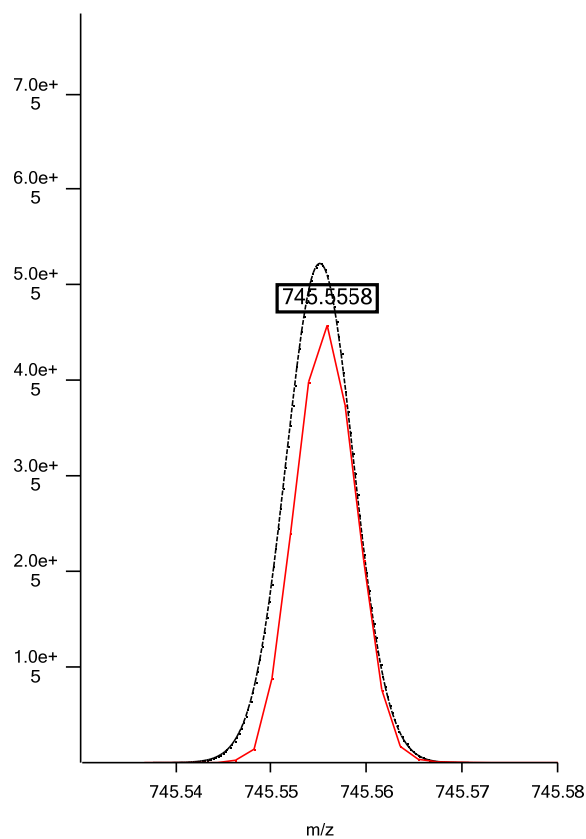


Positive ESI: PE 36:2; C₄₁H₇₉NO₈P; theoretical m/z 744.5543, (M+H)⁺; isotopic fit 0.0096

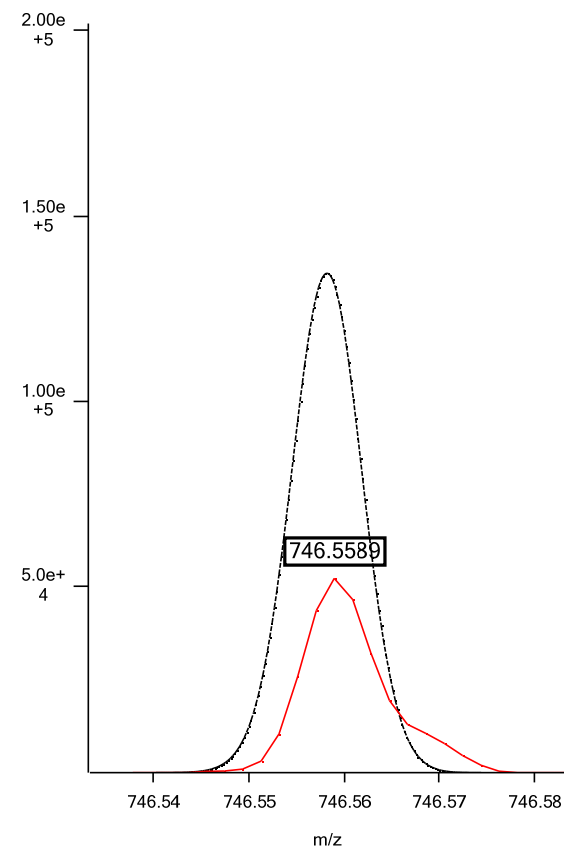
Isotope 1



Isotope 2

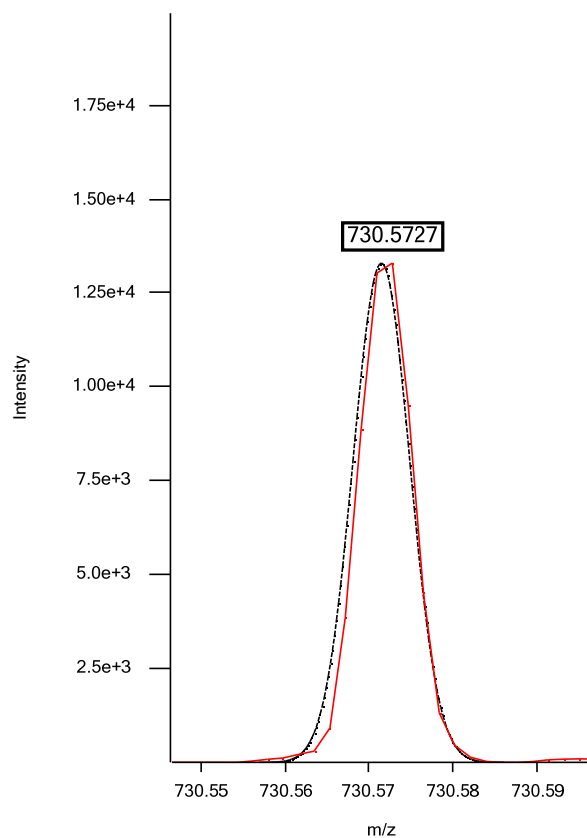


Isotope 3

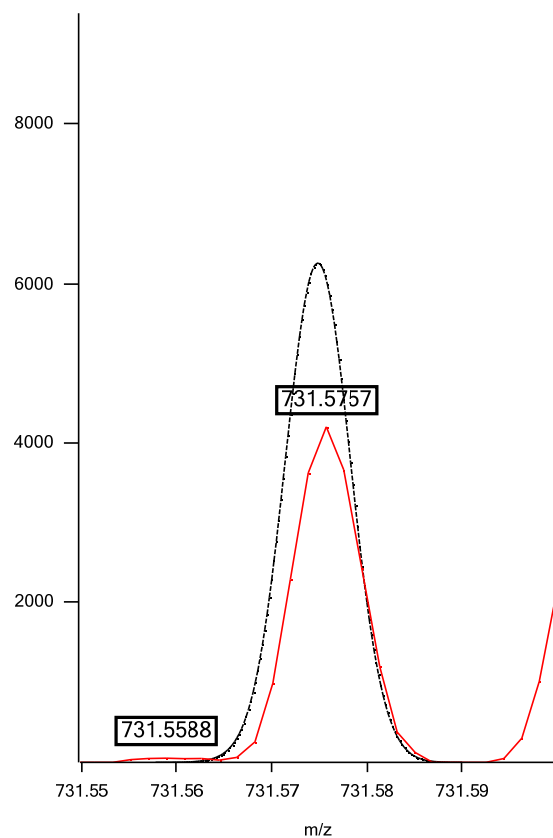


Positive ESI: PE 18:0p/18:1; C₄₁H₈₁NO₇P; theoretical *m/z* 730.5750, (M+H)⁺; isotopic fit 0.024

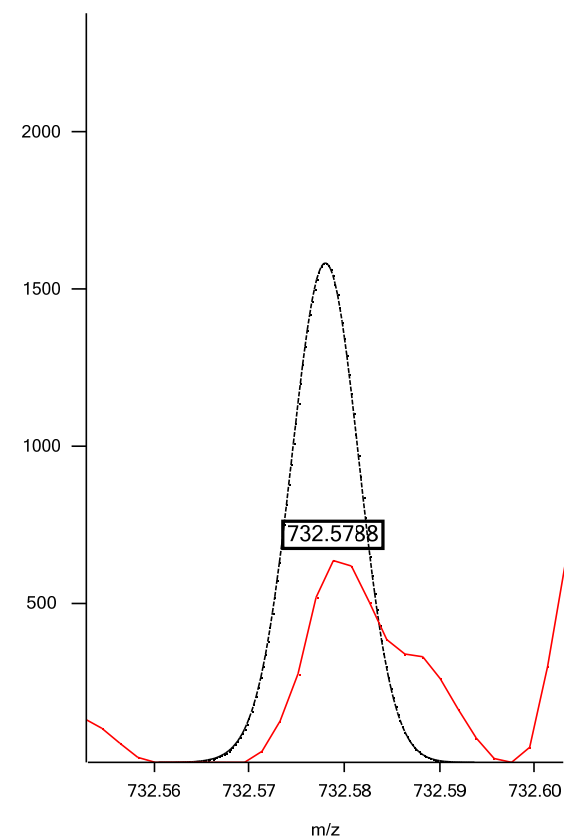
Isotope 1



Isotope 2

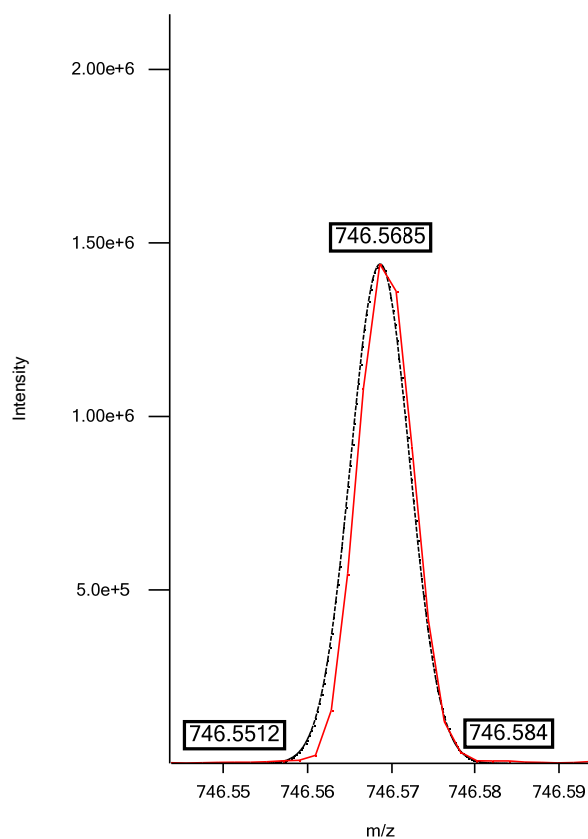


Isotope 3

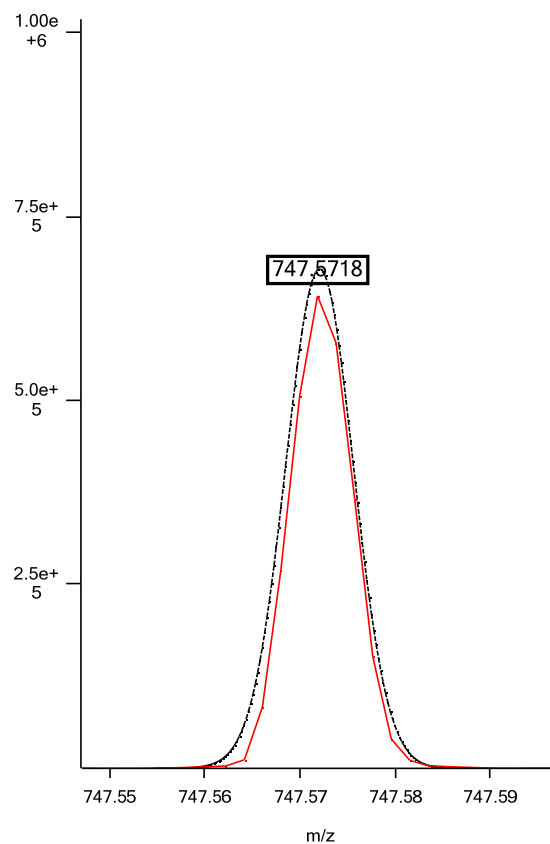


Positive ESI: PE 36:1; C₄₁H₈₁NO₈P; theoretical *m/z* 746.5700, (M+H)⁺; isotopic fit 0.0073

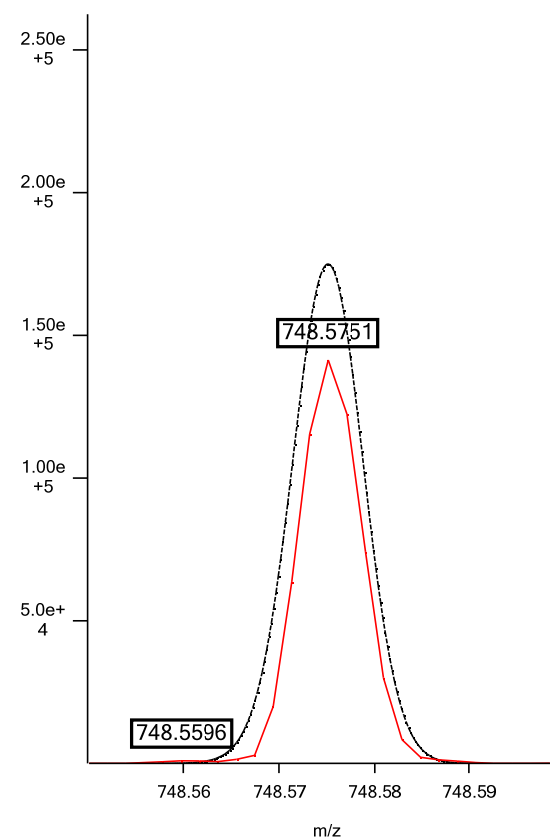
Isotope 1



Isotope 2

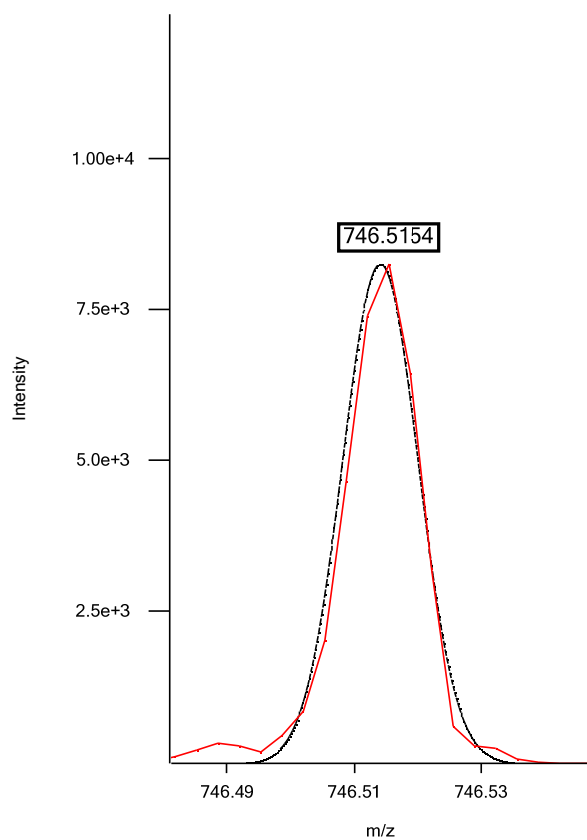


Isotope 3

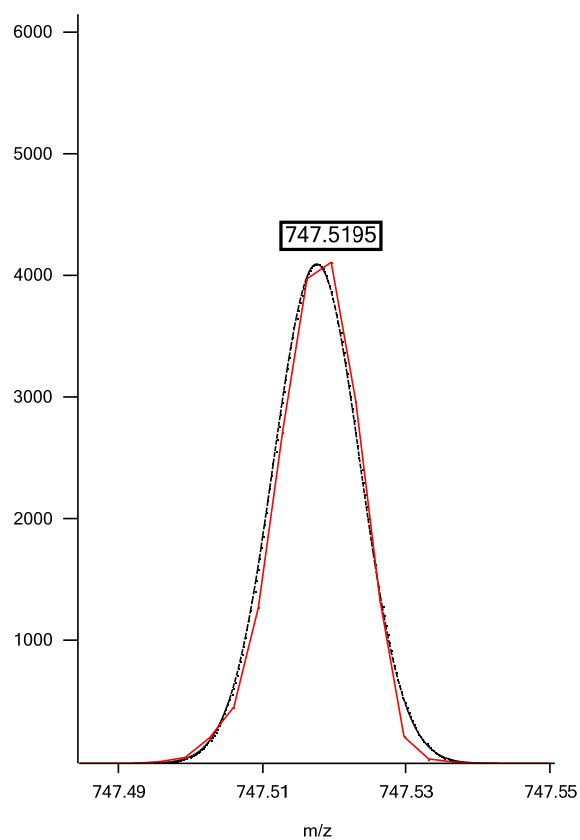


Negative ESI: PE 16:0p/22:6; C₄₃H₇₃NO₇P; theoretical *m/z* 746.5124, (M-H)⁻; isotopic fit 0.0028

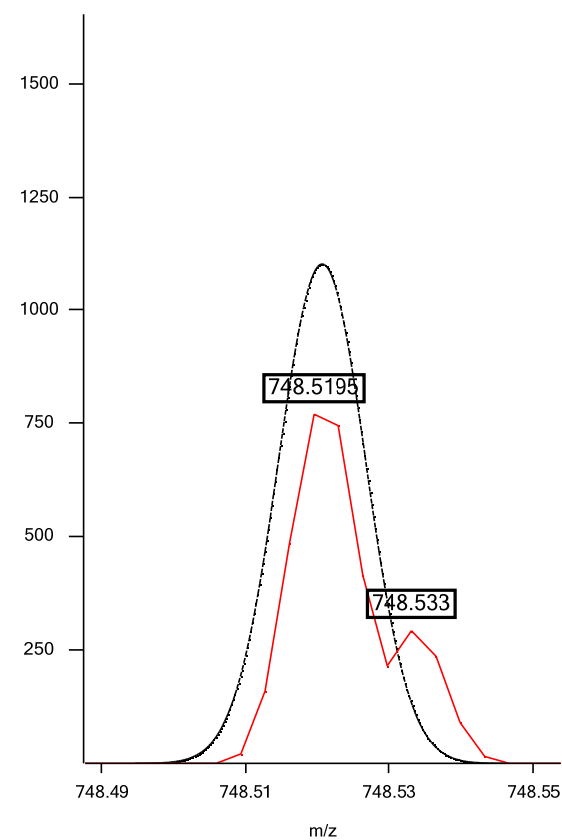
Isotope 1



Isotope 2

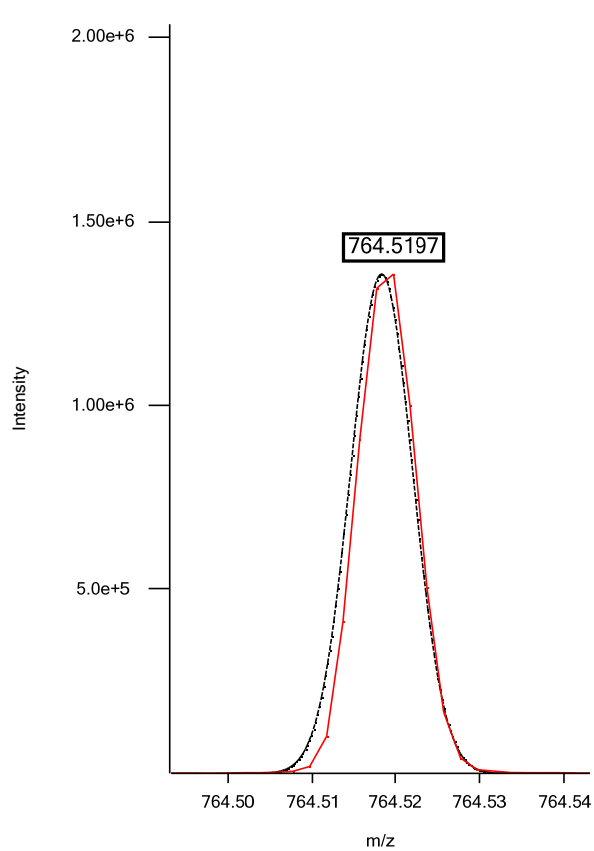


Isotope 3

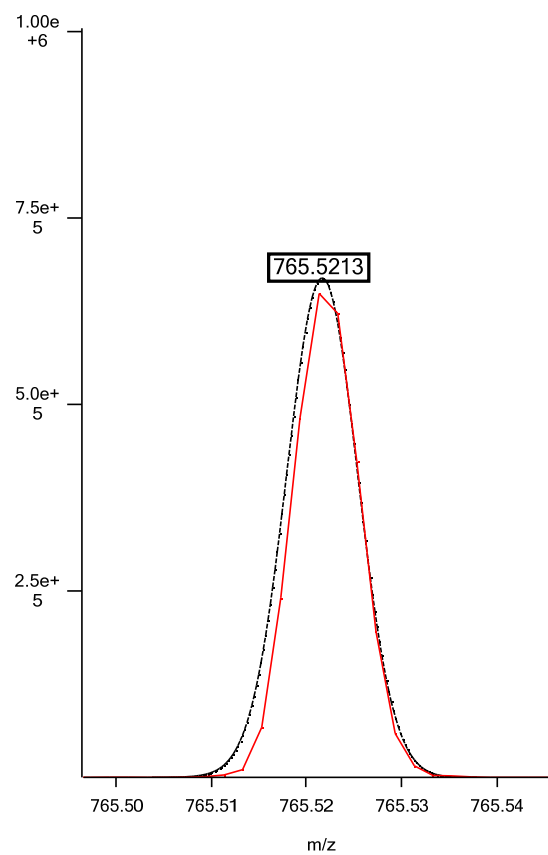


Positive ESI: PE 38:6; C₄₃H₇₅NO₈P; theoretical m/z 764.5230, (M+H)⁺; isotopic fit 0.0045

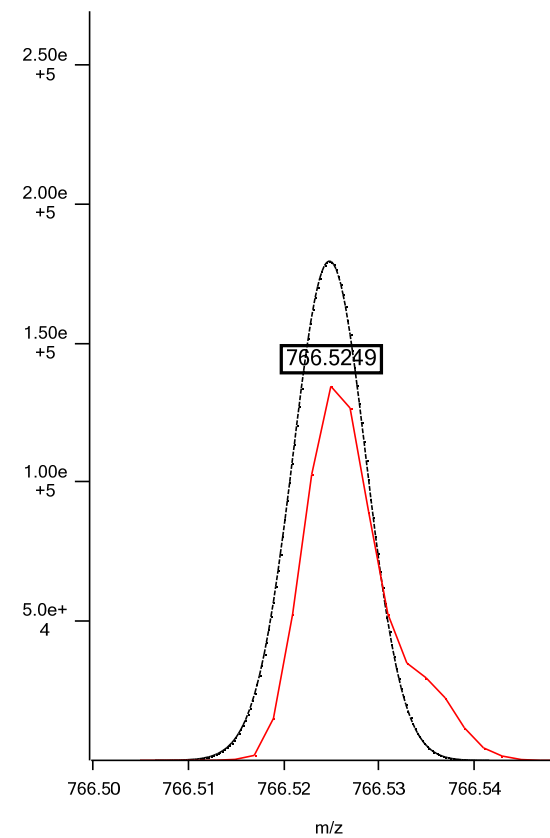
Isotope 1



Isotope 2

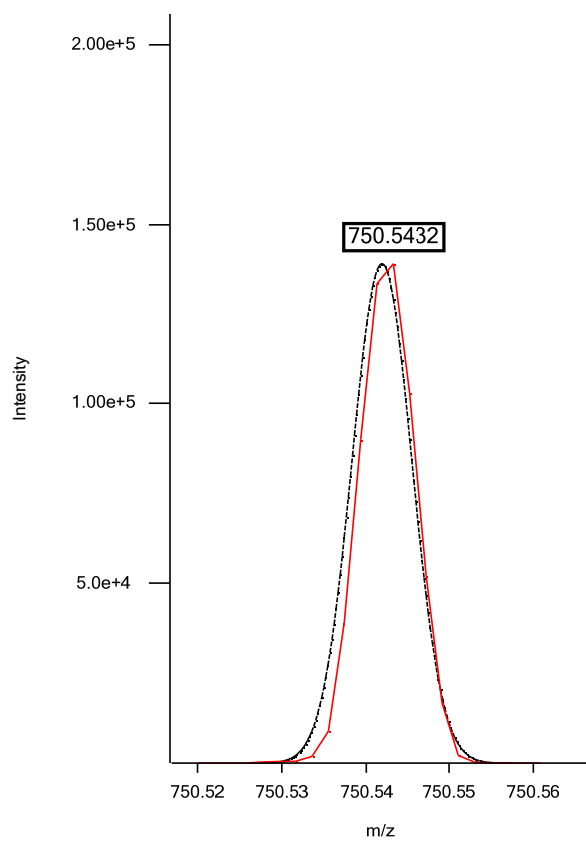


Isotope 3

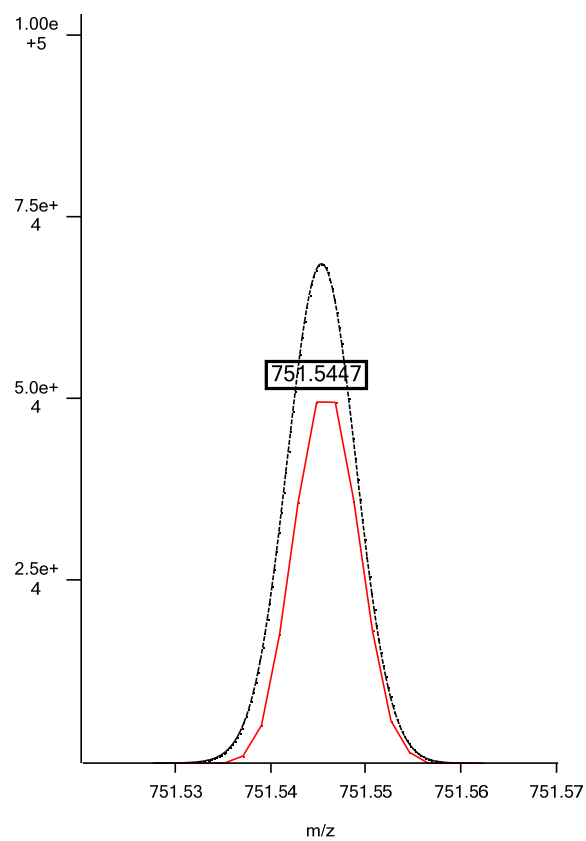


Positive ESI: PE 18:1p/20:4; C₄₃H₇₇NO₇P; theoretical *m/z* 750.5437, (M+H)⁺; isotopic fit 0.0172

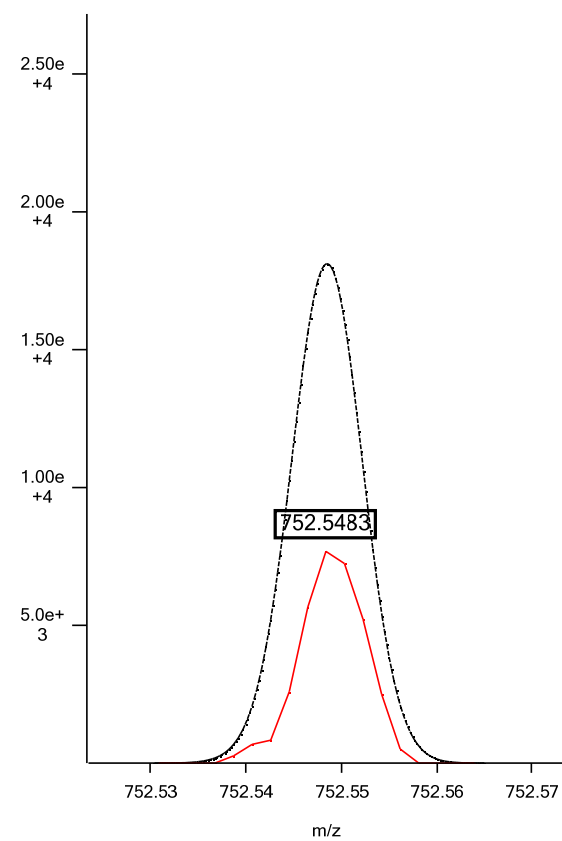
Isotope 1



Isotope 2

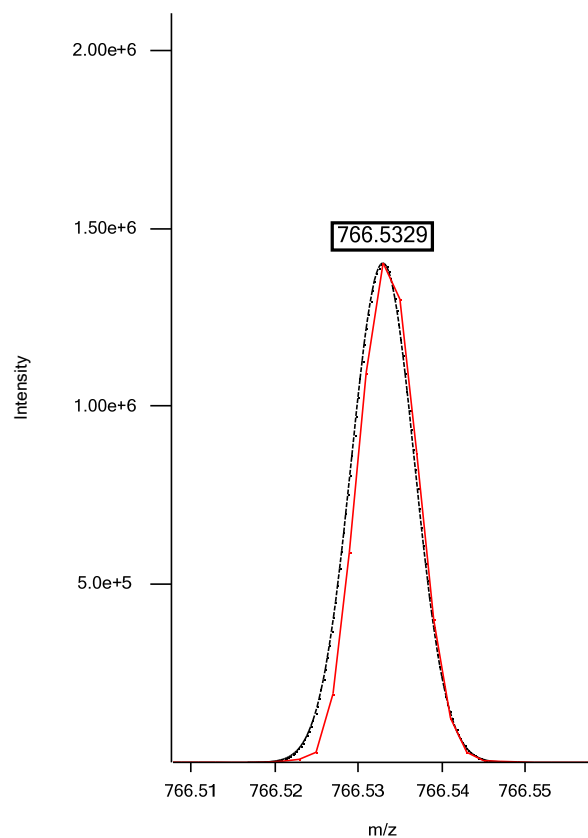


Isotope 3

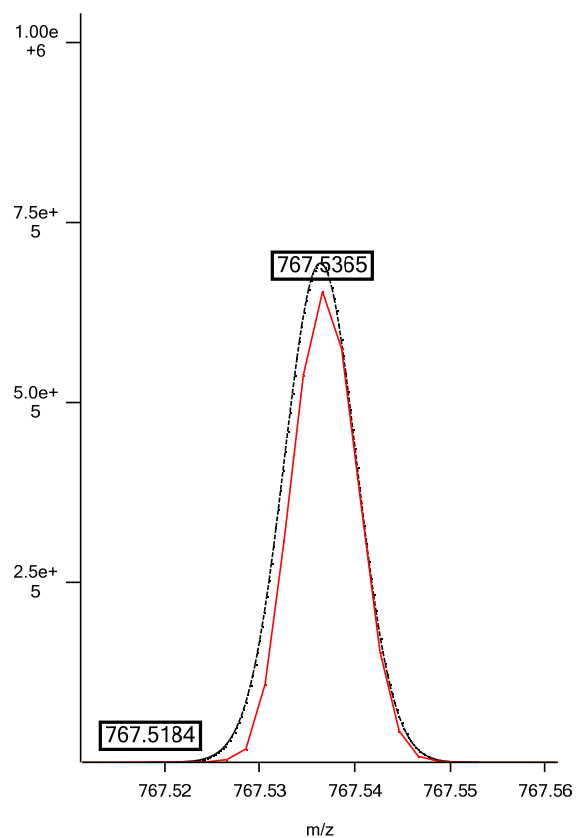


Positive ESI: PE 38:5; C₄₃H₇₇NO₈P; theoretical *m/z* 766.5387, (M+H)⁺; isotopic fit 0.0052

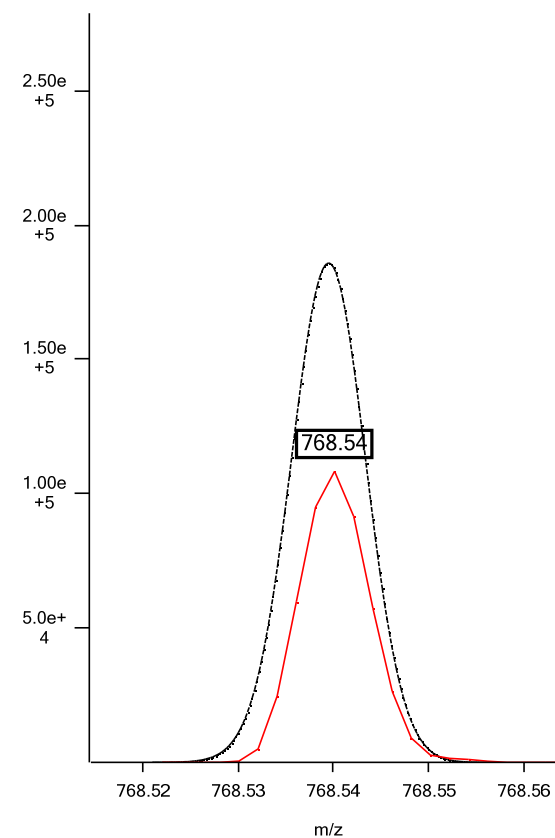
Isotope 1



Isotope 2

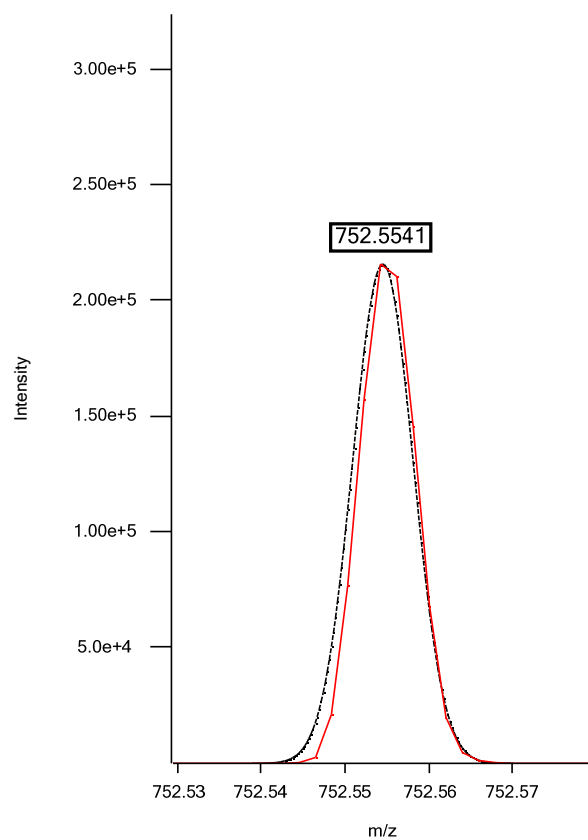


Isotope 3

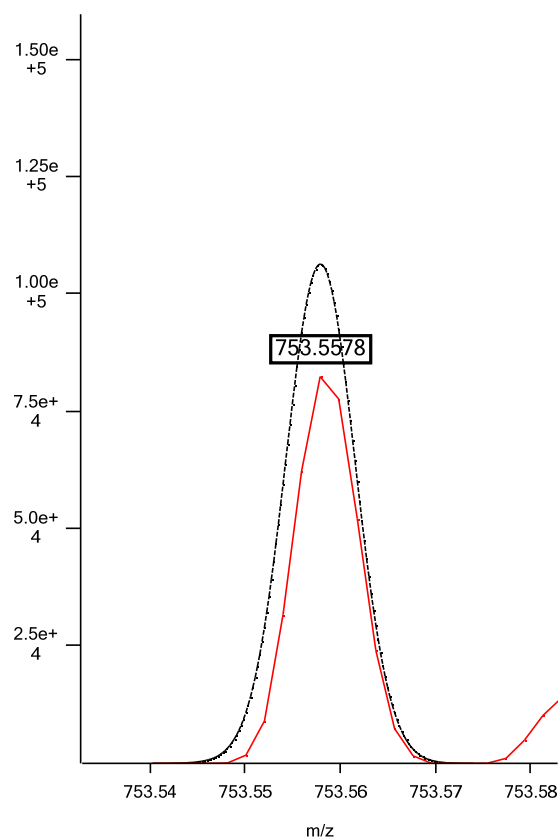


Positive ESI: PE 18:0p/20:4; C₄₃H₇₉NO₇P; theoretical *m/z* 752.5594, (M+H)⁺; isotopic fit 0.0156

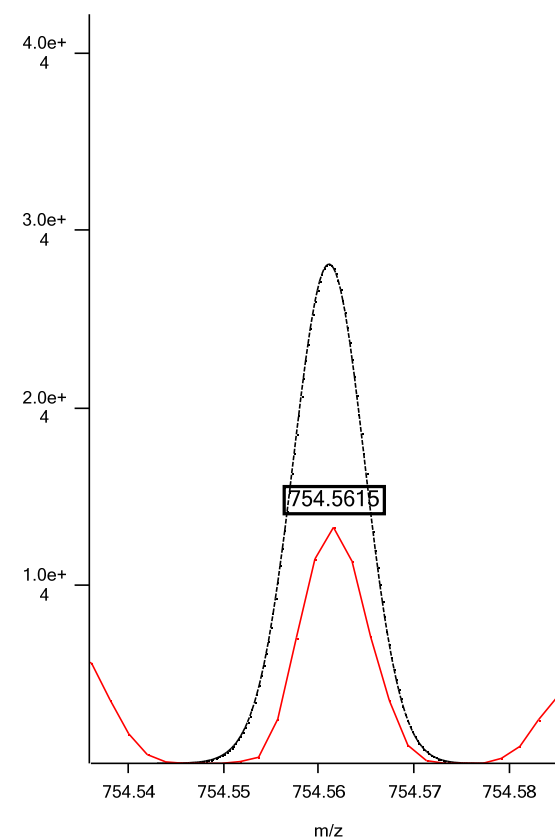
Isotope 1



Isotope 2

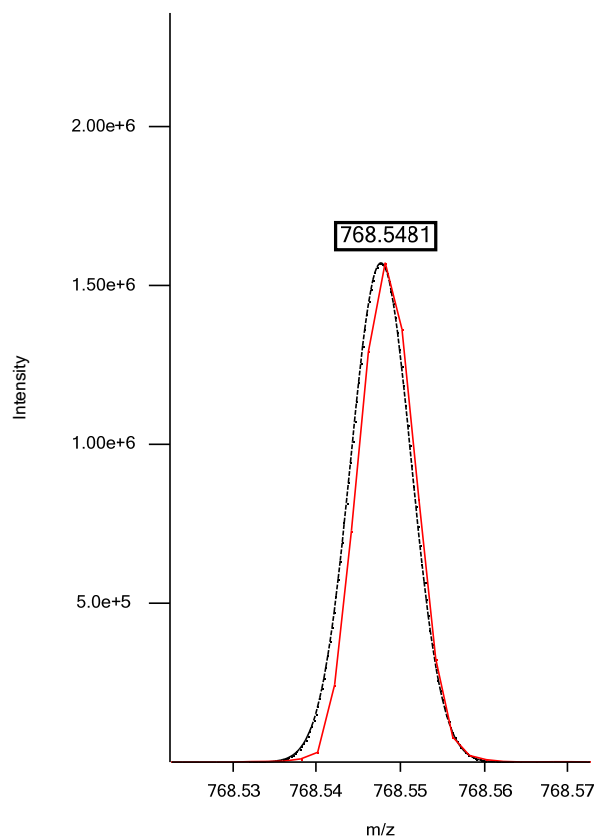


Isotope 3

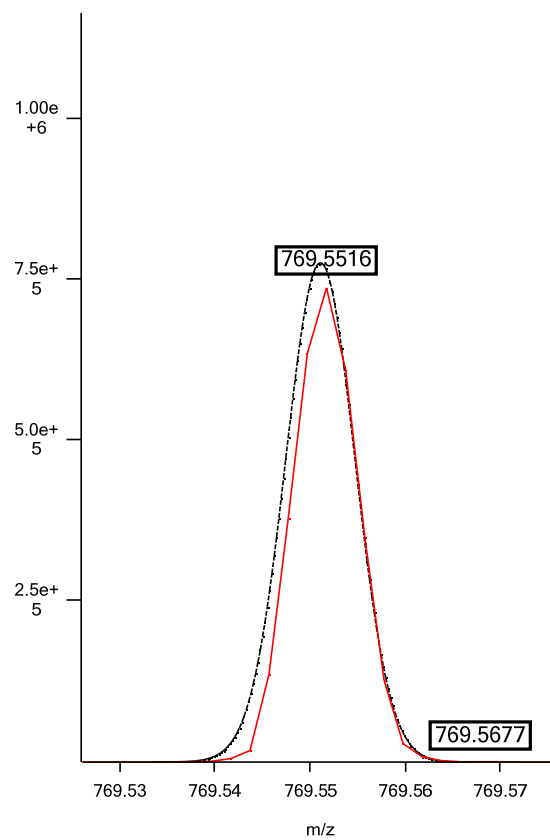


Positive ESI: PE 38:4; C₄₃H₇₉NO₈P; theoretical m/z 768.5543, (M+H)⁺; isotopic fit 0.0038

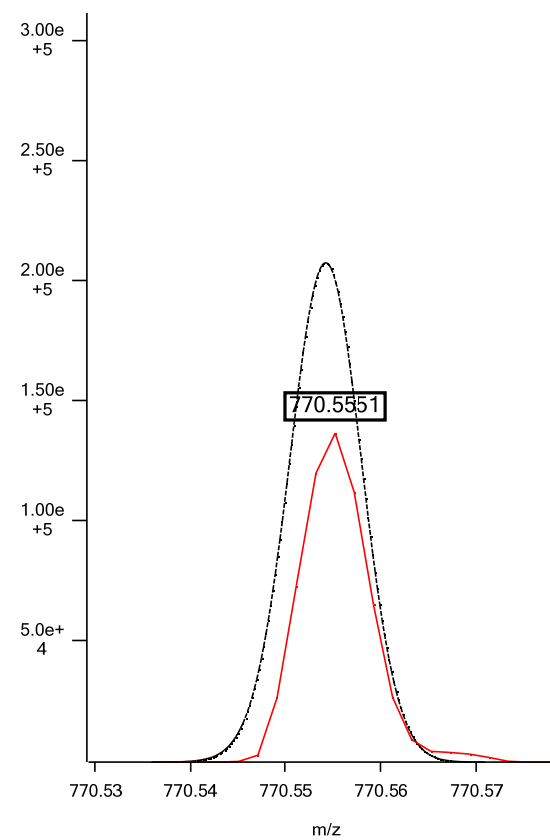
Isotope 1



Isotope 2

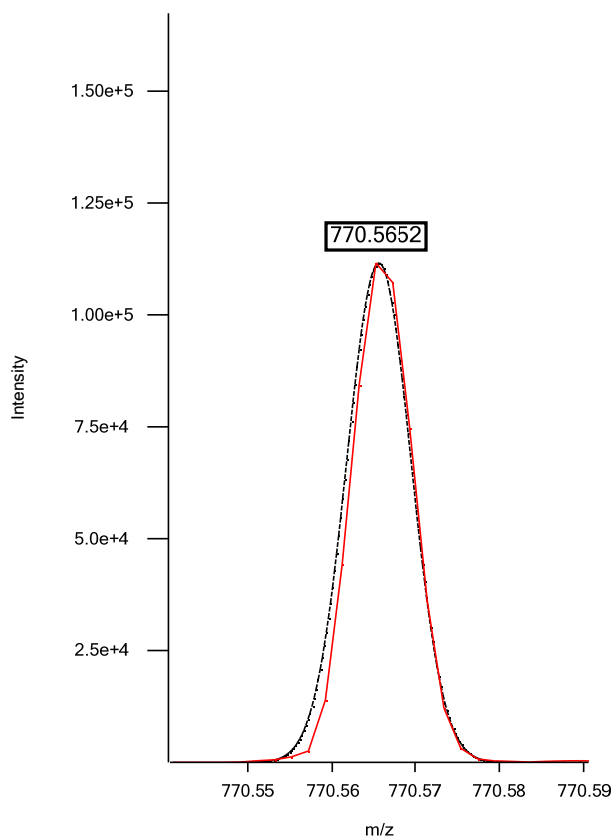


Isotope 3

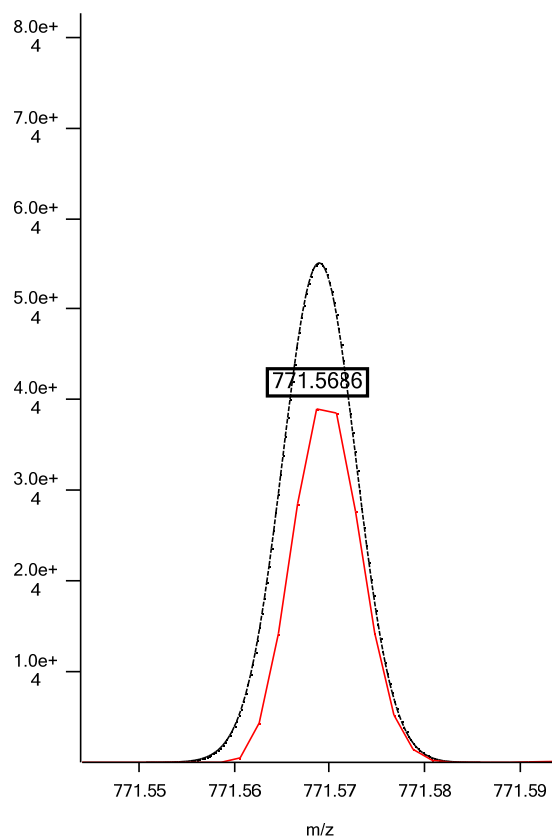


Positive ESI: PE 38:3; C₄₃H₈₁NO₈P; theoretical m/z 770.5700, (M+H)⁺; isotopic fit 0.0196

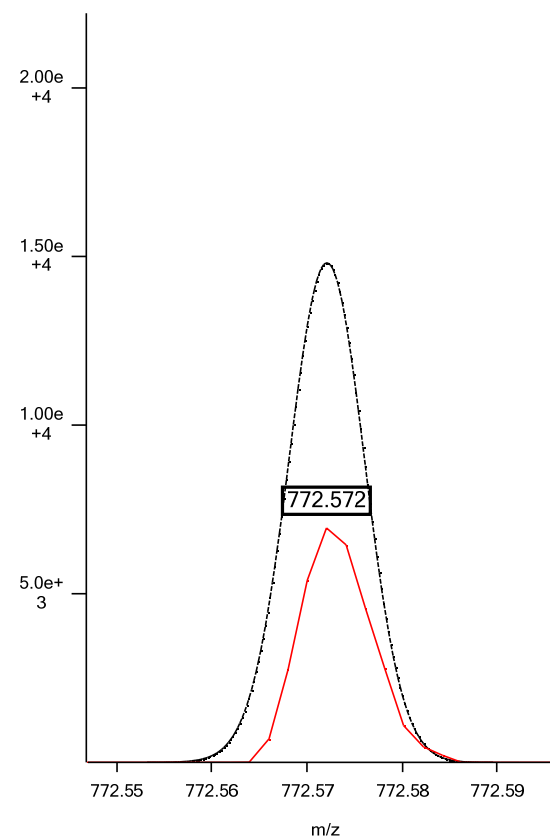
Isotope 1



Isotope 2



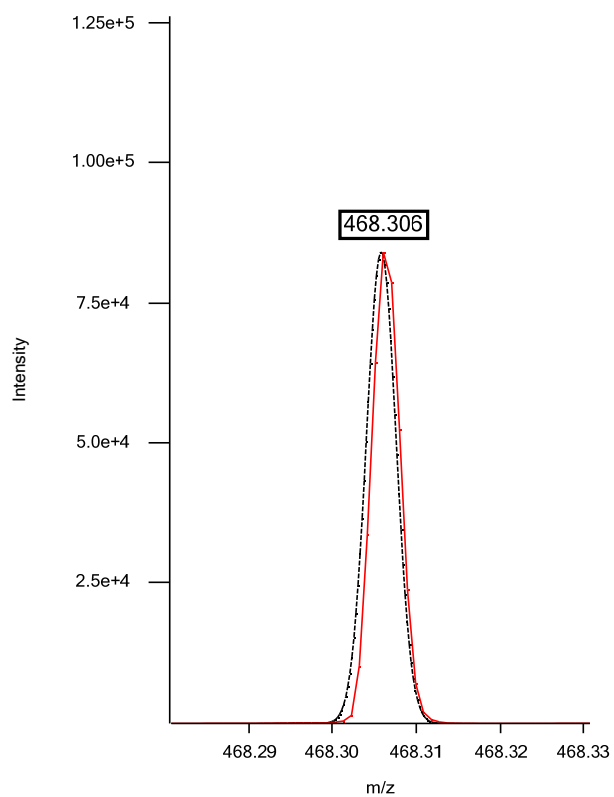
Isotope 3



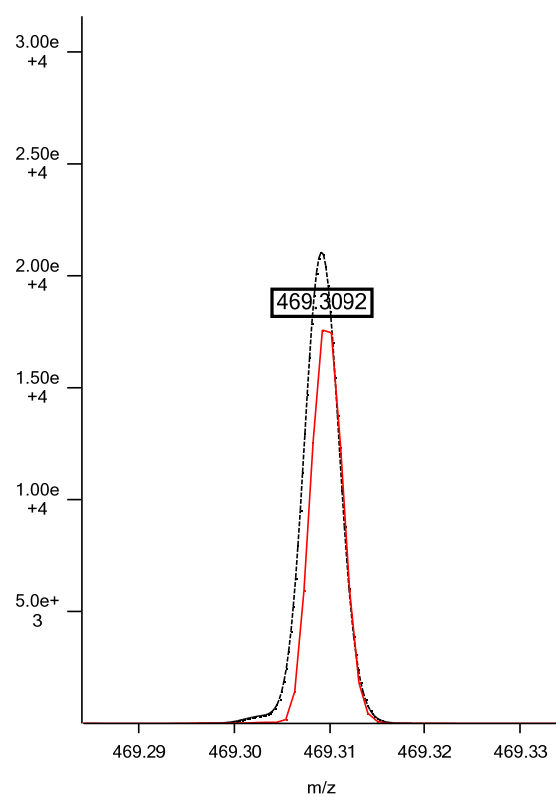
Glycerophosphocholines

Positive ESI: LPC 14:0; C₂₂H₄₇NO₇P; theoretical m/z 468.3090, (M+H)⁺; isotopic fit 0.0208

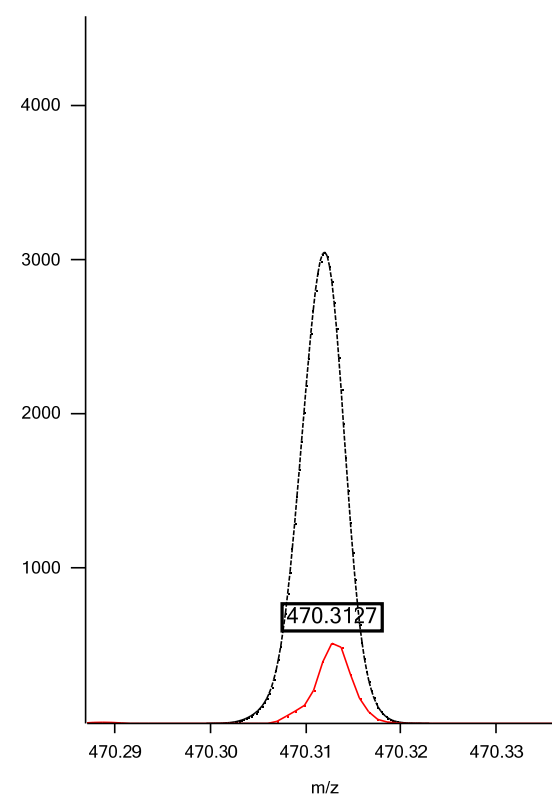
Isotope 1



Isotope 2

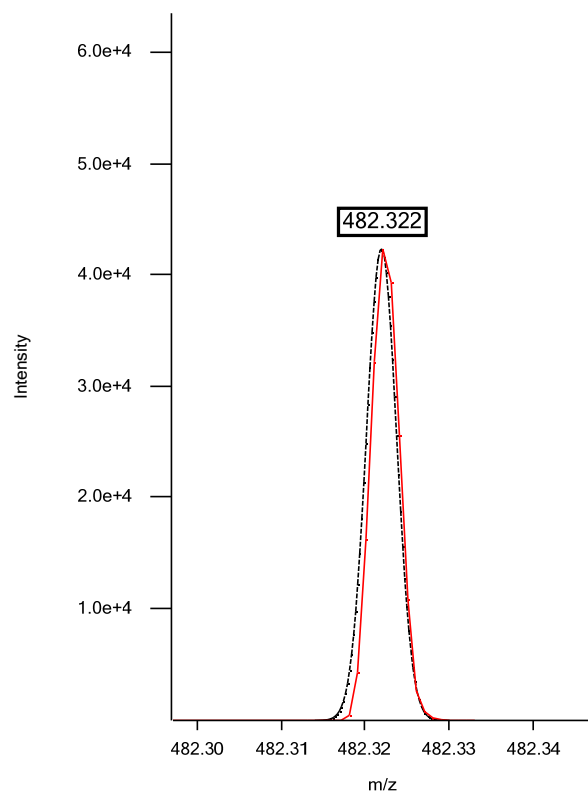


Isotope 3

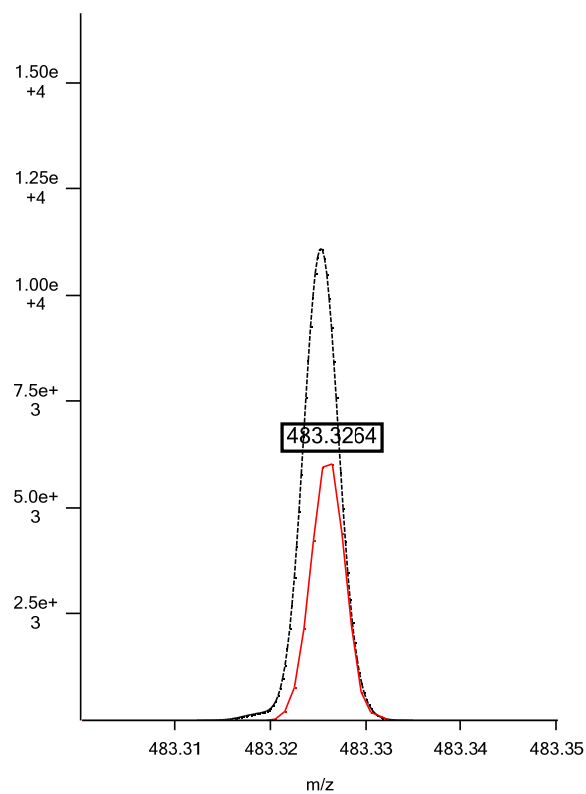


Positive ESI: LPC 15:0; C₂₃H₄₉NO₇P; theoretical m/z 482.3247, (M+H)⁺; isotopic fit 0.0302

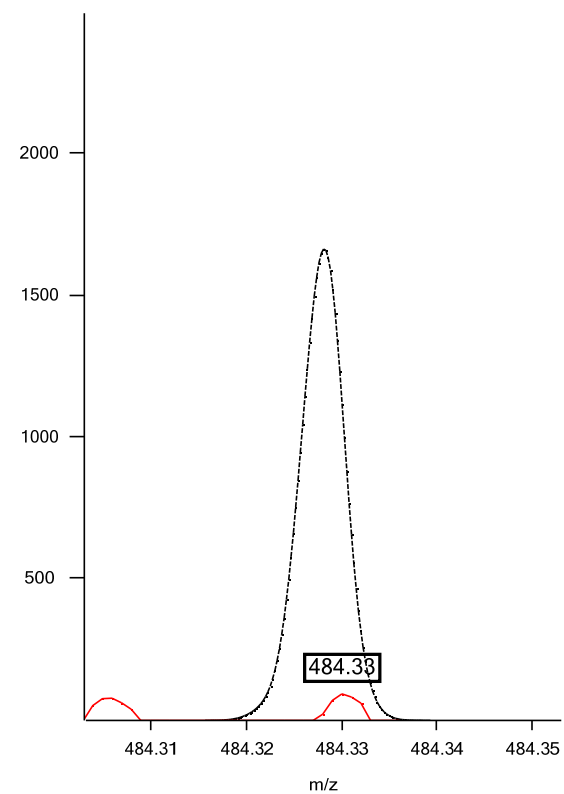
Isotope 1



Isotope 2

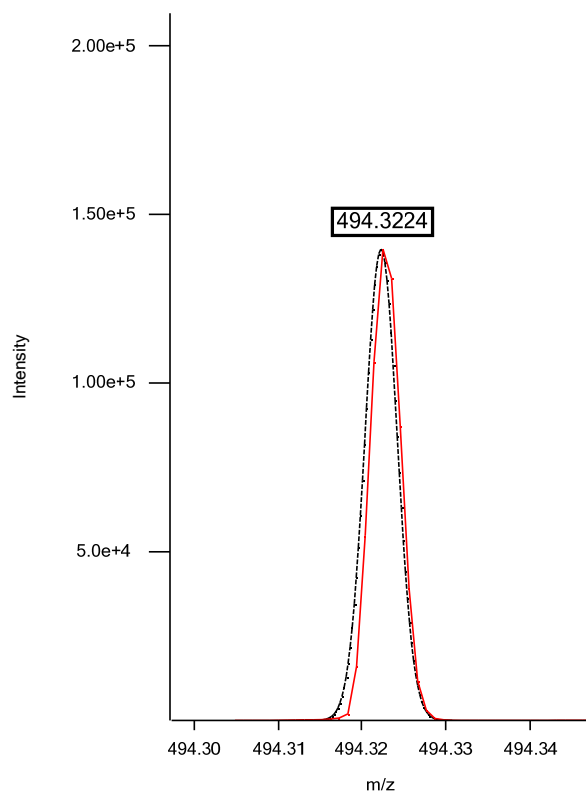


Isotope 3

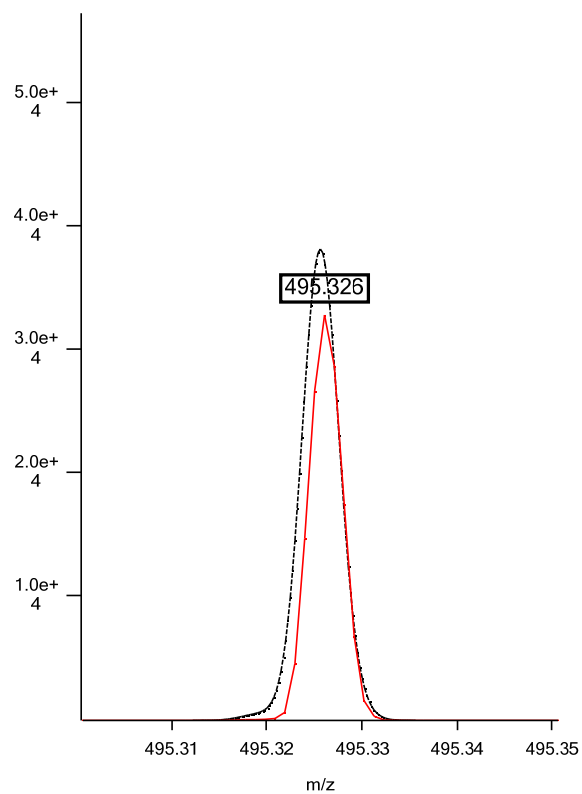


Positive ESI: LPC 16:1; C₂₄H₄₉NO₇P; theoretical *m/z* 494.3247, (M+H)⁺; isotopic fit 0.0034

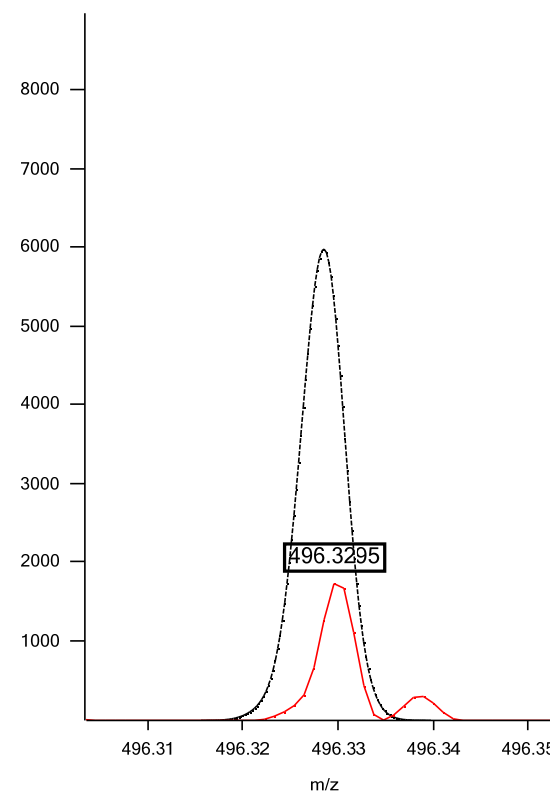
Isotope 1



Isotope 2

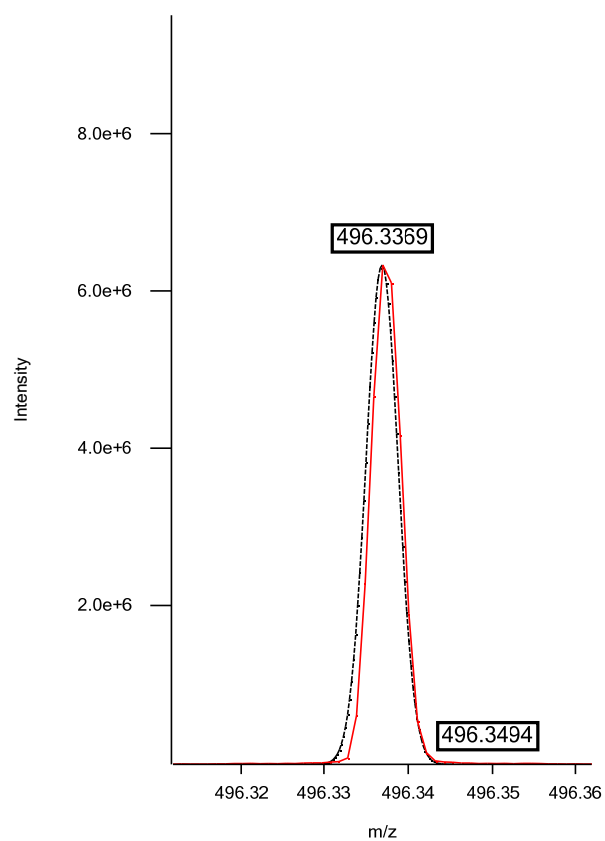


Isotope 3

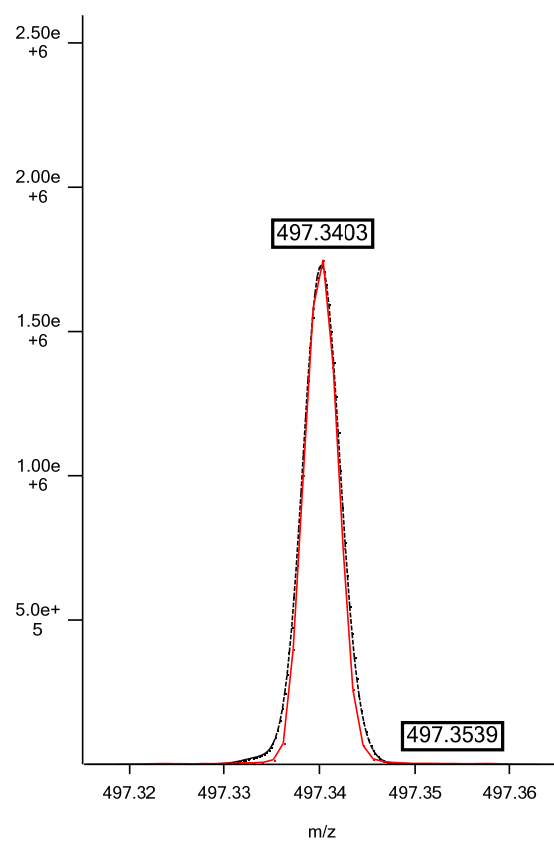


Positive ESI: LPC 16:0; C₂₄H₅₁NO₇P; theoretical m/z 496.3403, (M+H)⁺; isotopic fit 0.0036

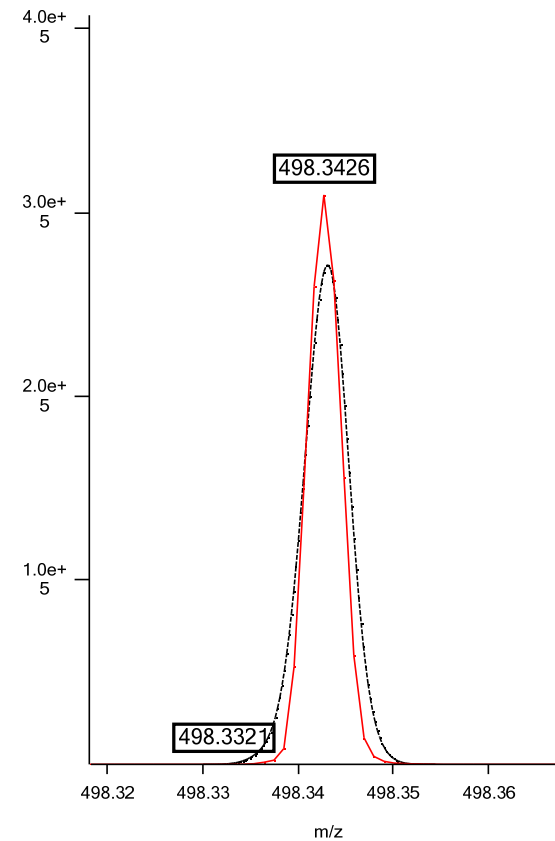
Isotope 1



Isotope 2

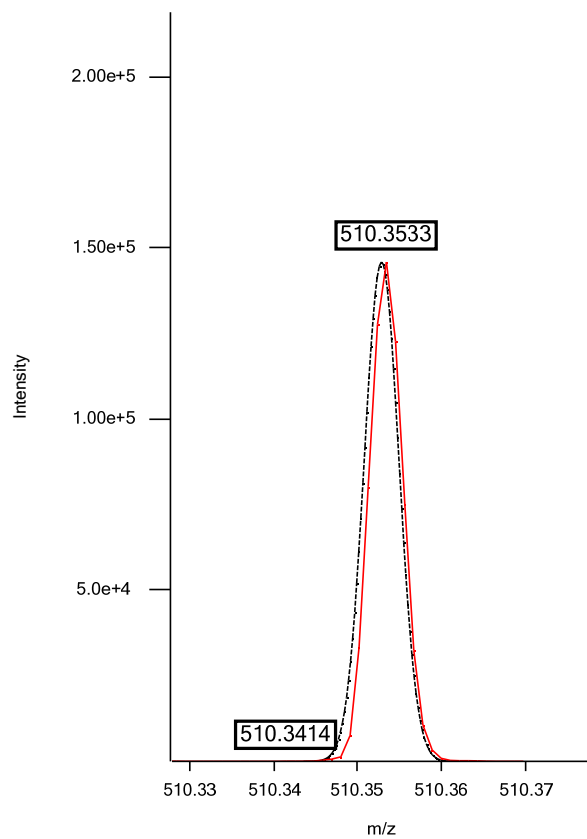


Isotope 3

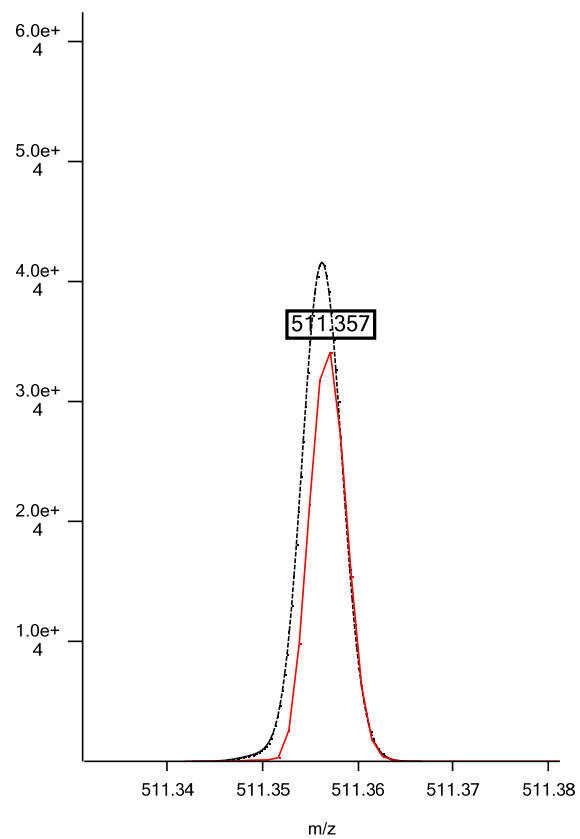


Positive ESI: LPC 17:0; C₂₅H₅₃NO₇P; theoretical m/z 510.3560, (M+H)⁺; isotopic fit 0.0037

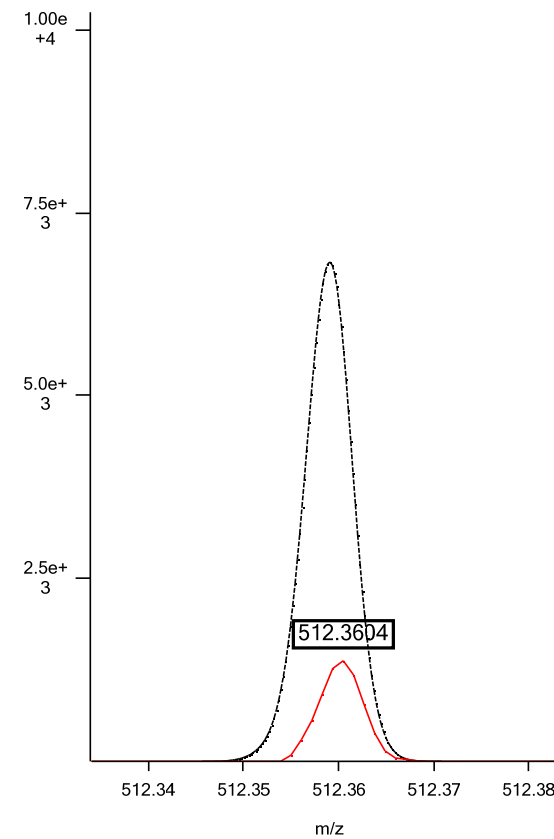
Isotope 1



Isotope 2

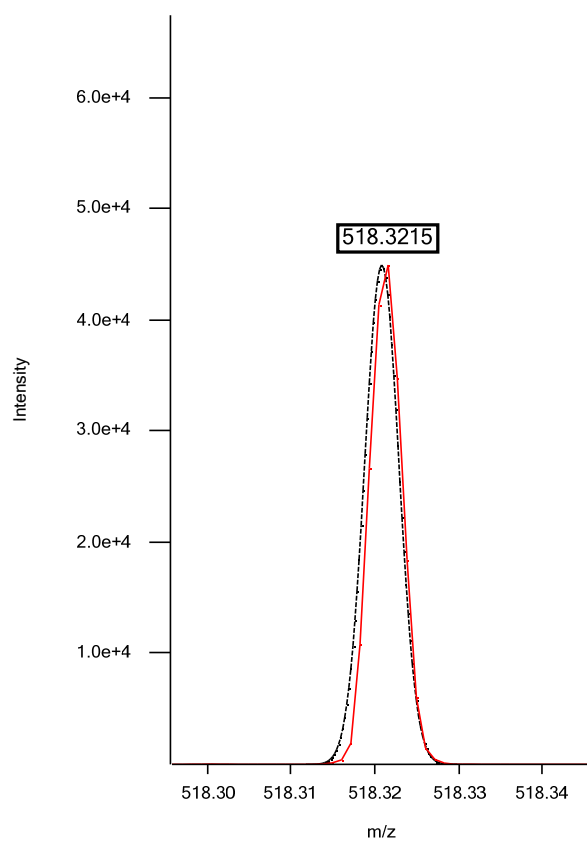


Isotope 3

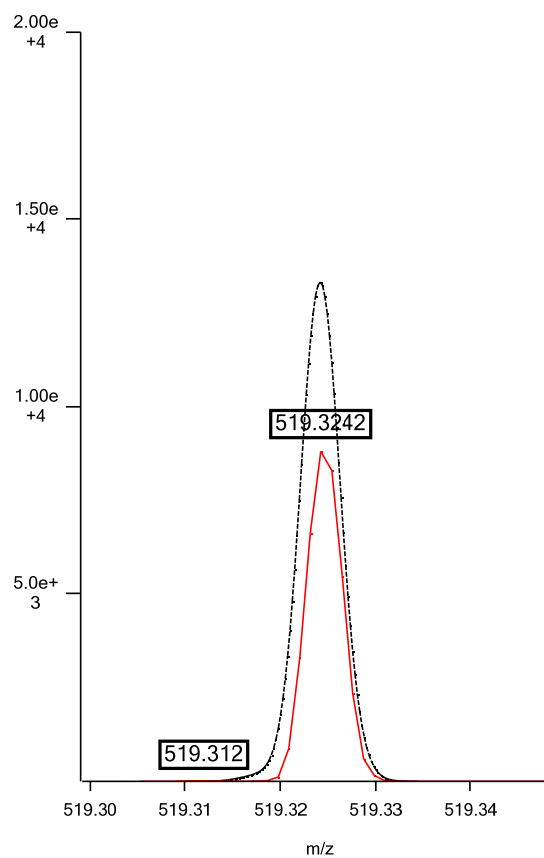


Positive ESI: LPC 18:3; C₂₆H₄₉NO₇P; theoretical m/z 518.3246, (M+H)⁺; isotopic fit 0.0326

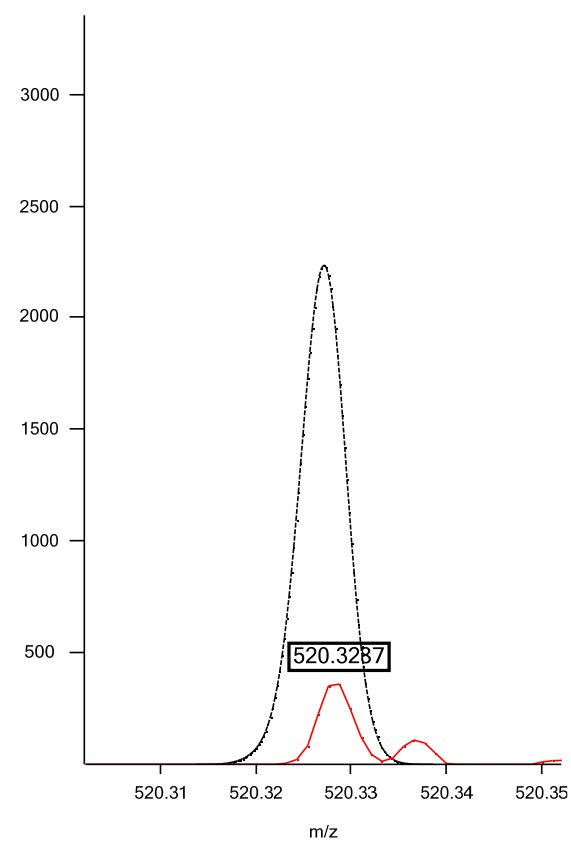
Isotope 1



Isotope 2

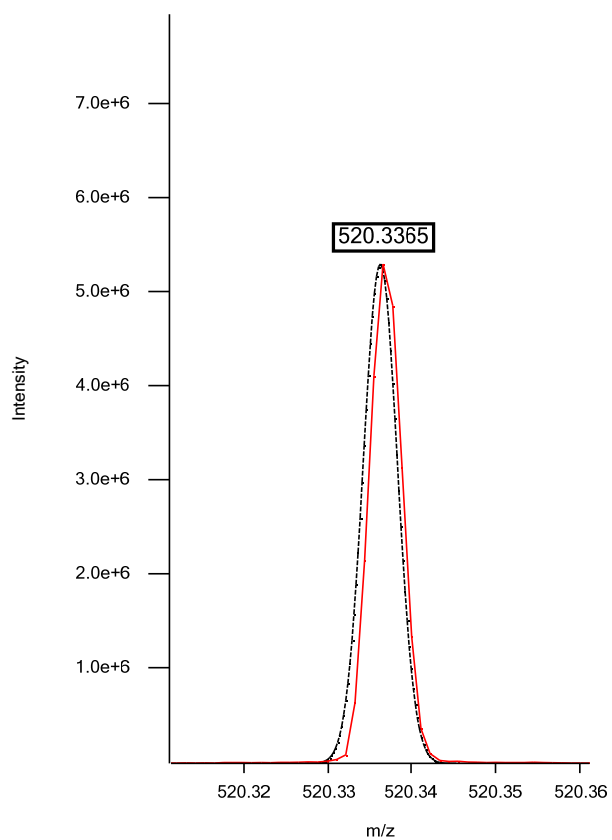


Isotope 3

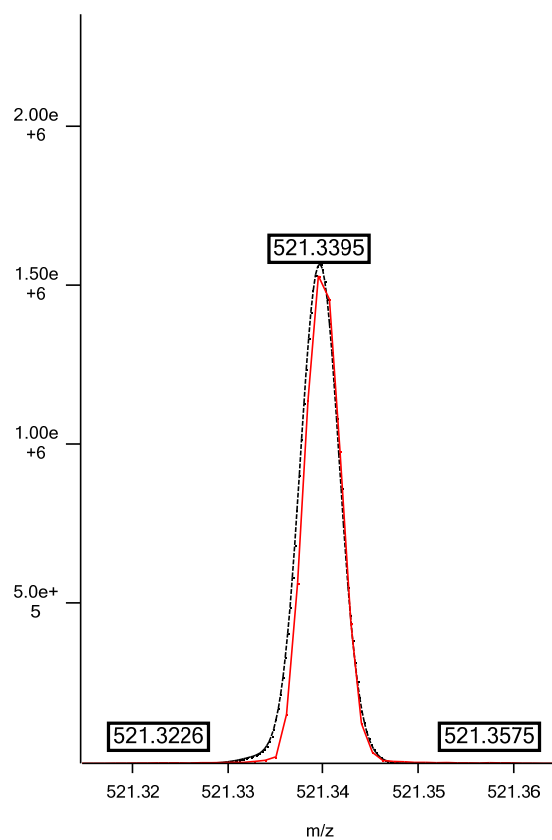


Positive ESI: LPC 18:2; C₂₆H₅₁NO₇P; theoretical m/z 520.3403, (M+H)⁺; isotopic fit 0.0113

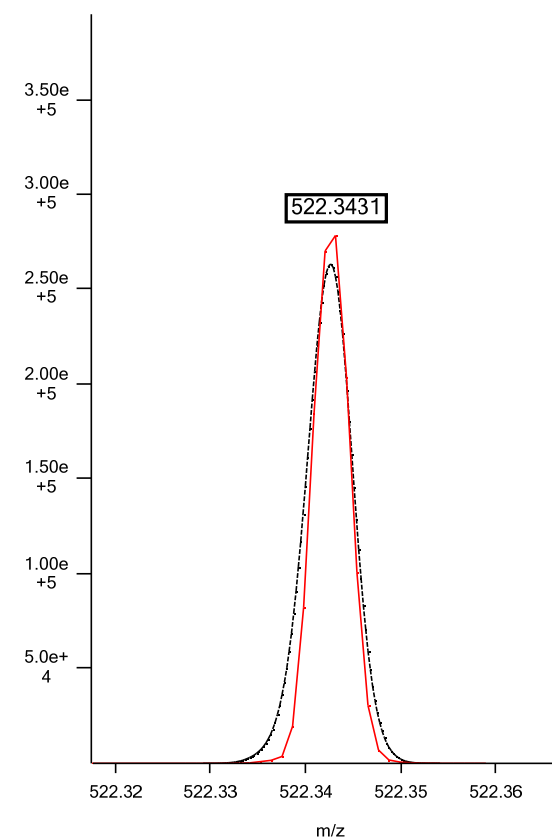
Isotope 1



Isotope 2

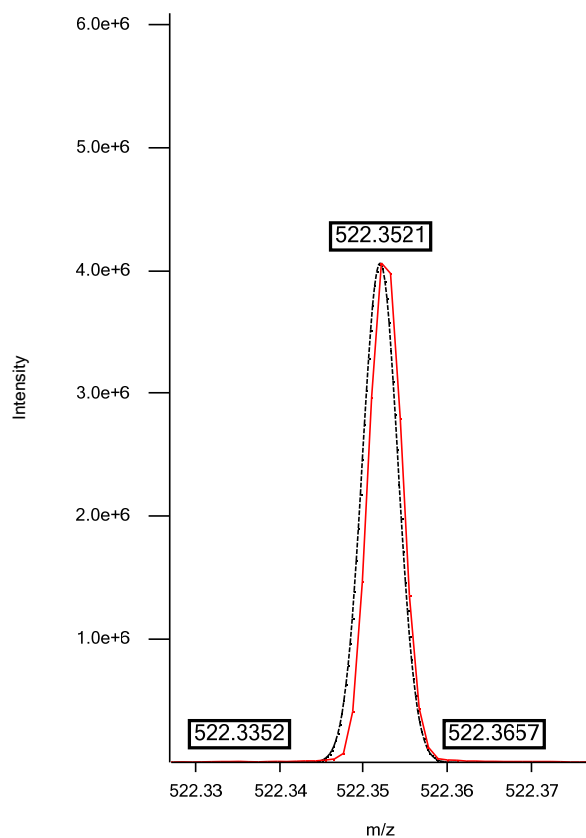


Isotope 3

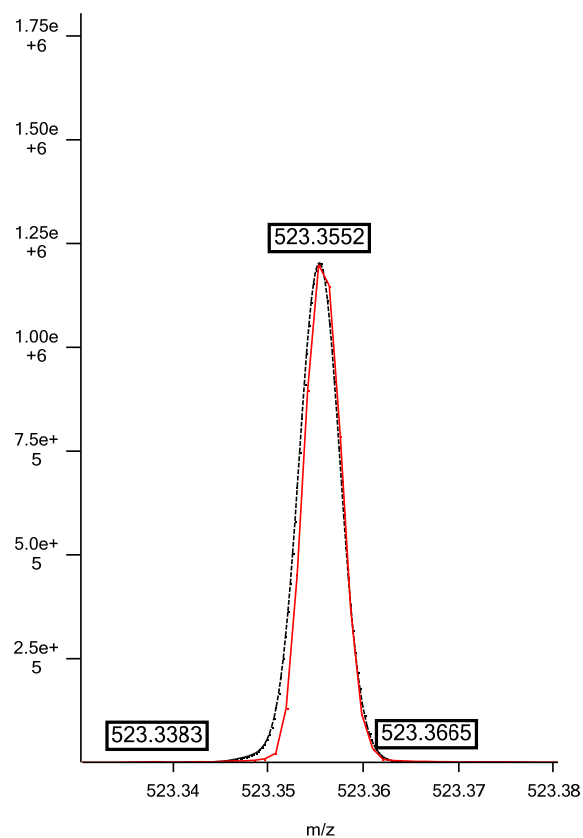


Positive ESI: LPC 18:1; C₂₆H₅₃NO₇P; theoretical m/z 522.3559, (M+H)⁺; isotopic fit 0.0032

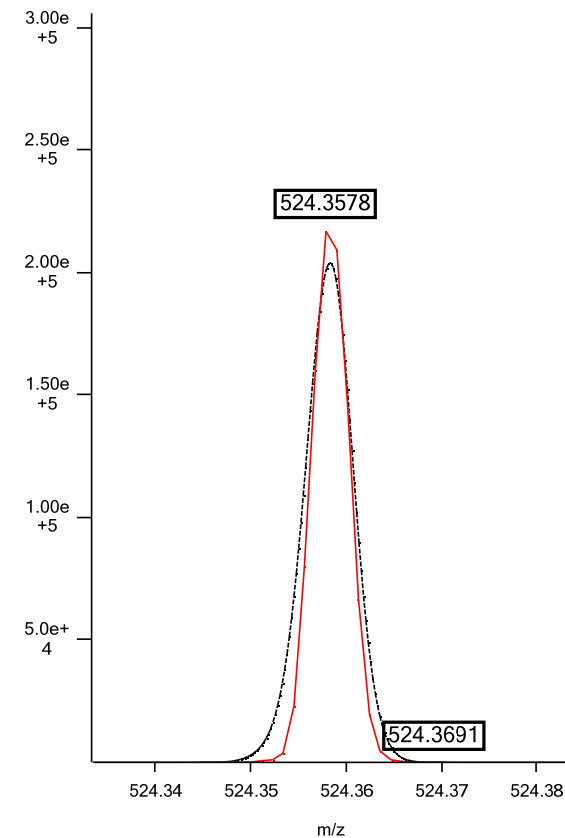
Isotope 1



Isotope 2

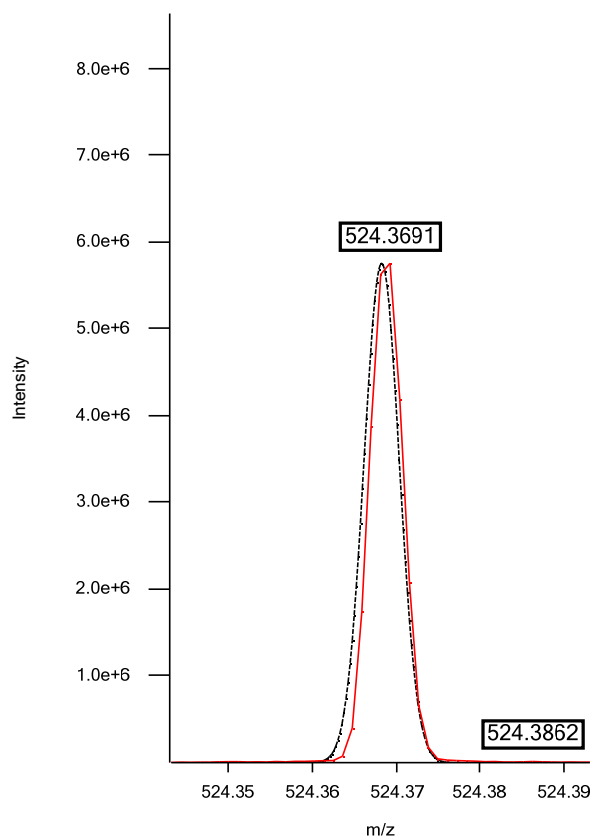


Isotope 3

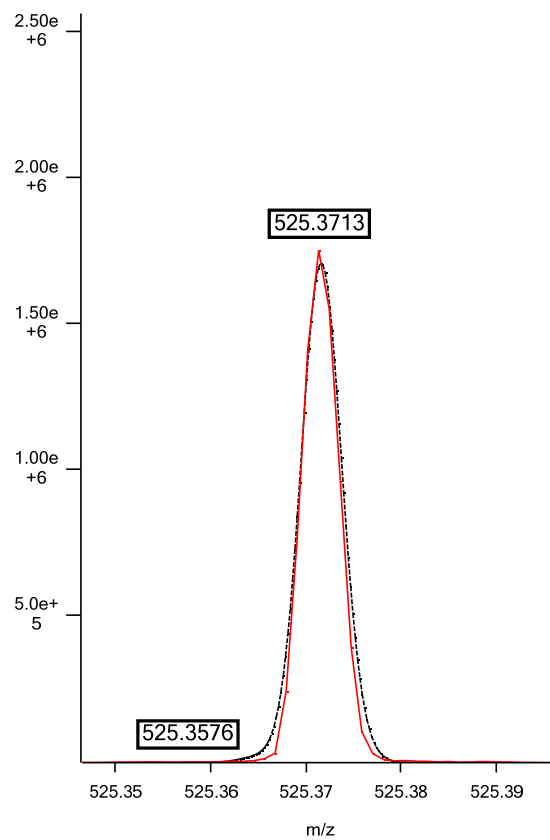


Positive ESI: LPC 18:0; C₂₆H₅₅NO₇P; theoretical *m/z* 524.3716, (M+H)⁺; isotopic fit 0.0014

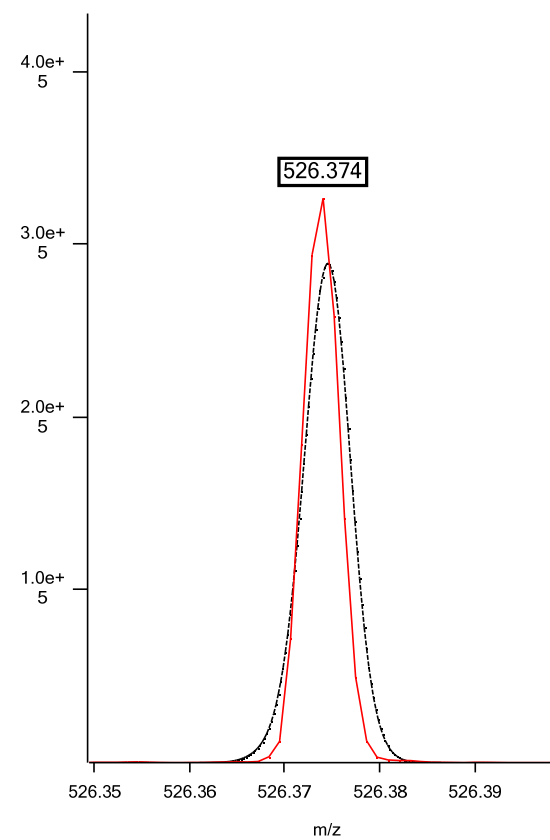
Isotope 1



Isotope 2

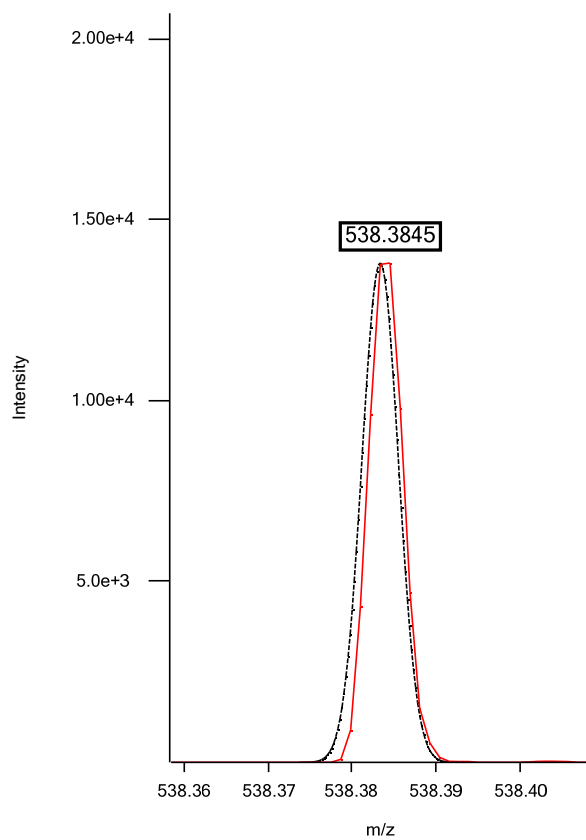


Isotope 3

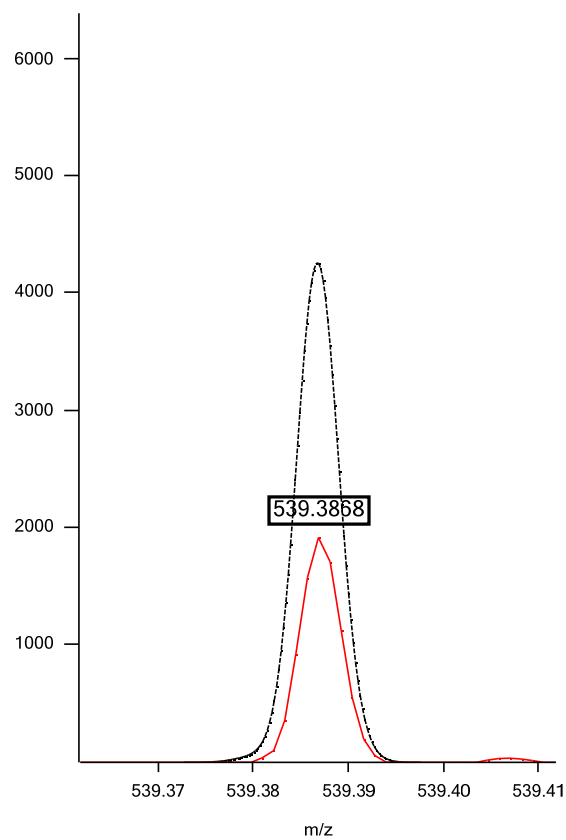


Positive ESI: LPC 19:0; C₂₇H₅₇NO₇P; theoretical *m/z* 538.3872, (M+H)⁺; isotopic fit 0.0186

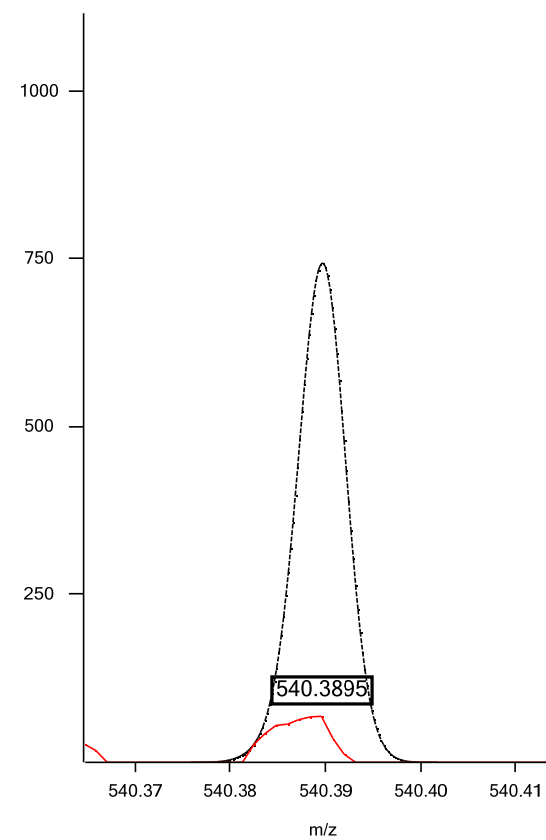
Isotope 1



Isotope 2

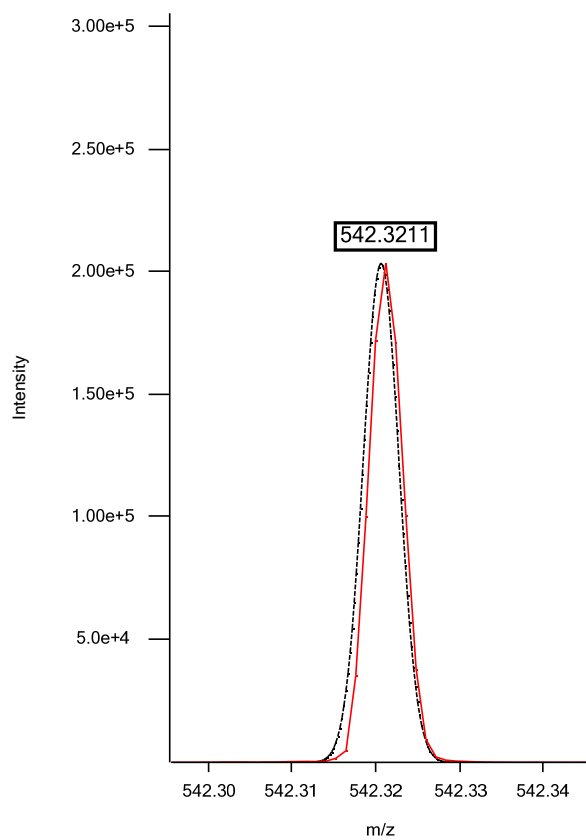


Isotope 3

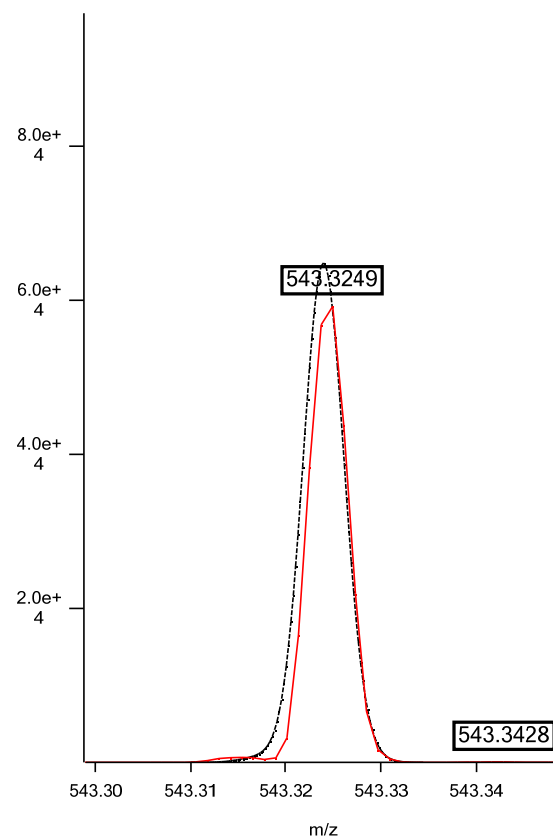


Positive ESI: LPC 20:5; C₂₈H₄₉NO₇P; theoretical *m/z* 542.3246, (M+H)⁺; isotopic fit 0.0029

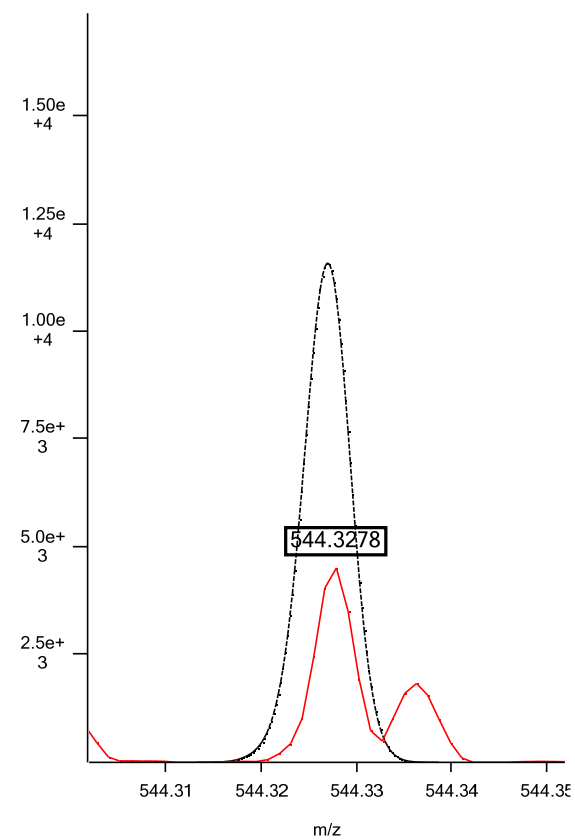
Isotope 1



Isotope 2

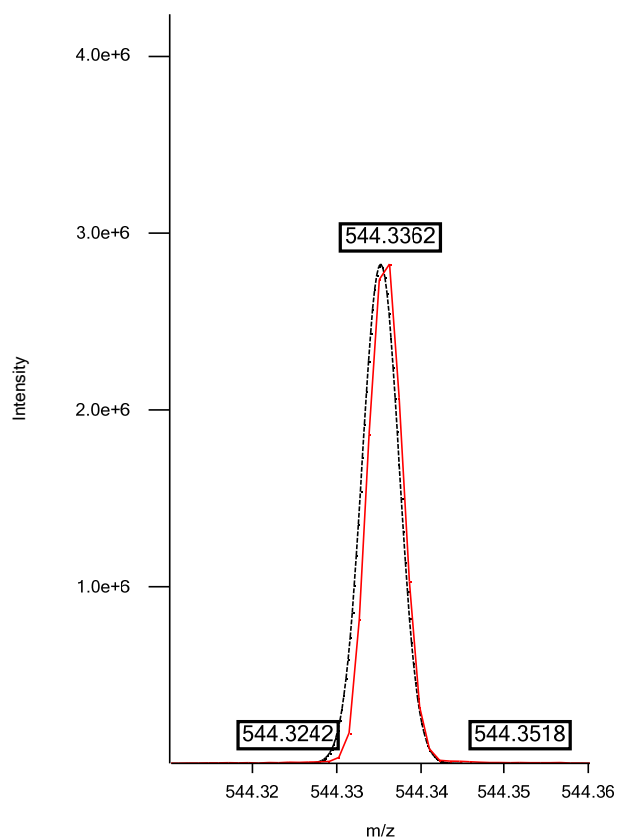


Isotope 3

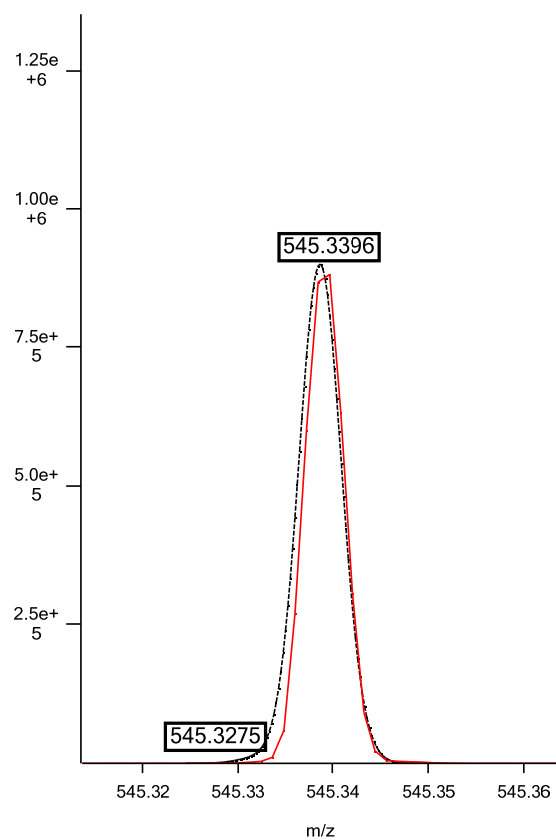


Positive ESI: LPC 20:4; C₂₈H₅₁NO₇P; theoretical m/z 544.3403, (M+H)⁺; isotopic fit 0.0006

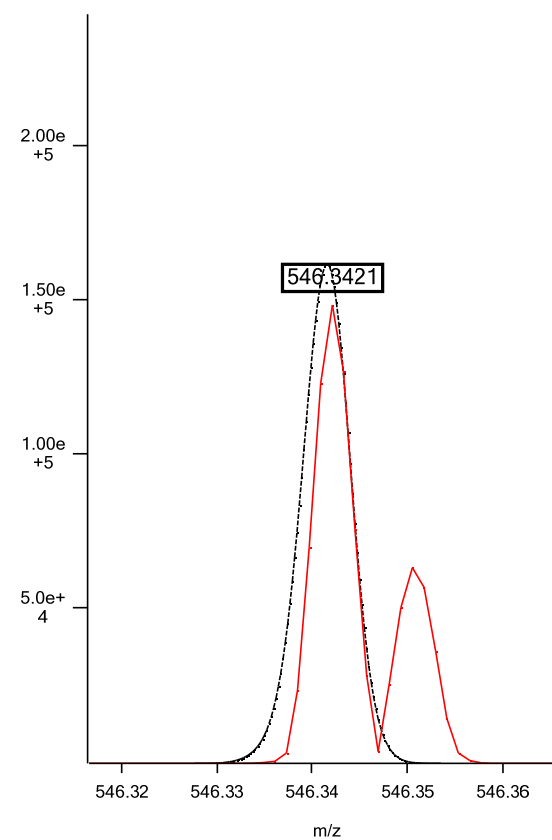
Isotope 1



Isotope 2

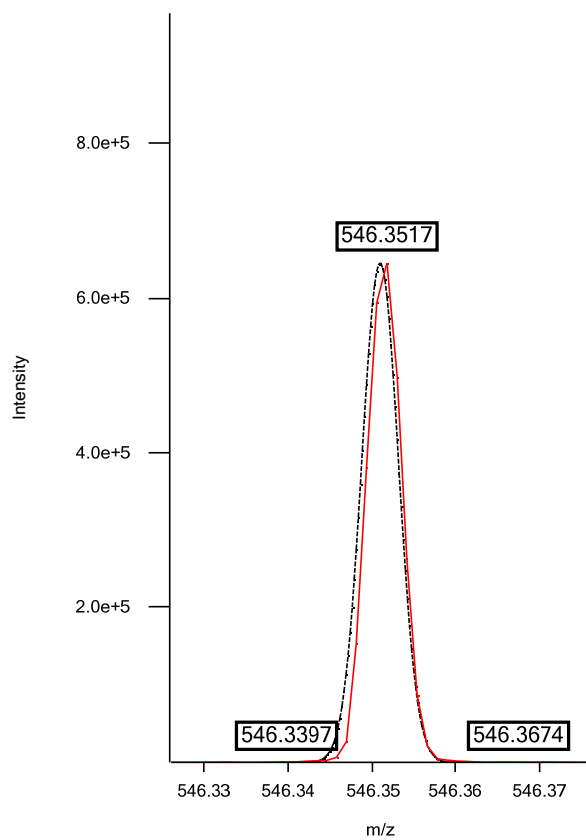


Isotope 3

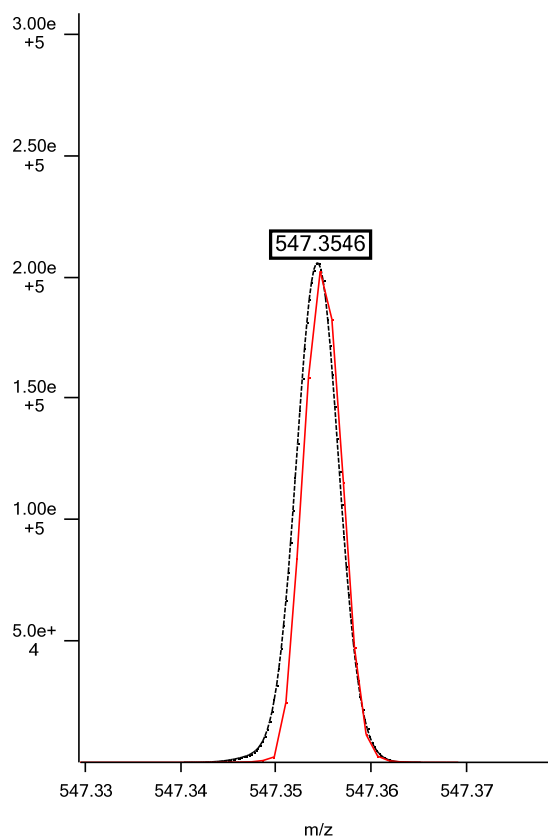


Positive ESI: LPC 20:3; C₂₈H₅₃NO₇P; theoretical *m/z* 546.3559, (M+H)⁺; isotopic fit 0.0038

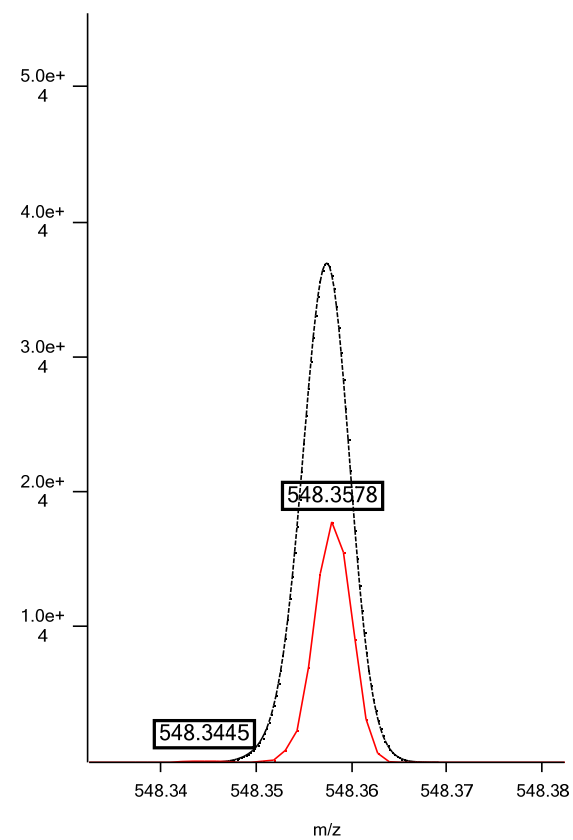
Isotope 1



Isotope 2

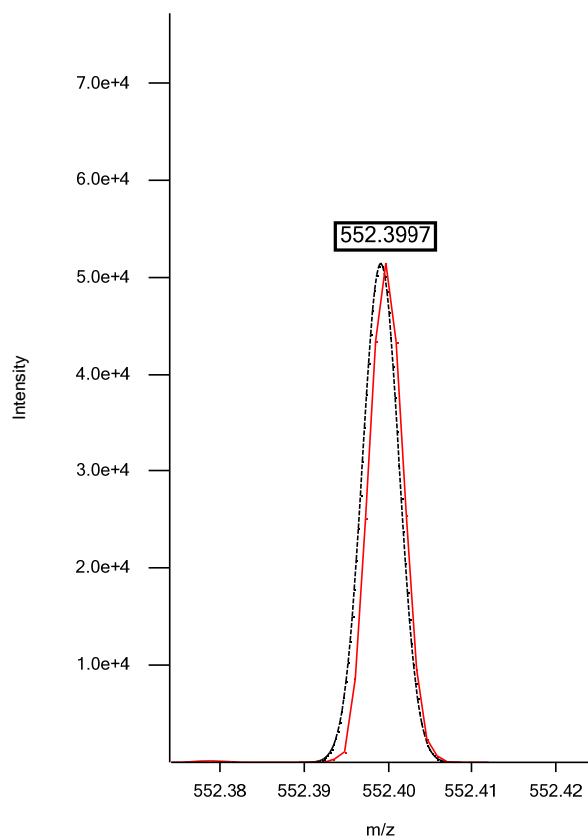


Isotope 3

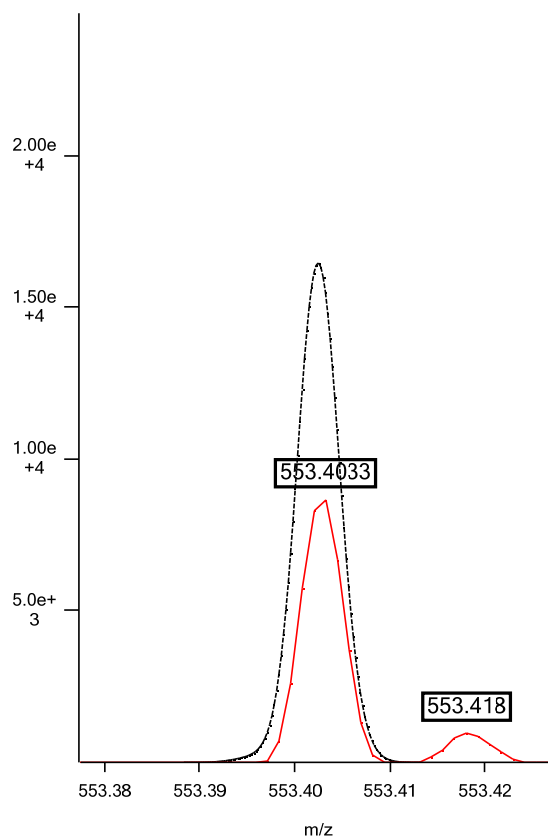


Positive ESI: LPC 20:0; C₂₈H₅₉NO₇P; theoretical m/z 552.4029, (M+H)⁺; isotopic fit 0.0211

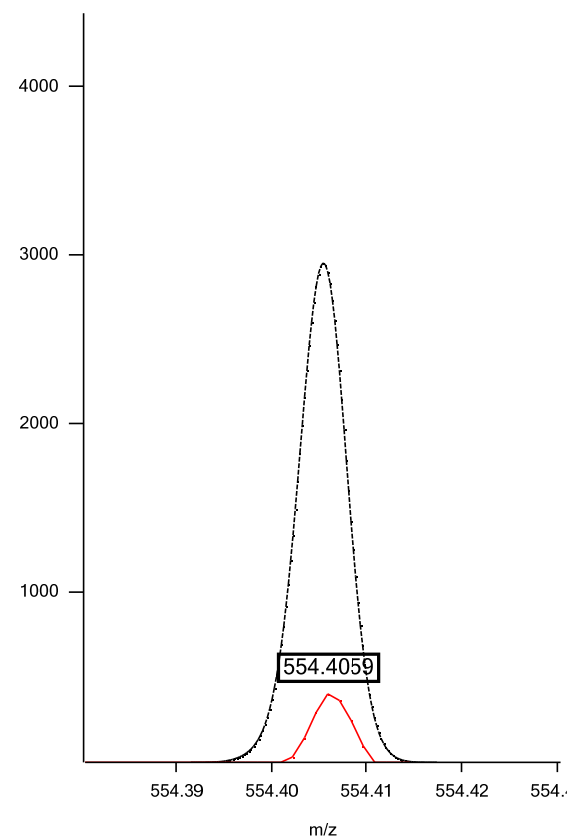
Isotope 1



Isotope 2

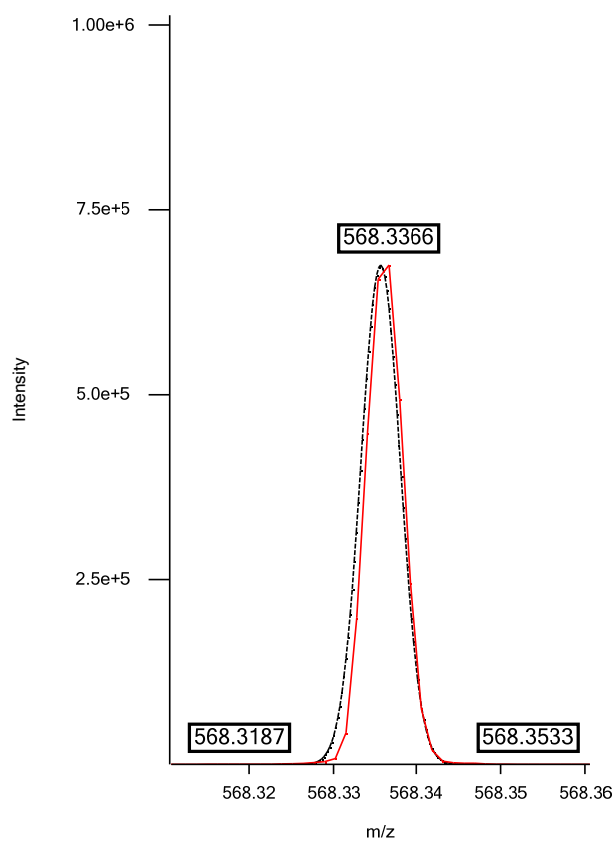


Isotope 3

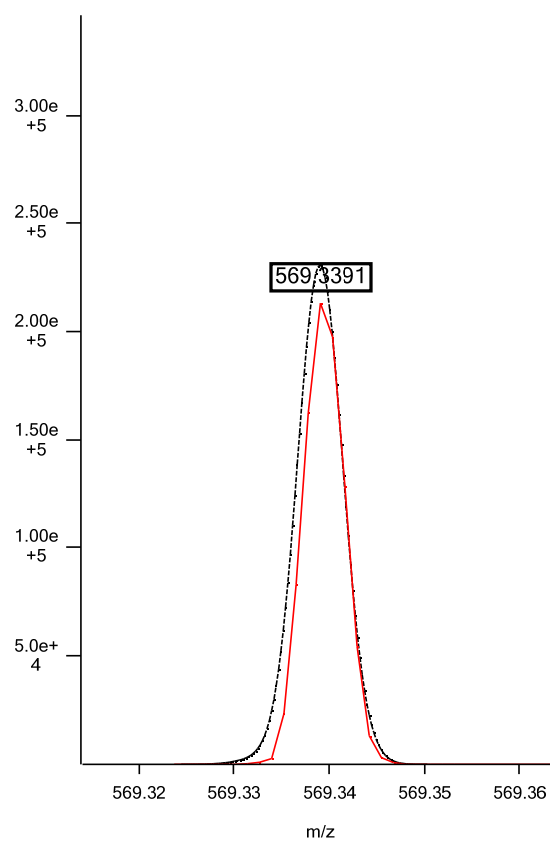


Positive ESI: LPC 22:6; C₃₀H₅₁NO₇P; theoretical m/z 568.3403, (M+H)⁺; isotopic fit 0.0089

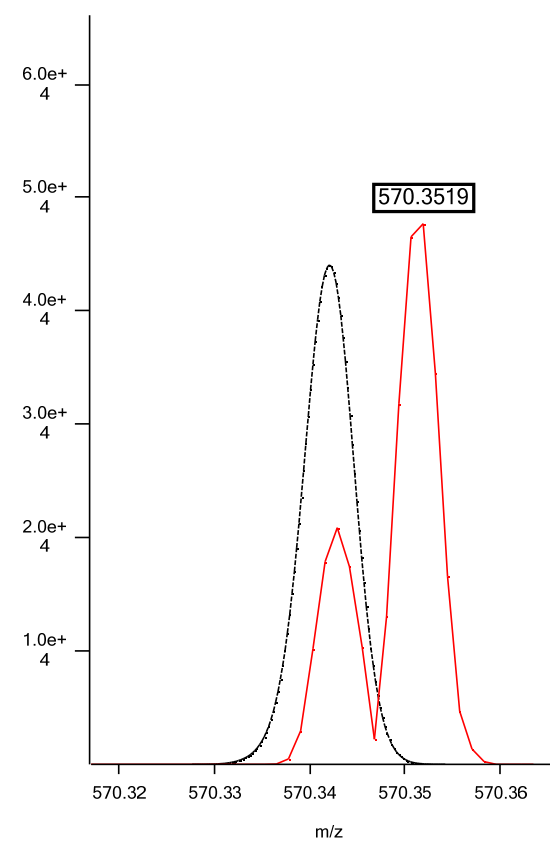
Isotope 1



Isotope 2

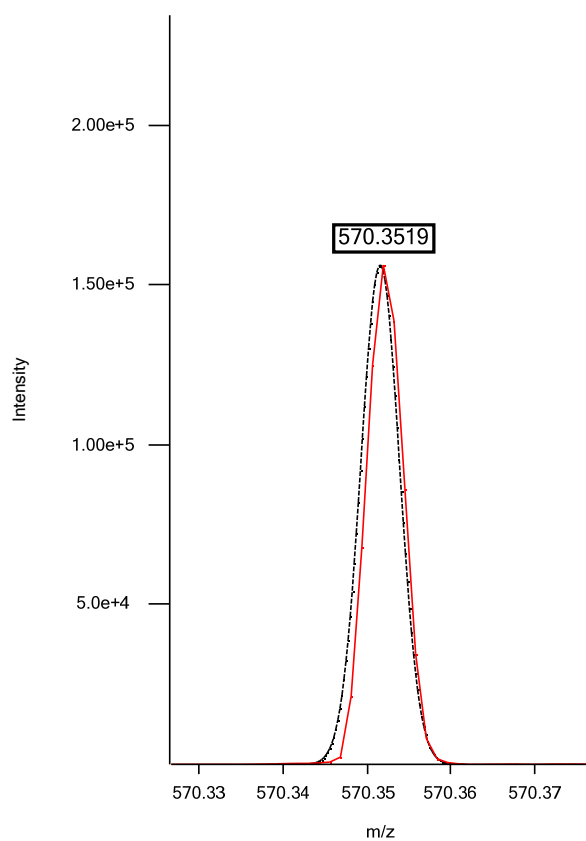


Isotope 3

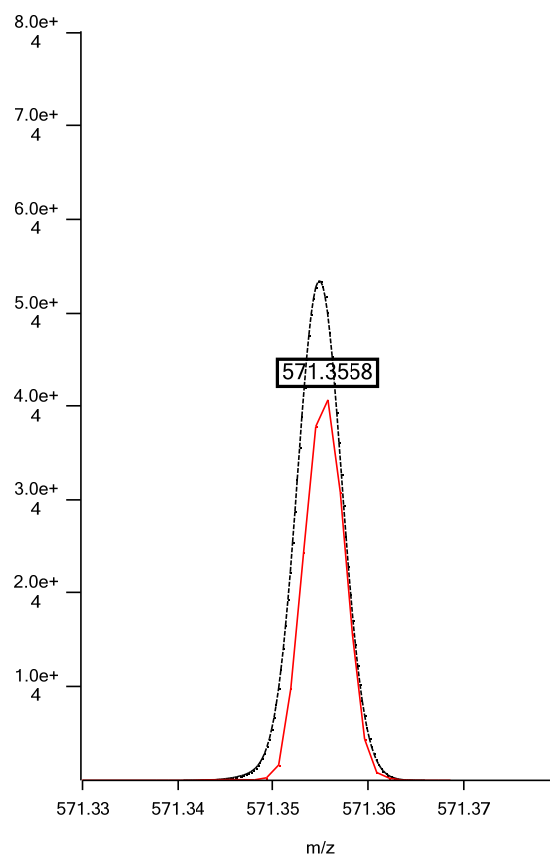


Positive ESI: LPC 22:5; C₃₀H₅₃NO₇P; theoretical m/z 570.3560, (M+H)⁺; isotopic fit 0.0200

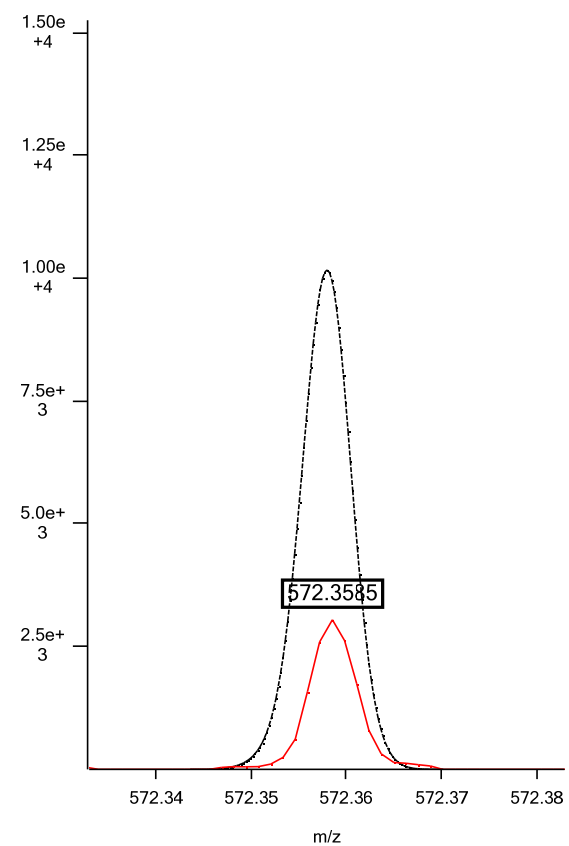
Isotope 1



Isotope 2

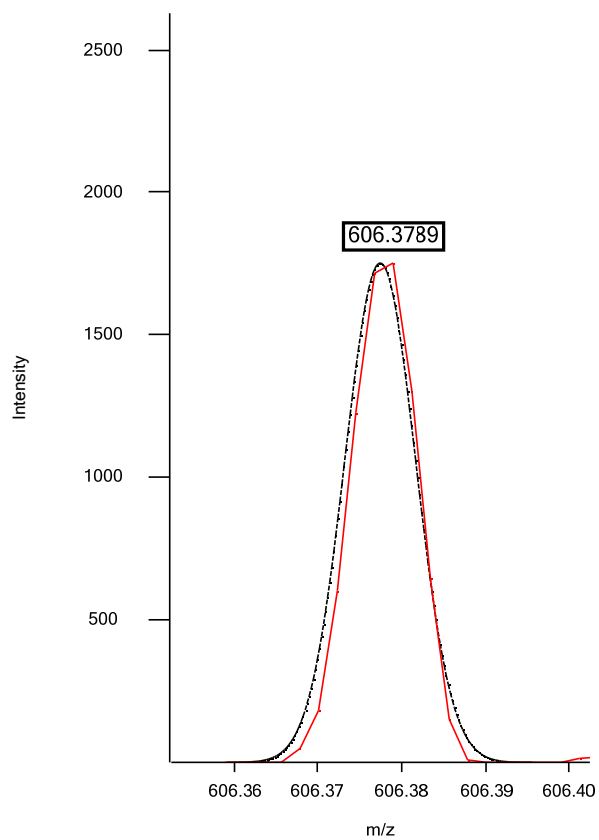


Isotope 3

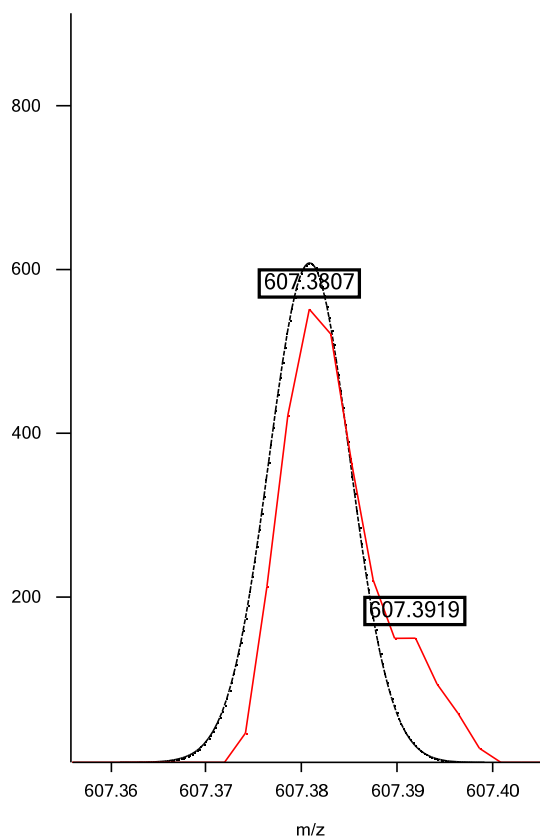


Positive ESI: Oxidized PC 17:1/Keto-5:0; $C_{30}H_{57}NO_9P$; theoretical m/z 606.3771, (M+H)⁺; isotopic fit 0.0050

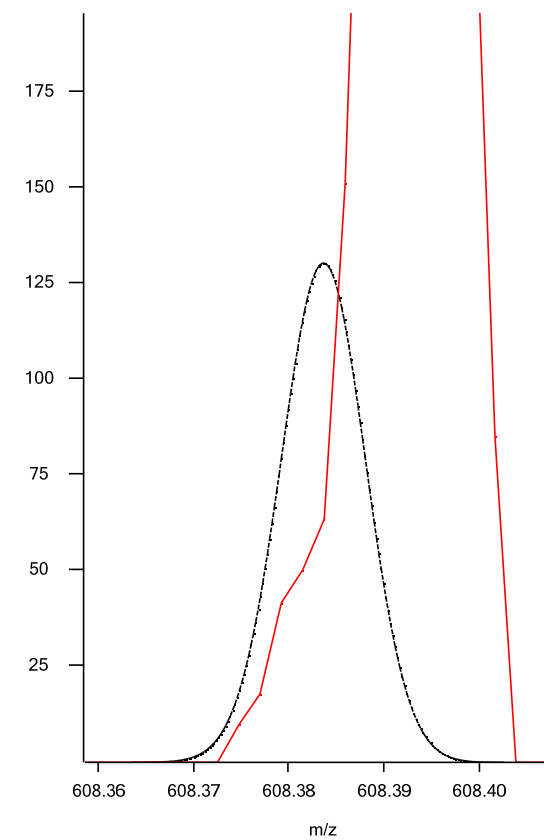
Isotope 1



Isotope 2

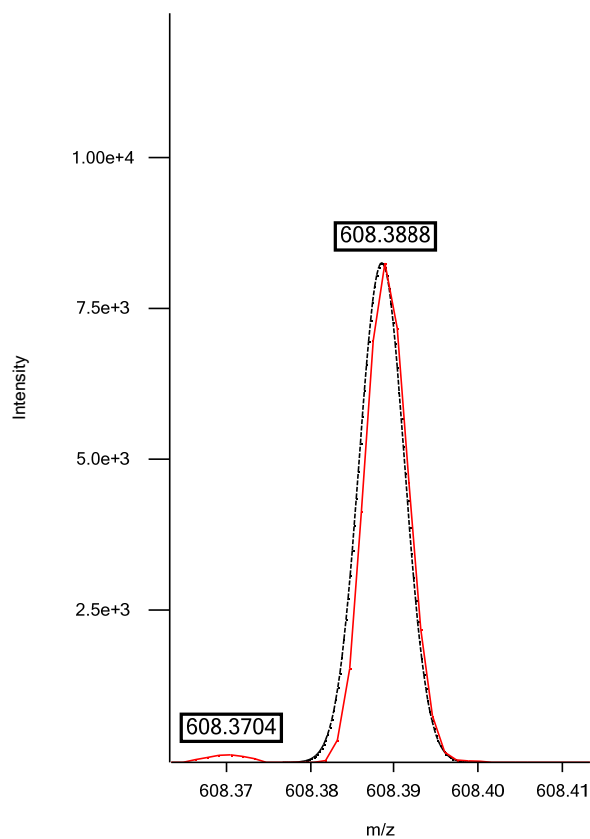


Isotope 3

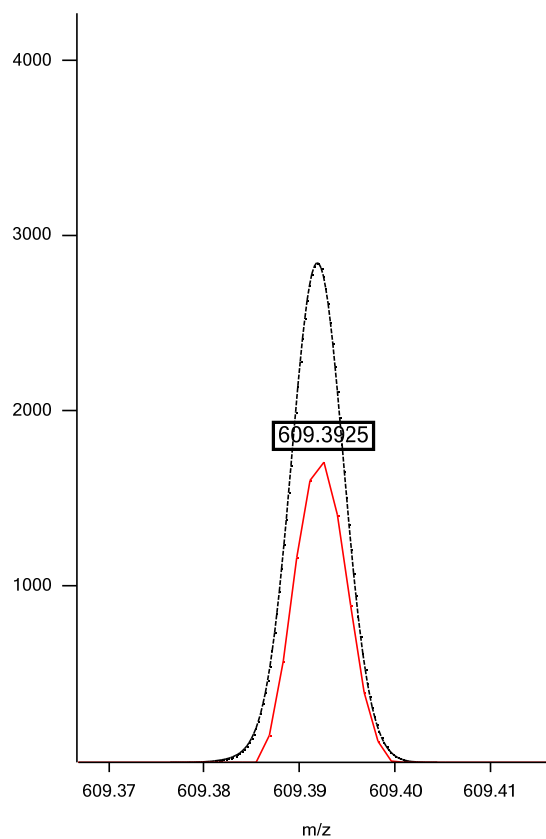


Positive ESI: Oxidized PC 17:0/Keto-5:0; $C_{30}H_{59}NO_9P$; theoretical m/z 608.3927, (M+H)⁺; isotopic fit 0.0249

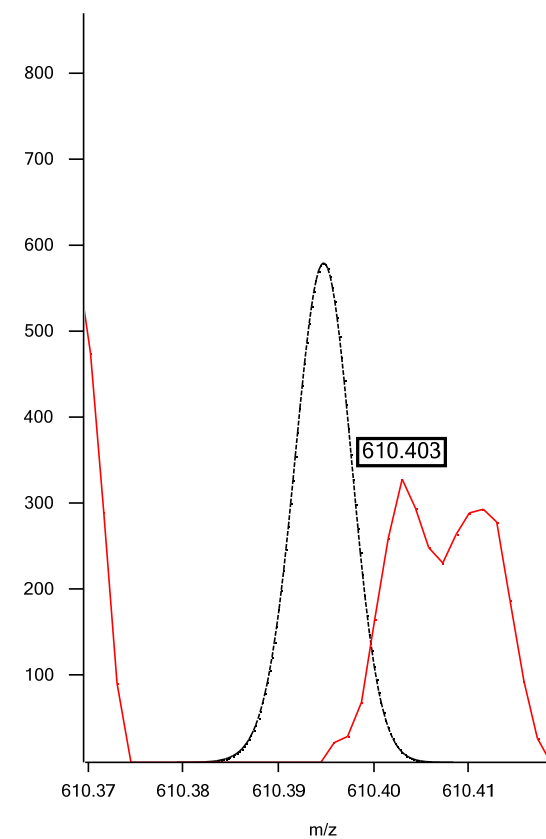
Isotope 1



Isotope 2

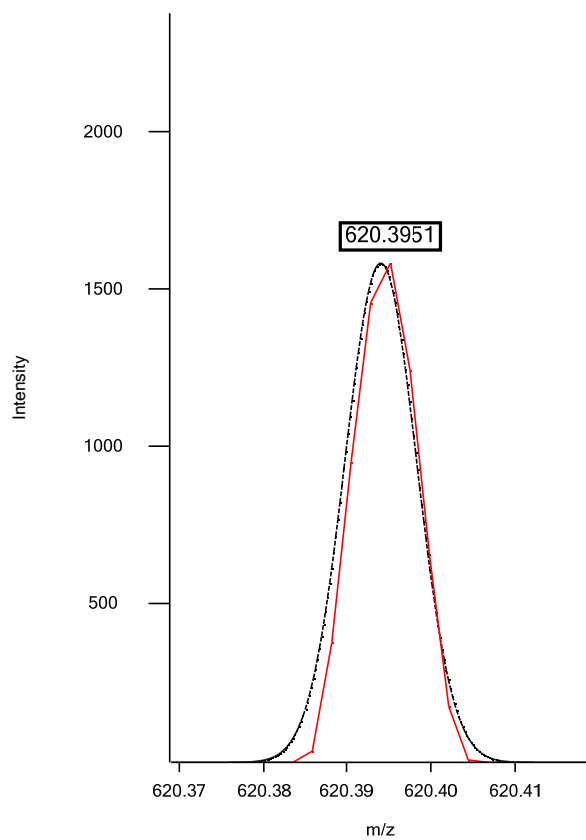


Isotope 3

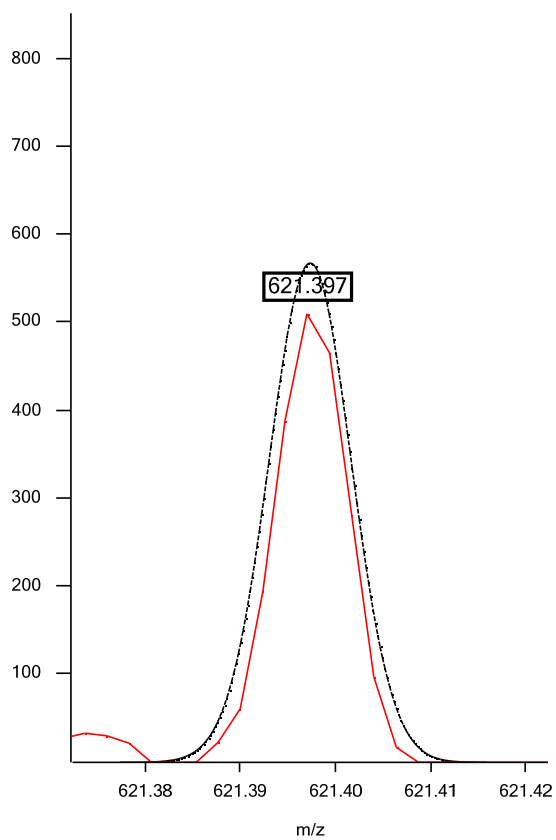


Positive ESI: Oxidized PC 18:1/Keto-5:0; $C_{31}H_{59}NO_9P$; theoretical m/z 620.3927, (M+H)⁺; isotopic fit 0.0045

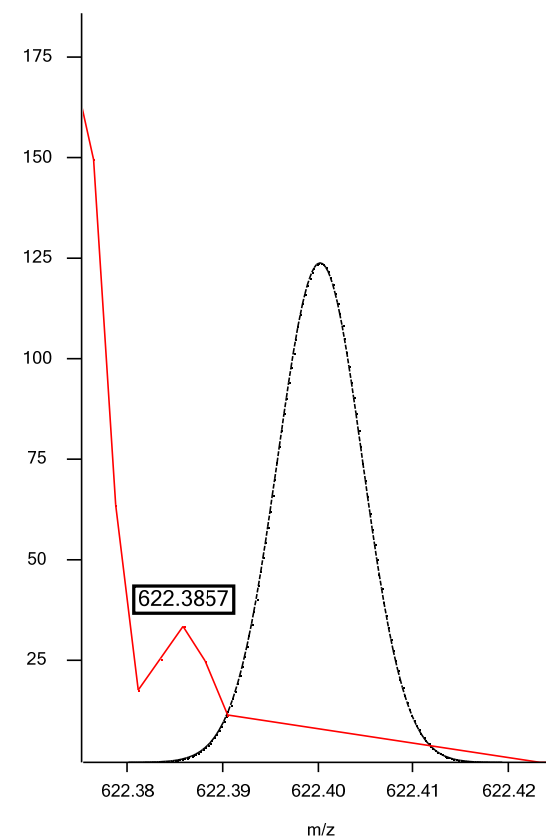
Isotope 1



Isotope 2

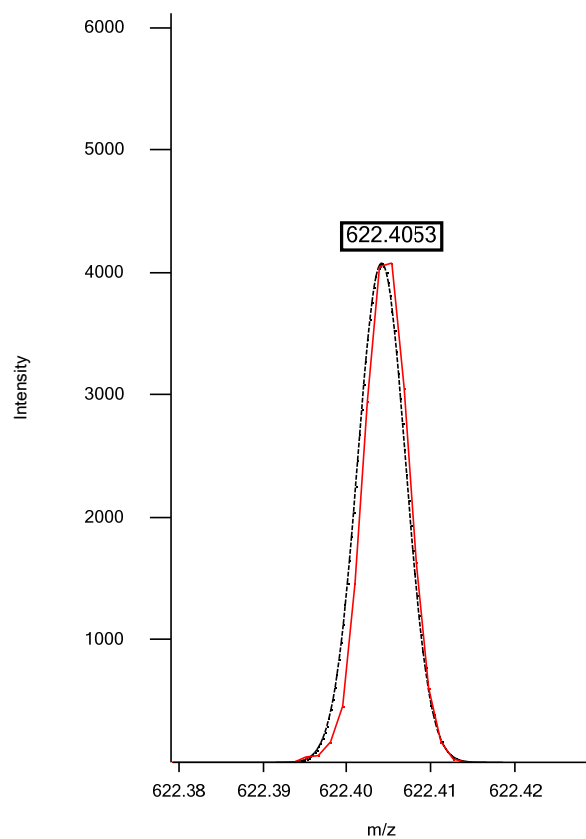


Isotope 3

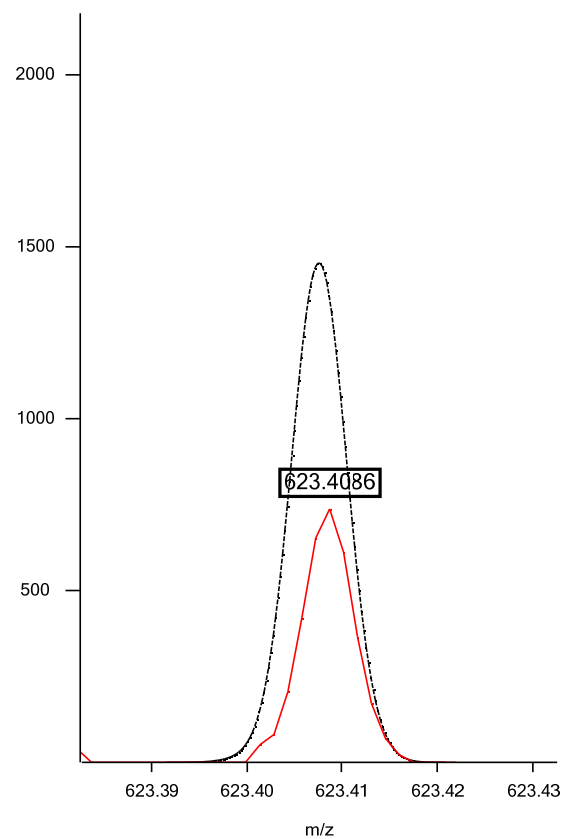


Positive ESI: Oxidized PC 18:0/Keto-5:0; $C_{31}H_{61}NO_9P$; theoretical m/z 622.4084, (M+H)⁺; isotopic fit 0.0263

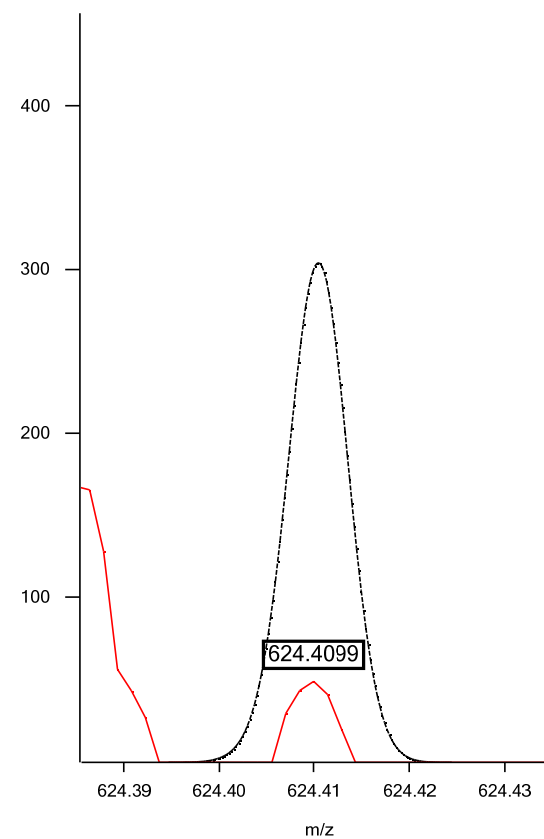
Isotope 1



Isotope 2

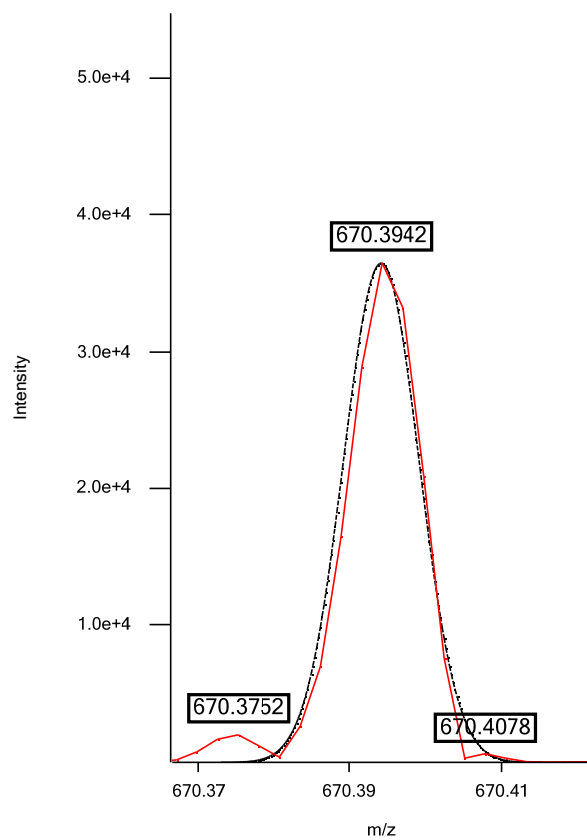


Isotope 3

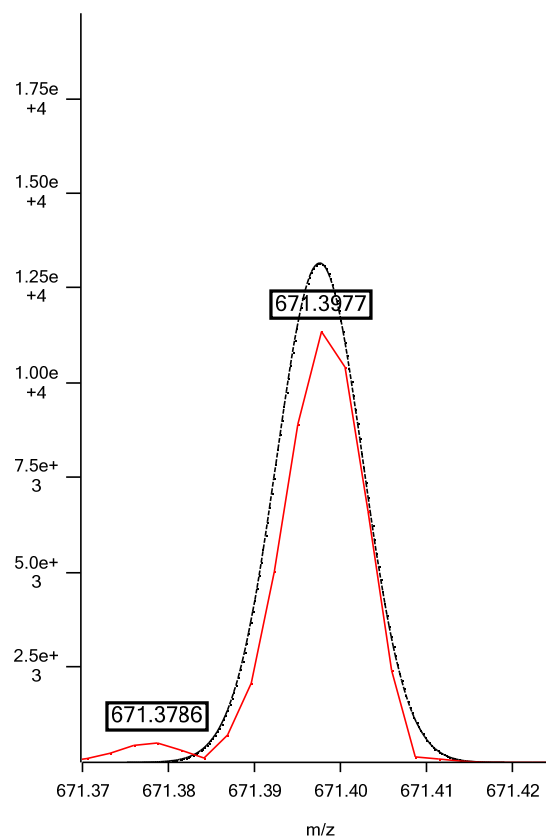


Negative ESI: Oxidized PC 16:0/Hydroperoxy-5:0; $C_{31}H_{61}NO_{12}P$; theoretical m/z 670.3931, $(M-H)^-$; isotopic fit 0.0059

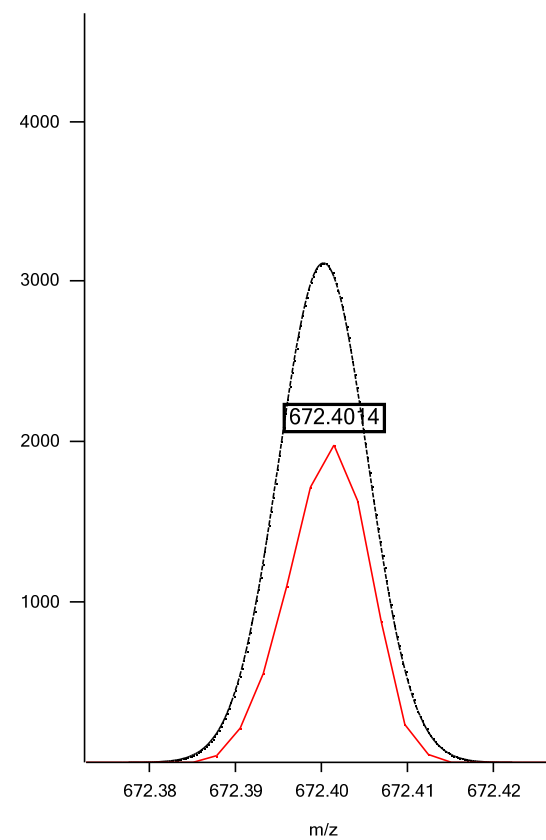
Isotope 1



Isotope 2

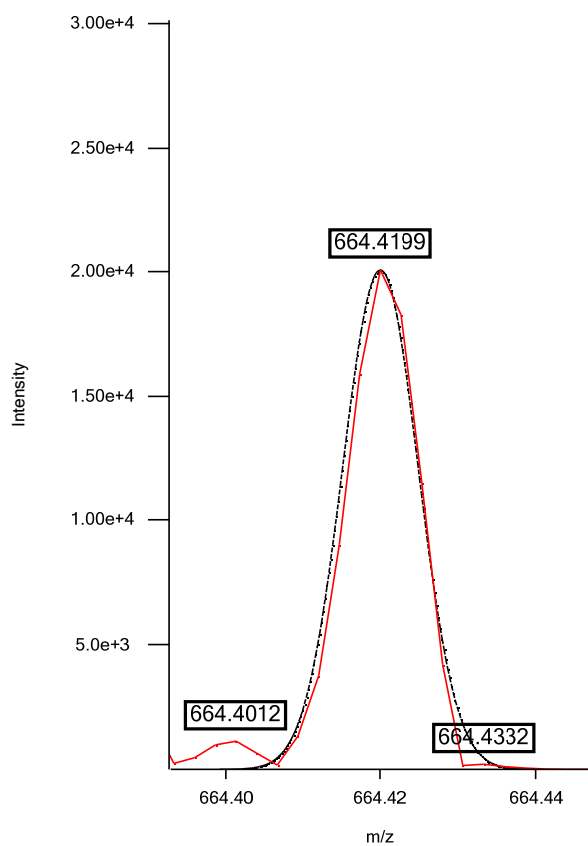


Isotope 3

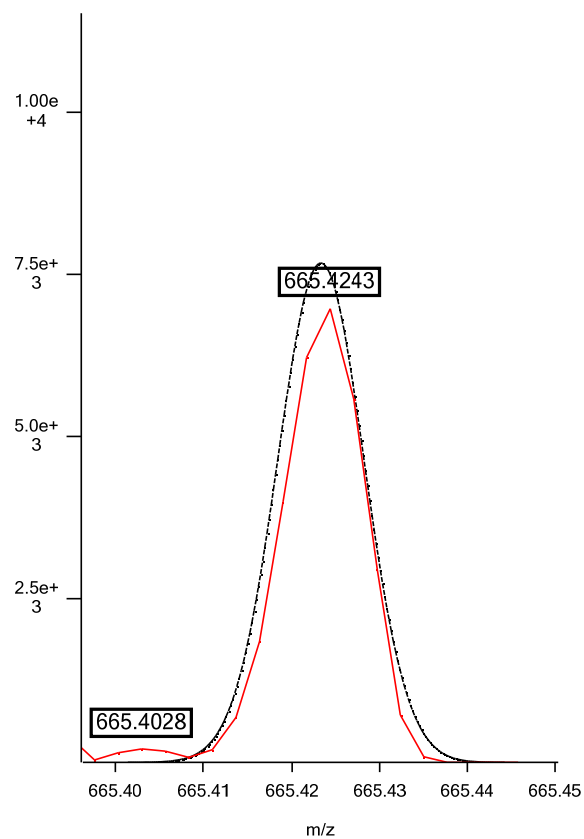


Negative ESI: Oxidized PC 16:0/Hydroxy-7:2e; $C_{33}H_{63}NO_{10}P$; theoretical m/z 664.4189, (M-H)⁻; isotopic fit 0.0035

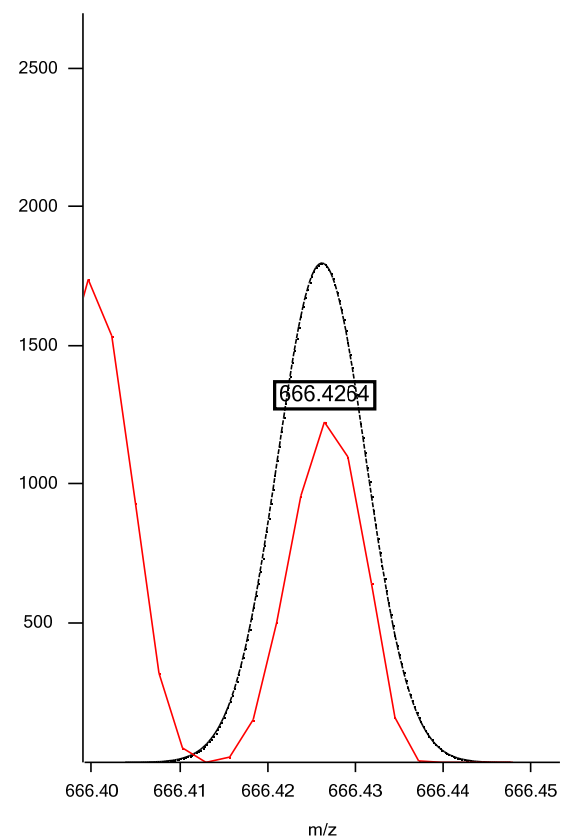
Isotope 1



Isotope 2

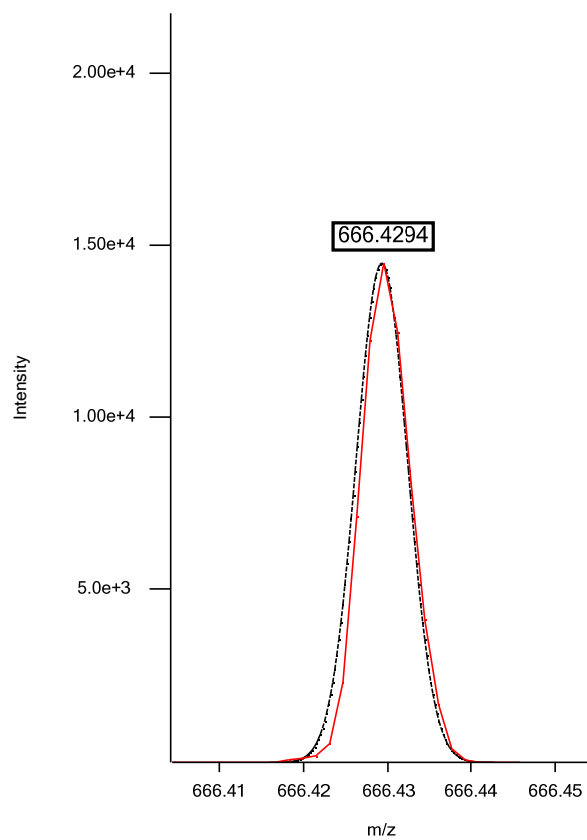


Isotope 3

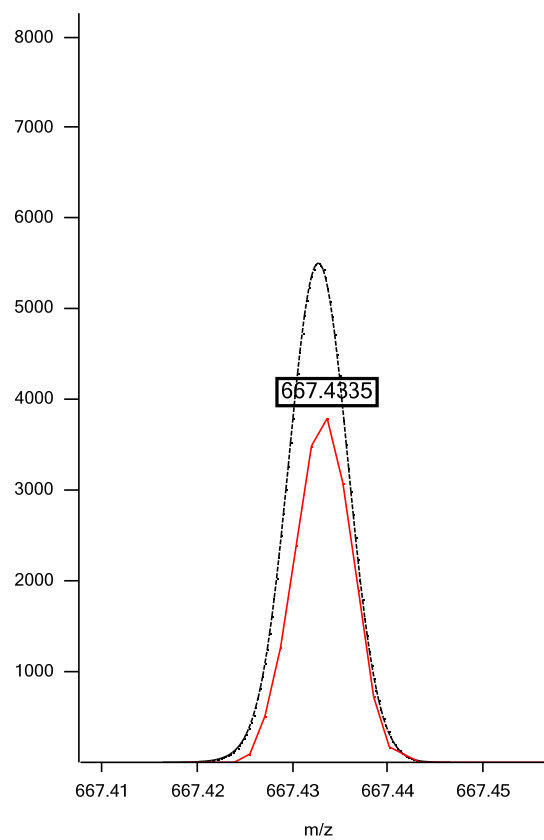


Positive ESI: Oxidized PC 18:0/Carboxy-7:0; $C_{33}H_{65}NO_{10}P$; theoretical m/z 666.4346, $(M+H)^+$; isotopic fit 0.0211

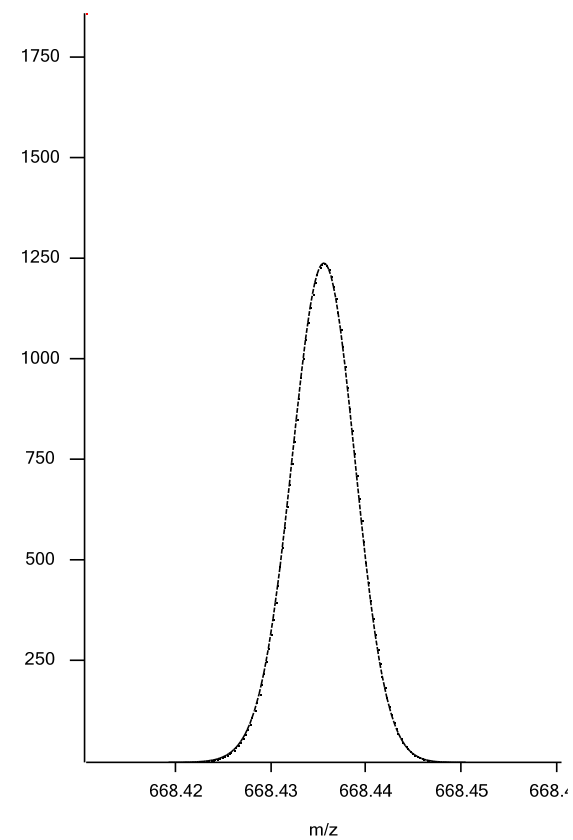
Isotope 1



Isotope 2

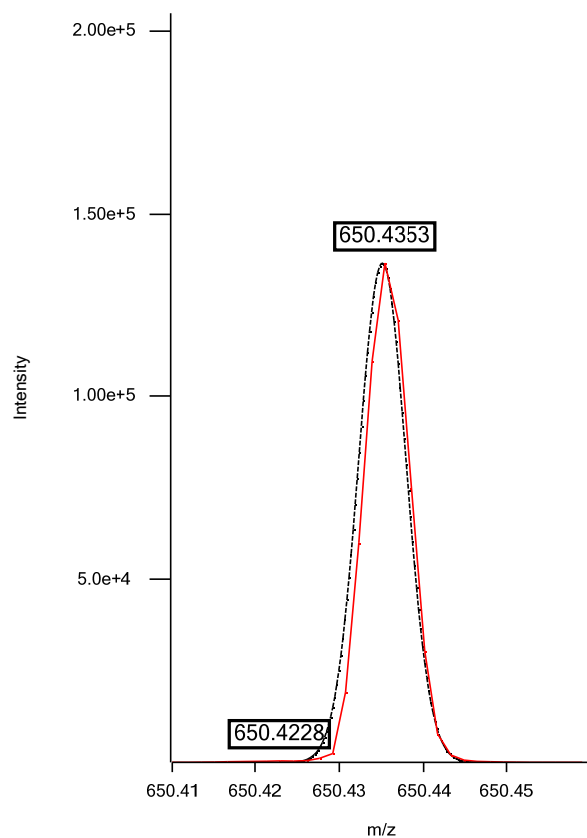


Isotope 3

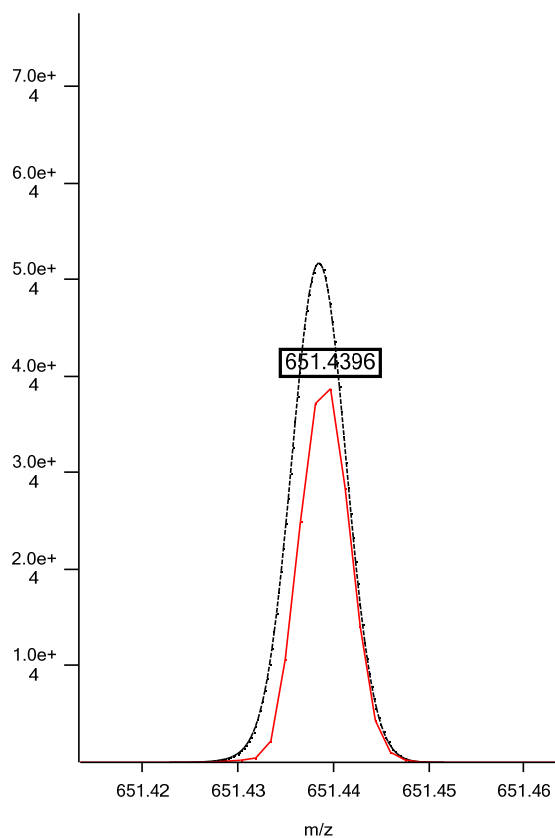


Positive ESI: Oxidized PC 18:0/Keto-7:0; $C_{33}H_{65}NO_9P$; theoretical m/z 650.4397, $(M+H)^+$; isotopic fit 0.0080

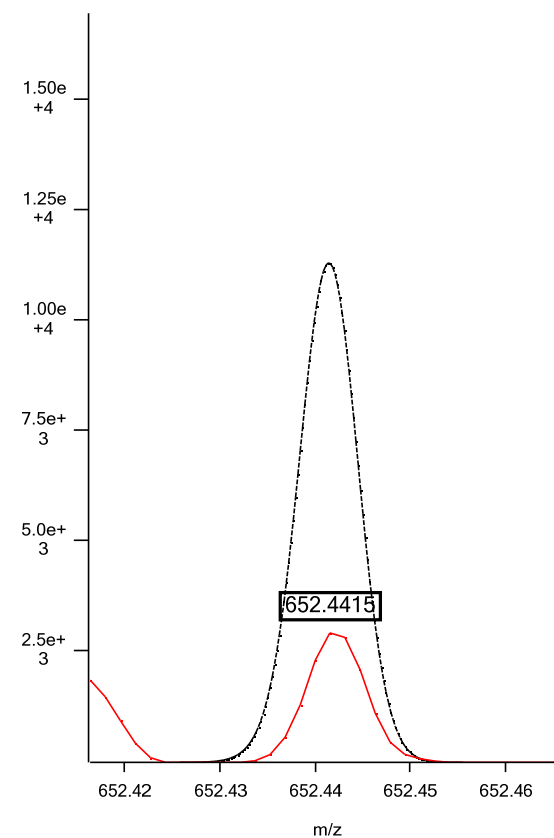
Isotope 1



Isotope 2

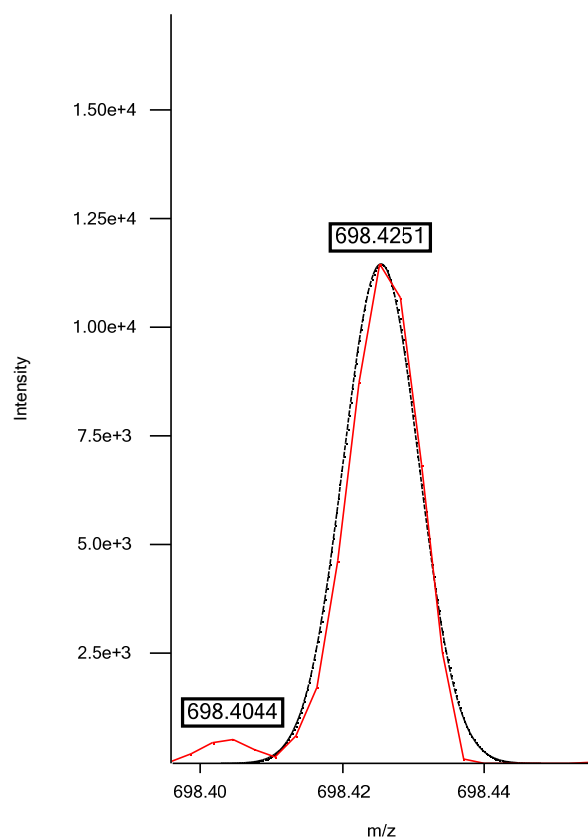


Isotope 3

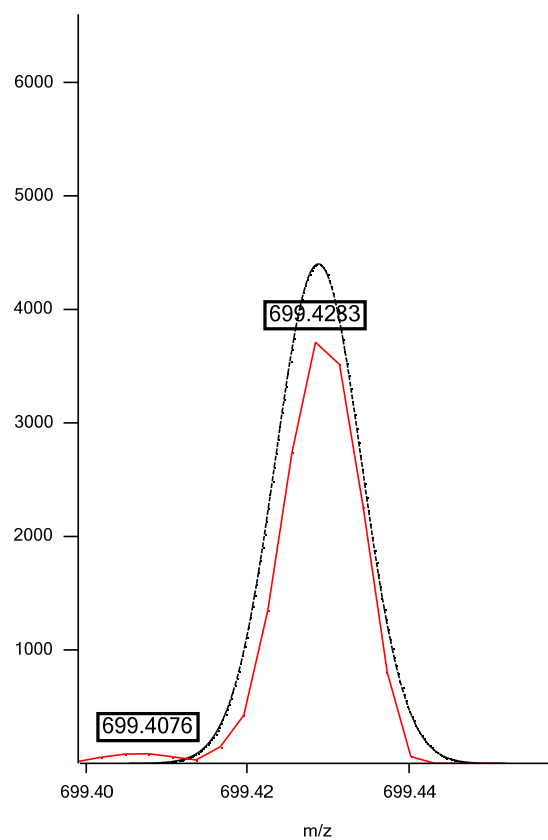


Negative ESI: Oxidized PC 18:0/Hydroperoxy-5:0; $C_{33}H_{65}NO_{12}P$; theoretical m/z 698.4244, $(M-H)^-$; isotopic fit 0.0057

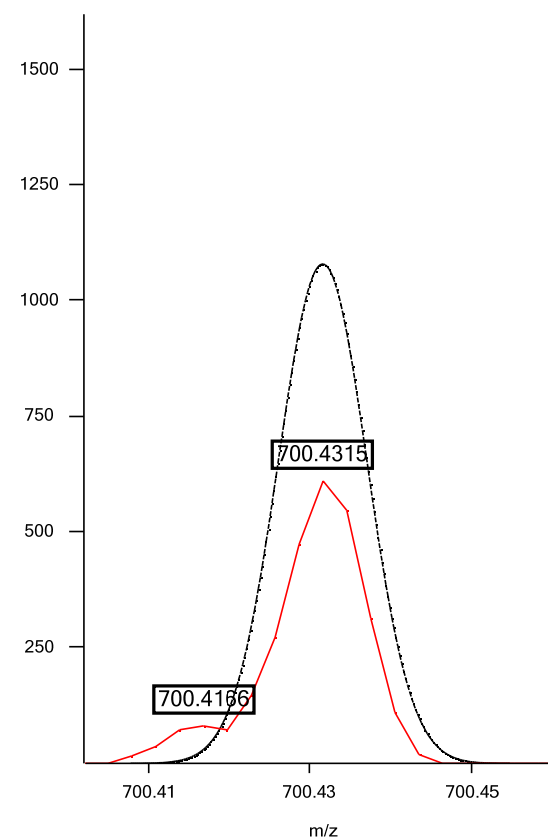
Isotope 1



Isotope 2

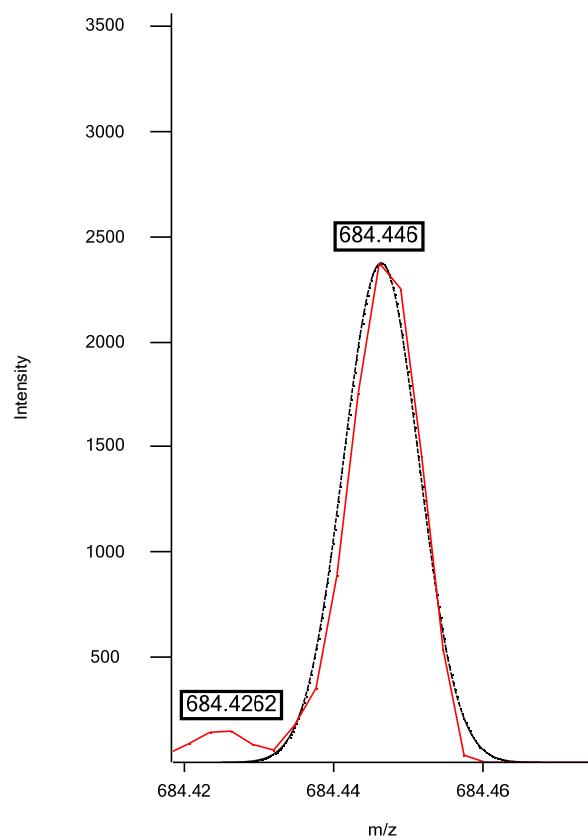


Isotope 3

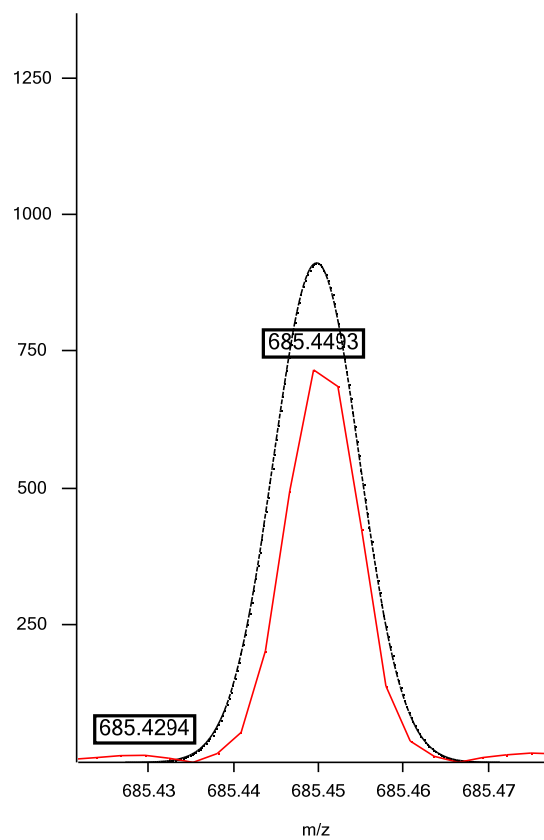


Negative ESI: Oxidized PC 18:0/Hydroperoxy-5:0e; C₃₃H₆₇NO₁₁P; theoretical *m/z* 684.4452, (M-H)⁻; isotopic fit 0.0092

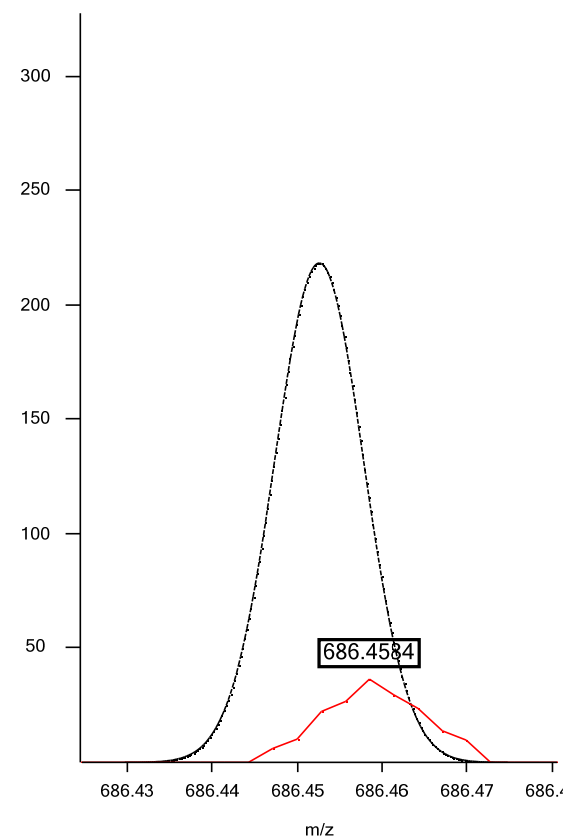
Isotope 1



Isotope 2

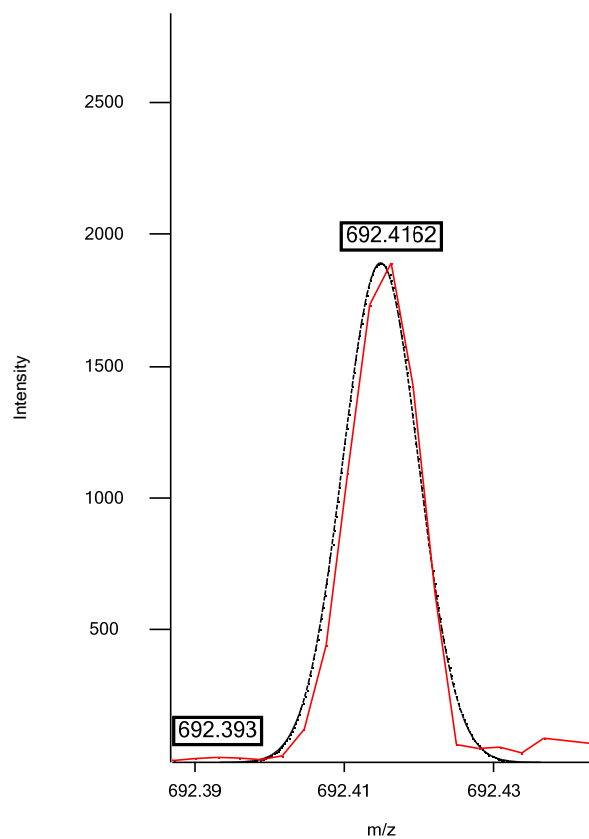


Isotope 3

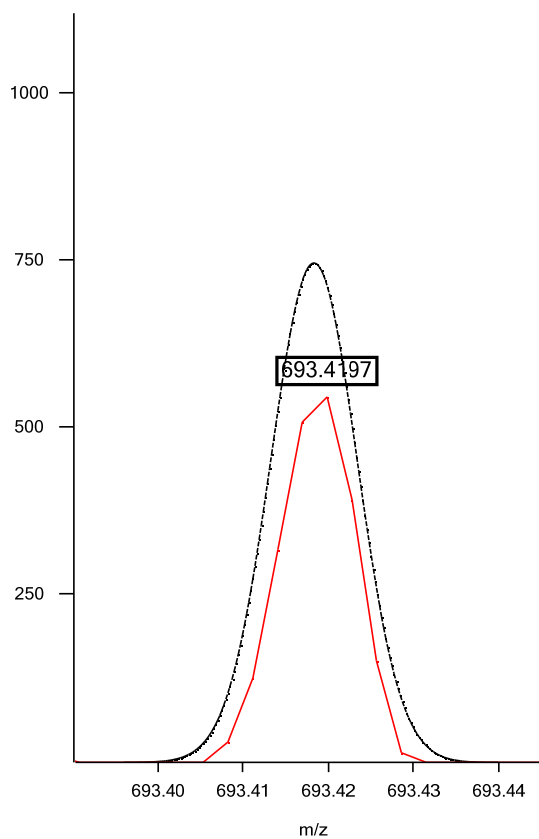


Negative ESI: Oxidized PC 18:0/Keto-6:1; C₃₄H₆₃NO₁₁P; theoretical *m/z* 692.4138, (M-H)⁻; isotopic fit 0.0134

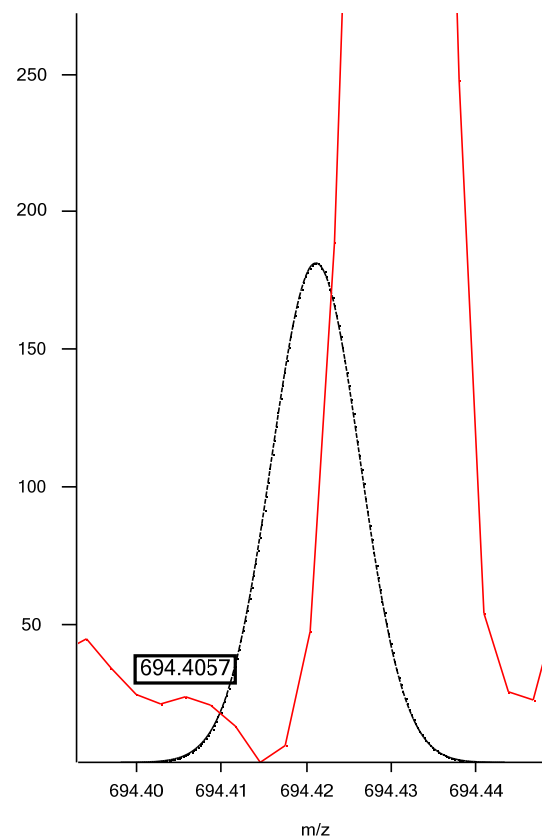
Isotope 1



Isotope 2

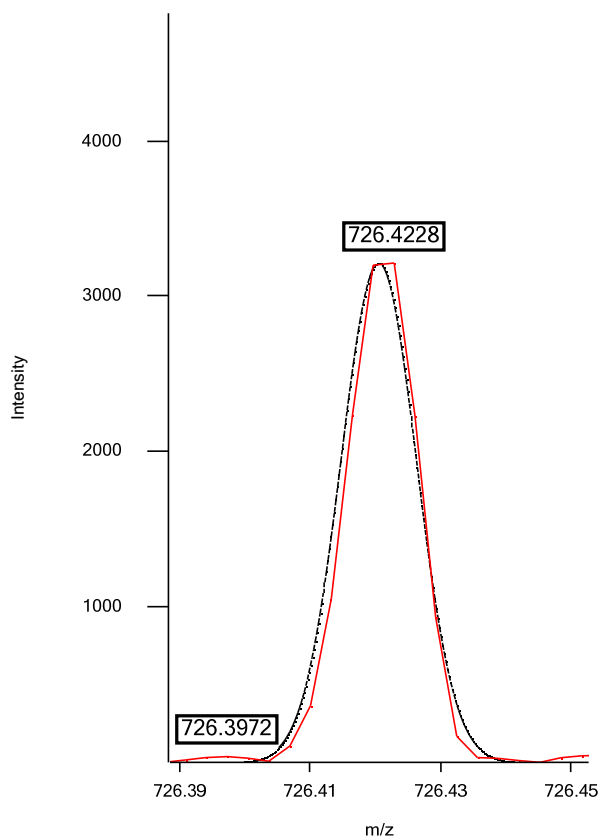


Isotope 3

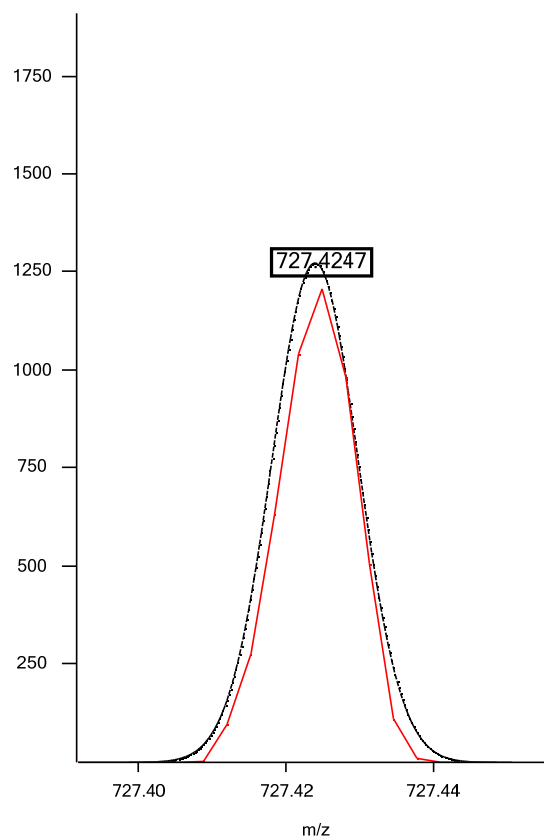


Negative ESI: Oxidized PC 18:1/Trihydroxy-6:0; $C_{34}H_{65}NO_{13}P$; theoretical m/z 726.4193, (M-H)⁻; isotopic fit 0.0041

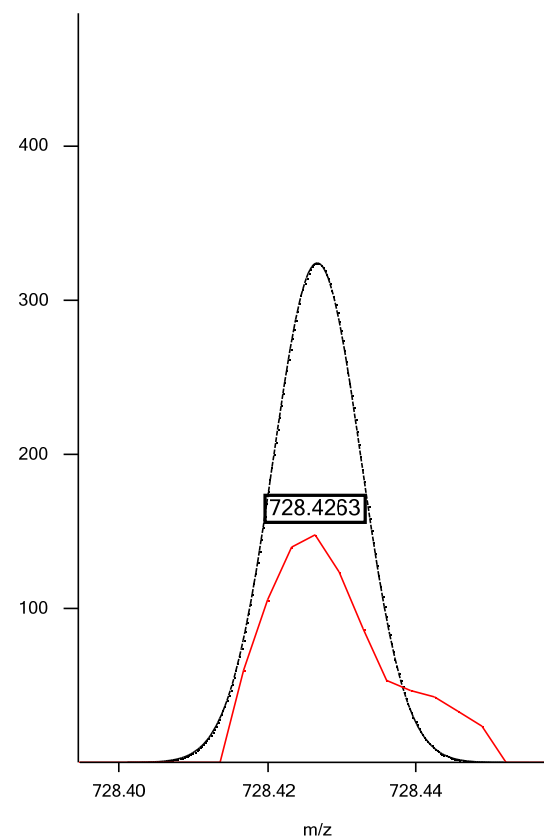
Isotope 1



Isotope 2

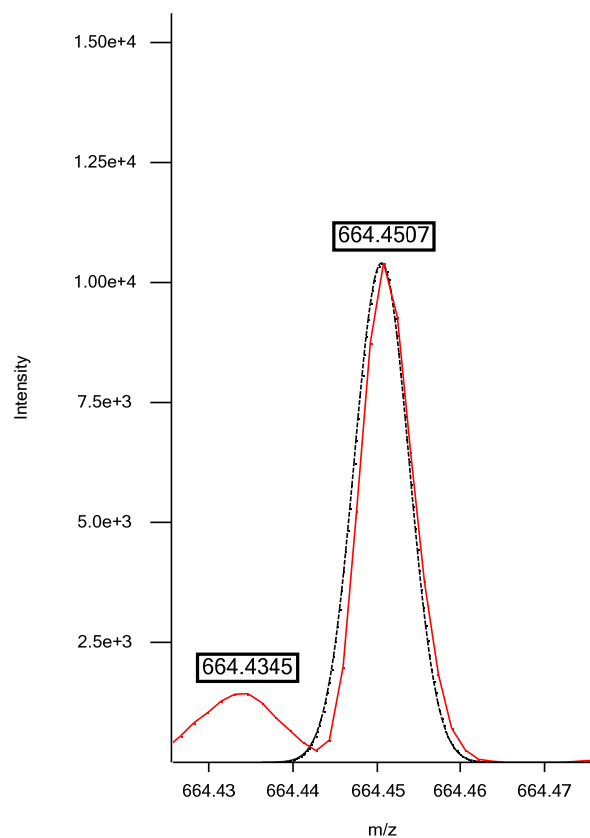


Isotope 3

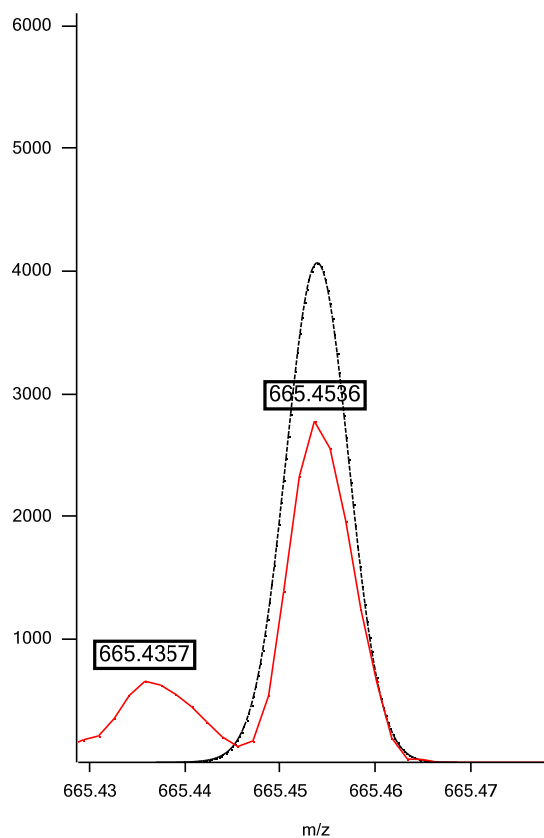


Positive ESI: Oxidized PC 19:0/Keto-7:0; $C_{34}H_{67}NO_9P$; theoretical m/z 664.4553, $(M+H)^+$; isotopic fit 0.0150

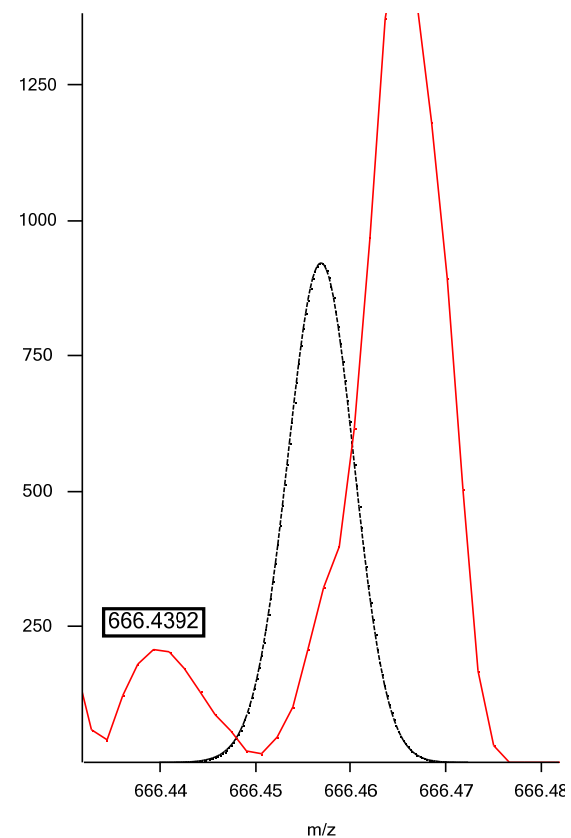
Isotope 1



Isotope 2

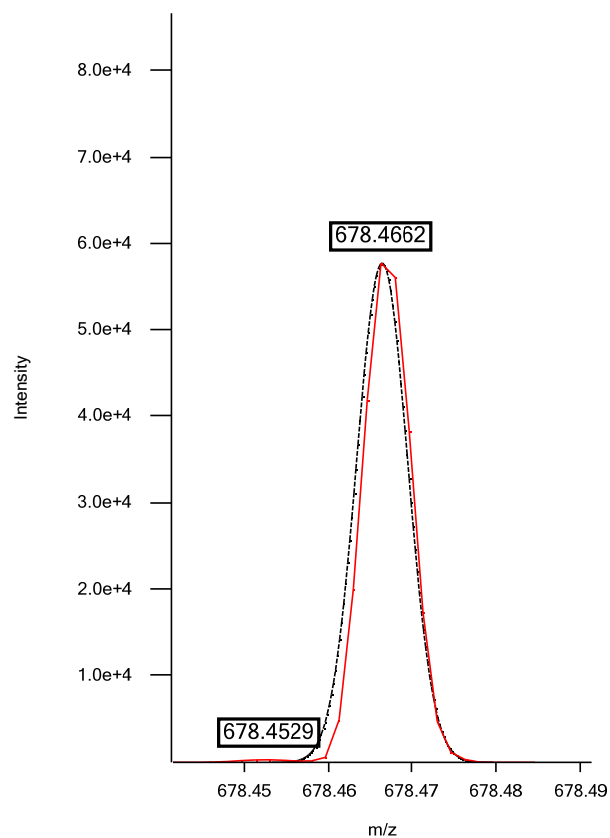


Isotope 3

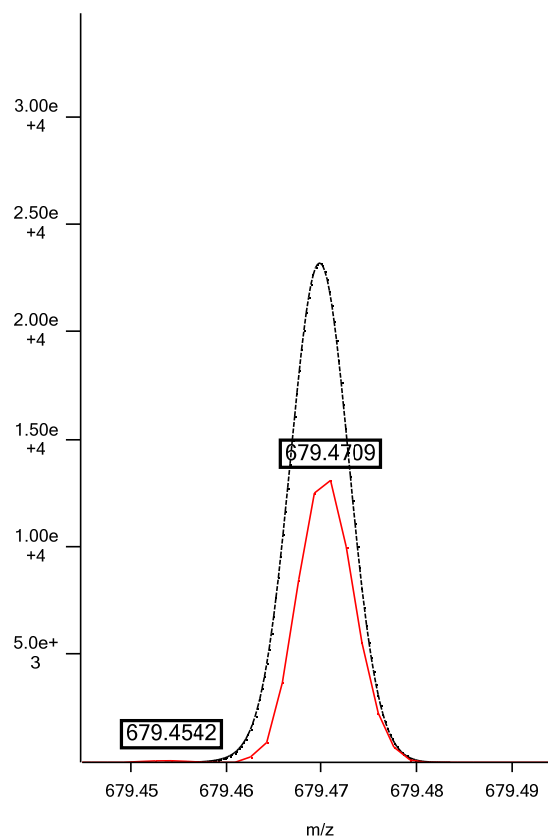


Positive ESI: Oxidized PC 20:0/Keto-7:0; $C_{35}H_{69}NO_9P$; theoretical m/z 678.4710, (M+H)⁺; isotopic fit 0.0269

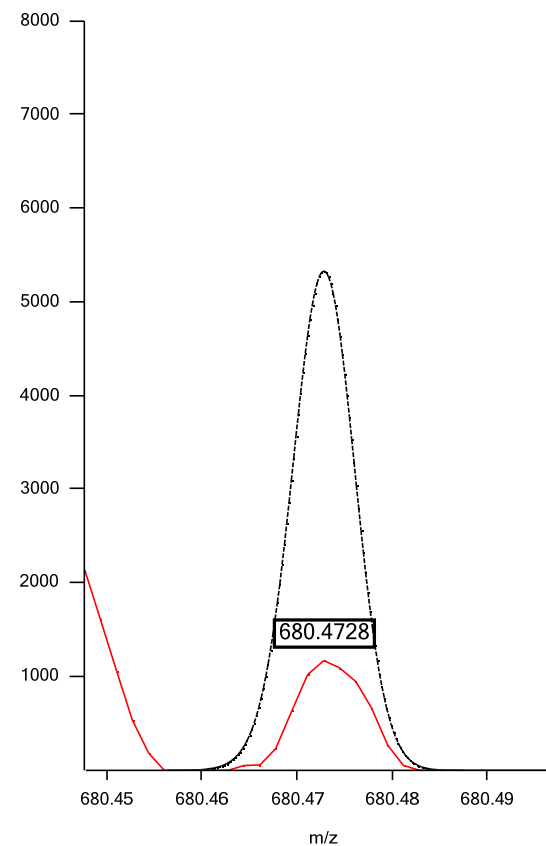
Isotope 1



Isotope 2

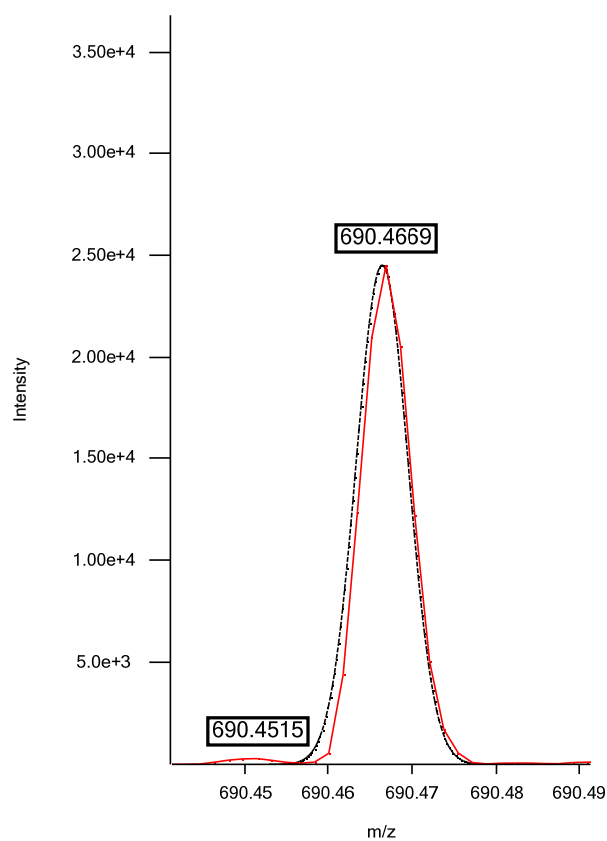


Isotope 3

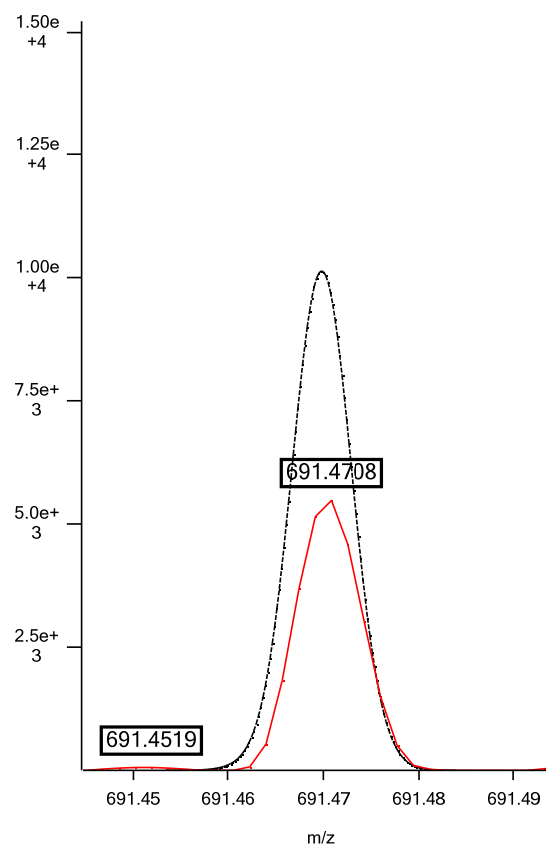


Positive ESI: Oxidized PC 21:1/Keto-7:0; C₃₆H₆₉NO₉P; theoretical *m/z* 690.4710, (M+H)⁺; isotopic fit 0.0372

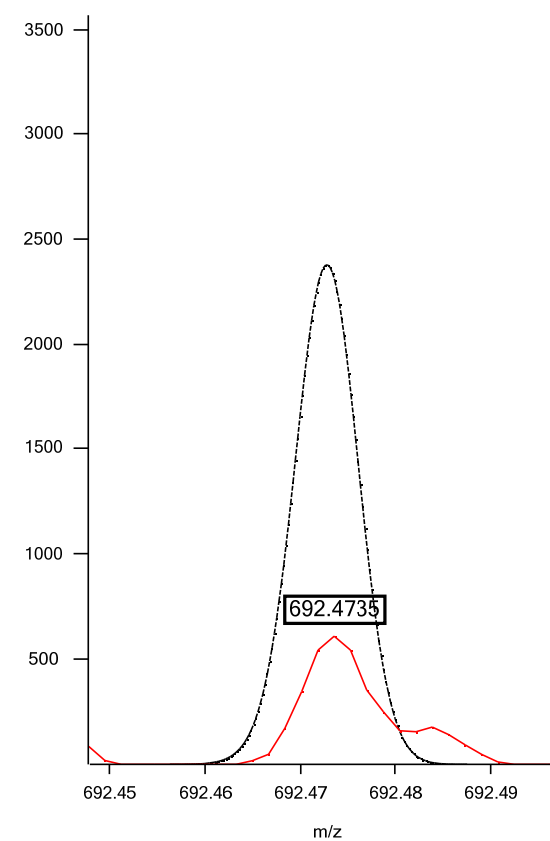
Isotope 1



Isotope 2

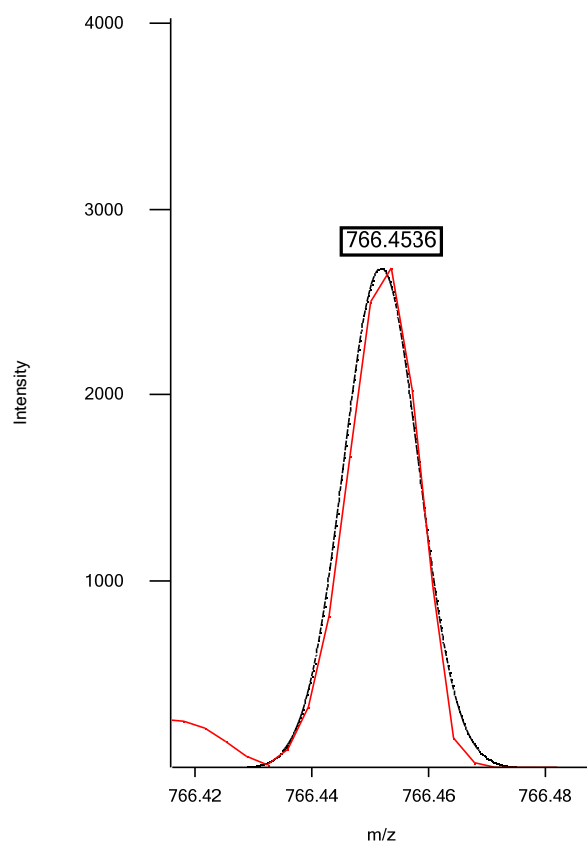


Isotope 3

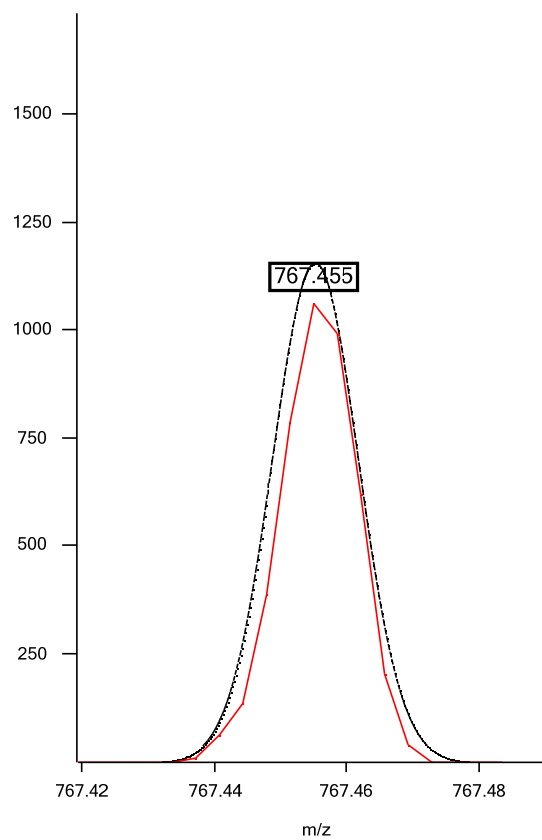


Negative ESI: Oxidized PC 18:2/Trihydroxy-9:0; $C_{37}H_{69}NO_{13}P$; theoretical m/z 766.4506, (M-H)⁻; isotopic fit 0.0372

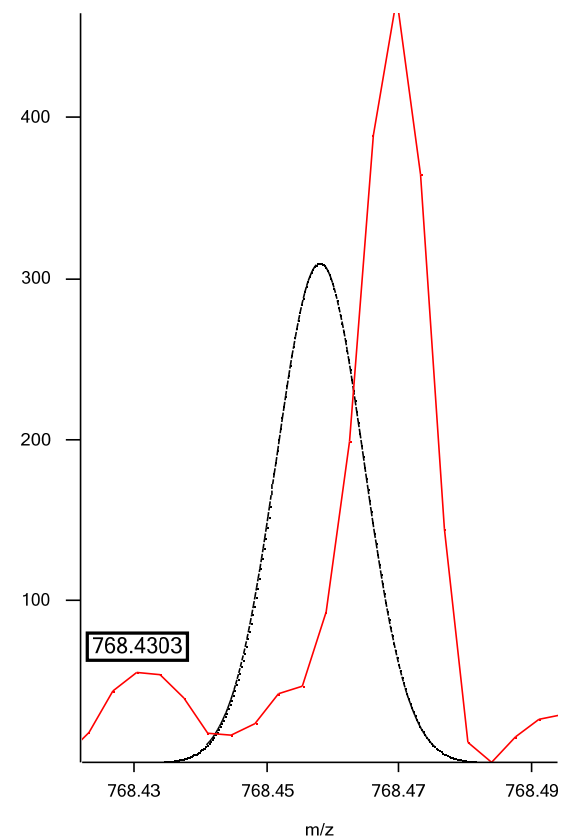
Isotope 1



Isotope 2

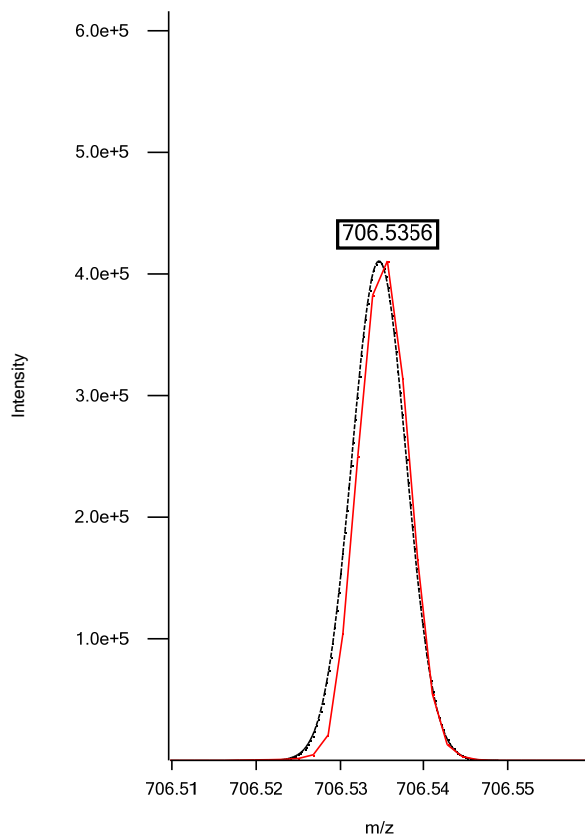


Isotope 3

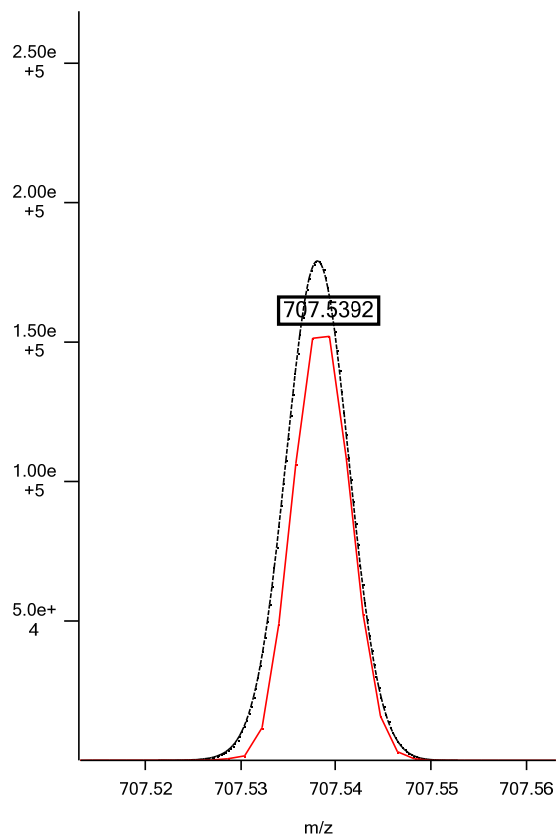


Positive ESI: PC 30:0; C₃₈H₇₇NO₈P; theoretical m/z 706.5387, (M+H)⁺; isotopic fit 0.0050

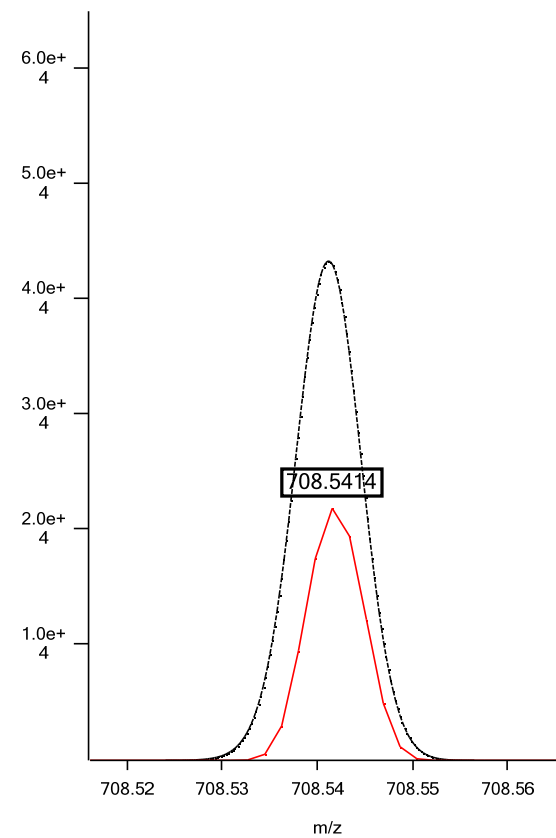
Isotope 1



Isotope 2

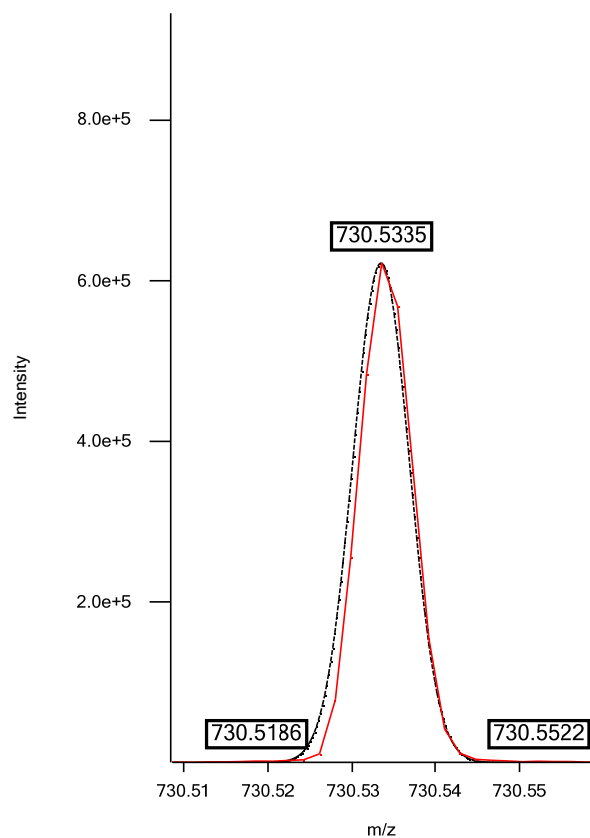


Isotope 3

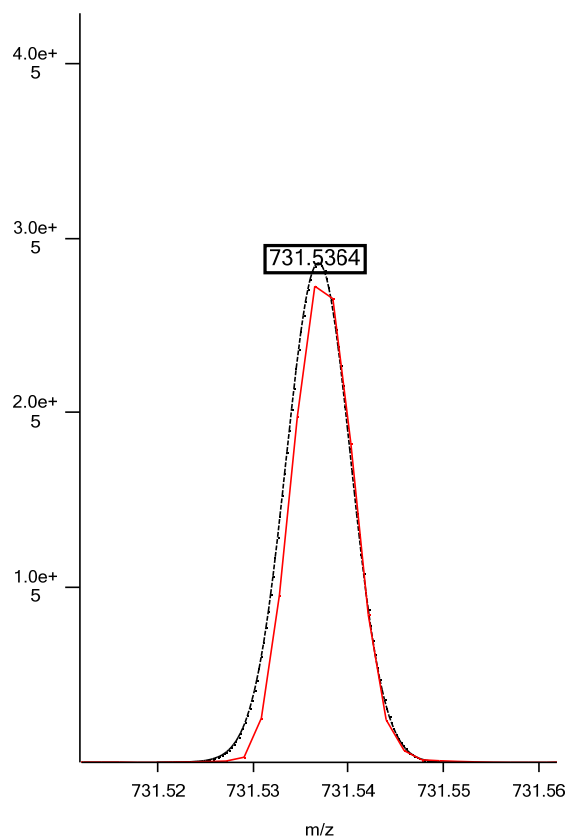


Positive ESI: PC 32:2; C₄₀H₇₇NO₈P; theoretical *m/z* 730.5387, (M+H)⁺; isotopic fit 0.0069

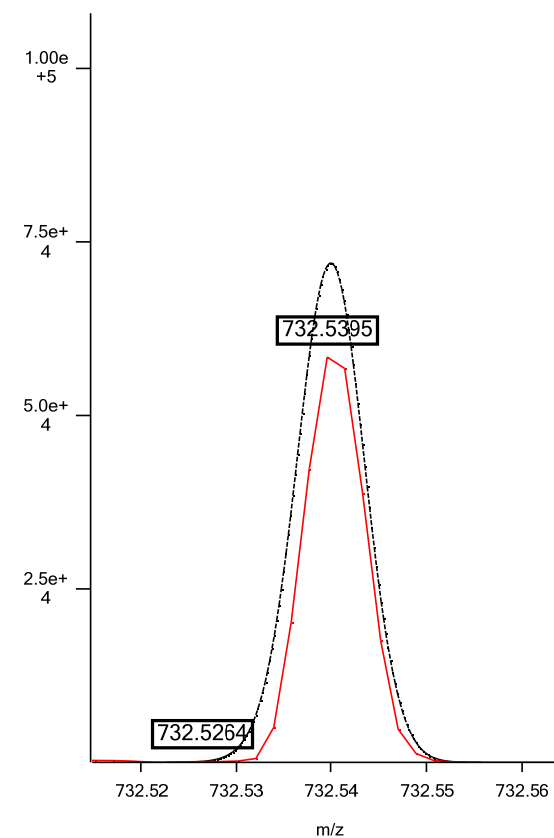
Isotope 1



Isotope 2

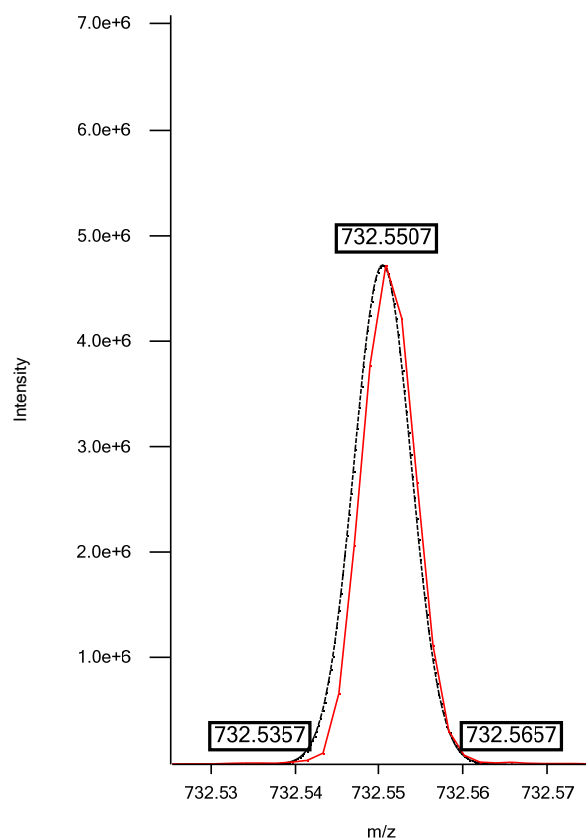


Isotope 3

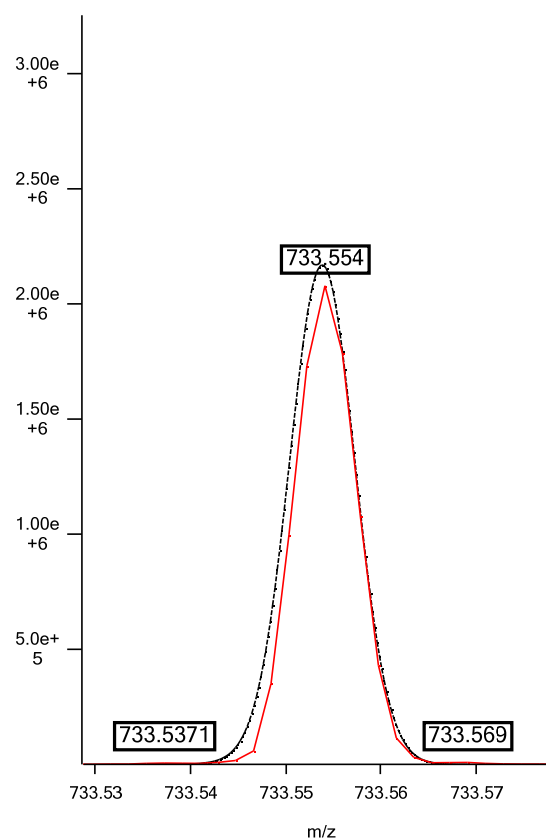


Positive ESI: PC 32:1; C₄₀H₇₉NO₈P; theoretical *m/z* 732.5543, (M+H)⁺; isotopic fit 0.0052

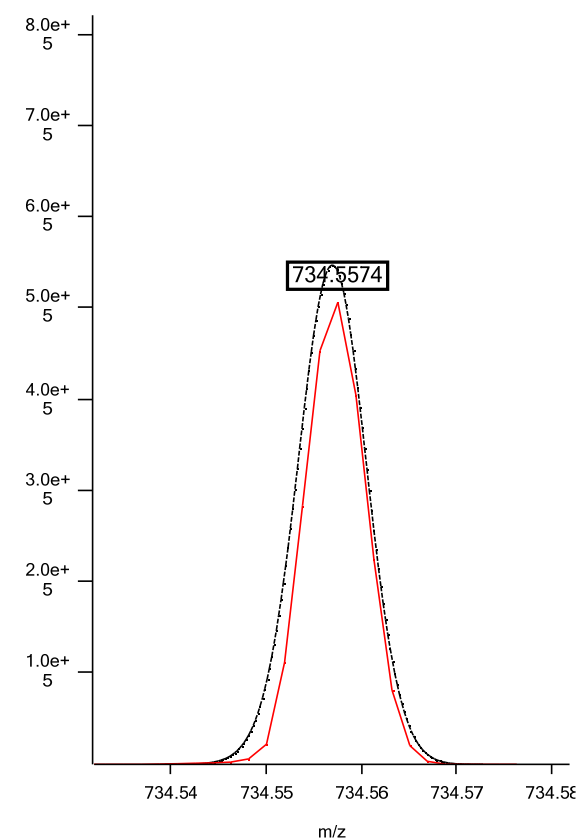
Isotope 1



Isotope 2

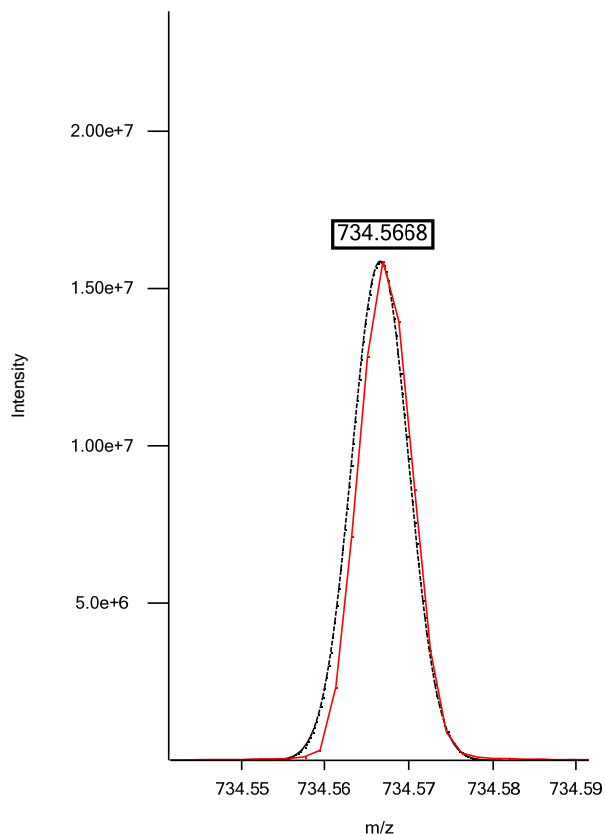


Isotope 3

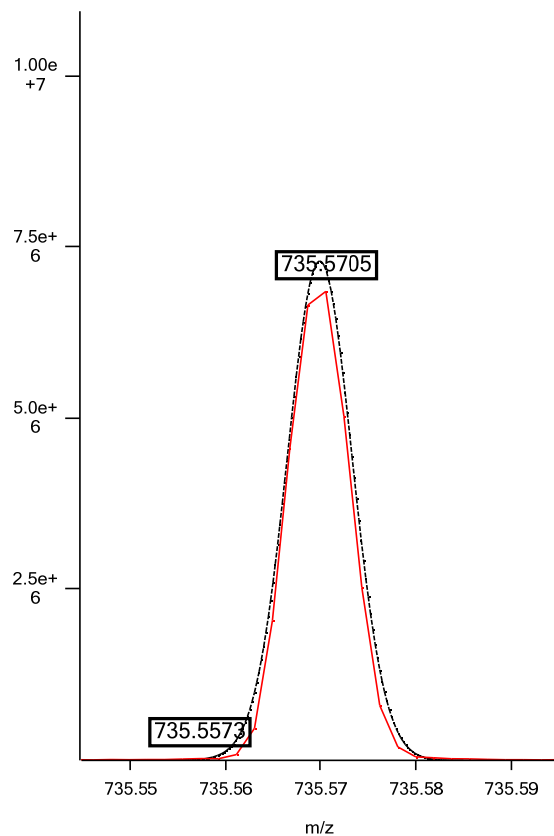


Positive ESI: PC 32:0; C₄₀H₈₁NO₈P; theoretical *m/z* 734.5699, (M+H)⁺; isotopic fit 0.0045

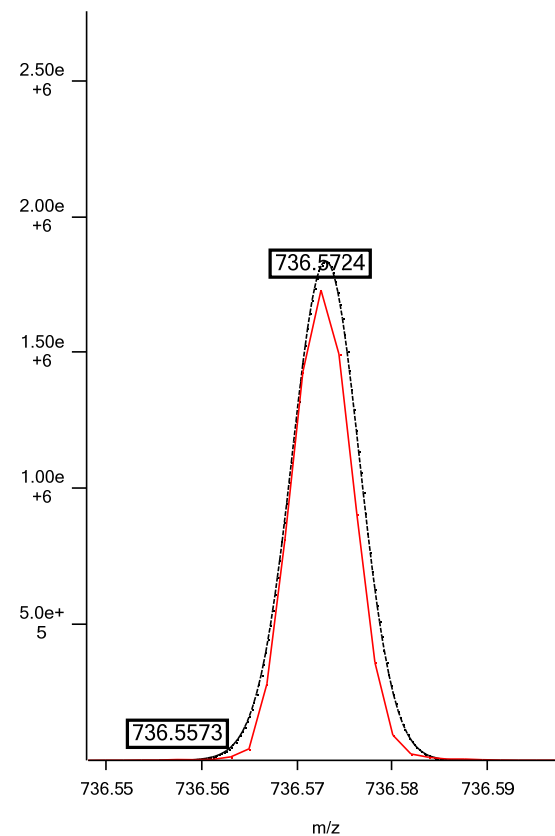
Isotope 1



Isotope 2

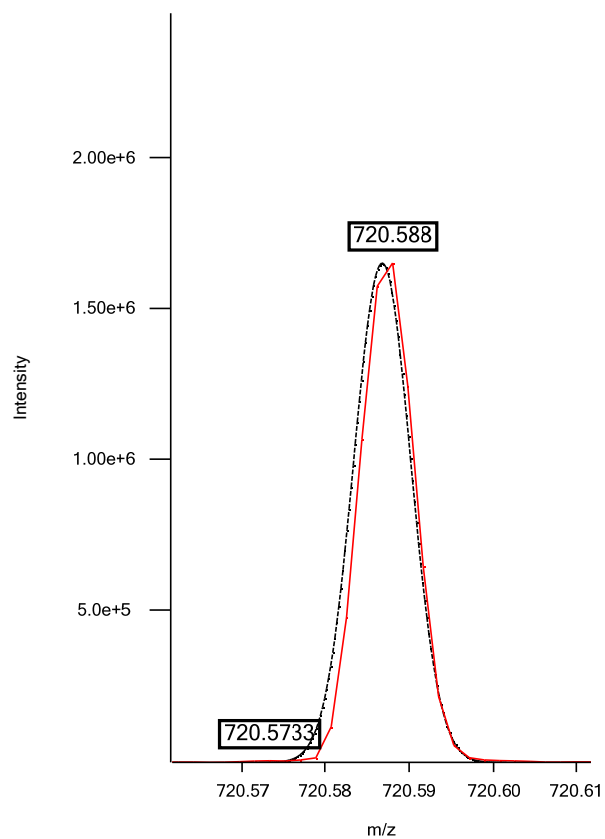


Isotope 3

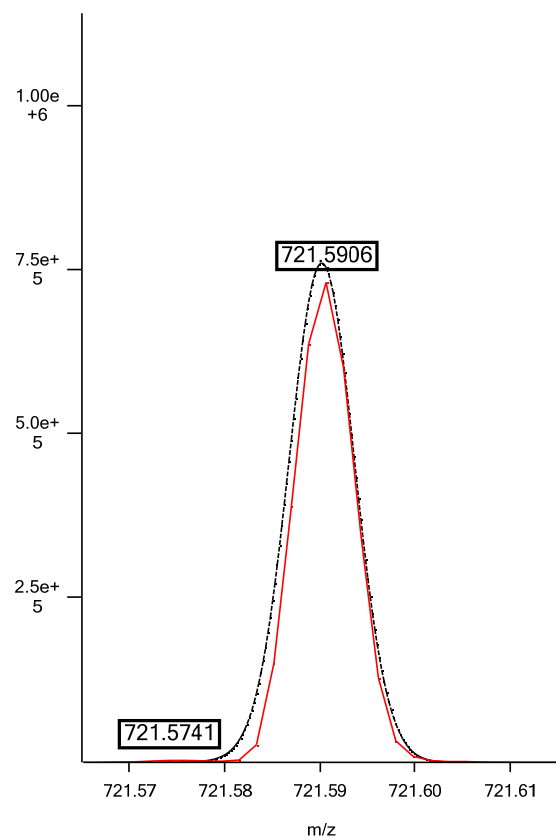


Positive ESI: PC 16:0e/16:0; C₄₀H₈₃NO₇P; theoretical m/z 720.5907, (M+H)⁺; isotopic fit 0.0039

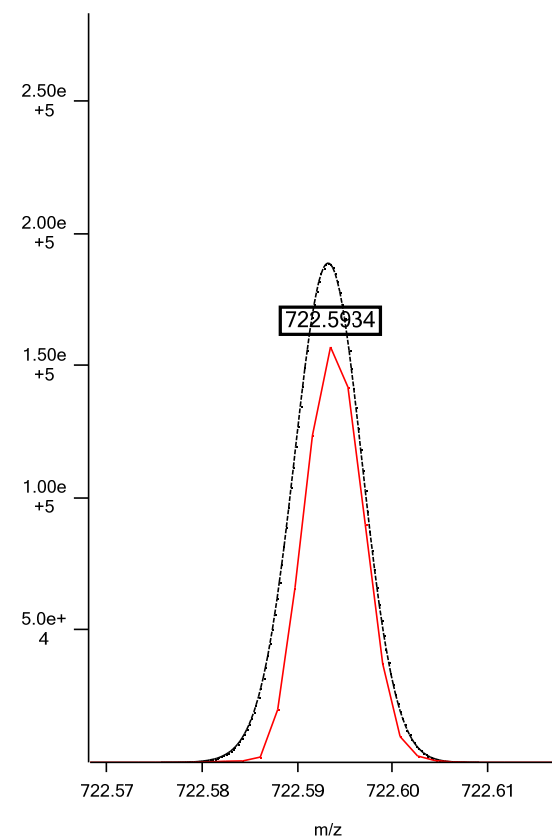
Isotope 1



Isotope 2

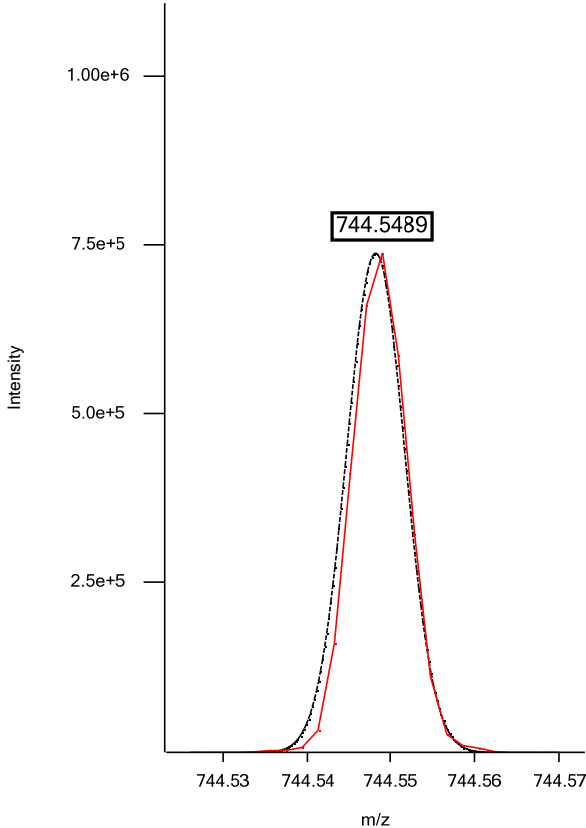


Isotope 3

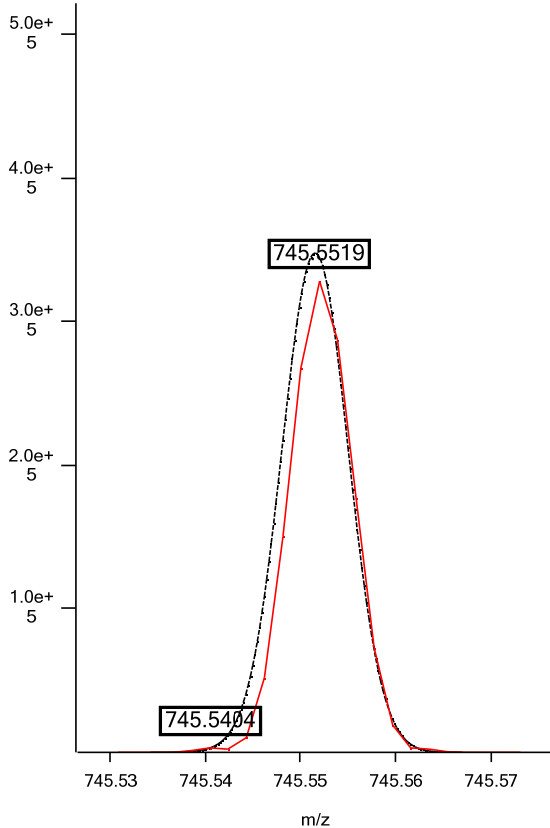


Positive ESI: PC 33:2; C₄₁H₇₉NO₈P; theoretical *m/z* 744.5543, (M+H)⁺; isotopic fit 0.0066

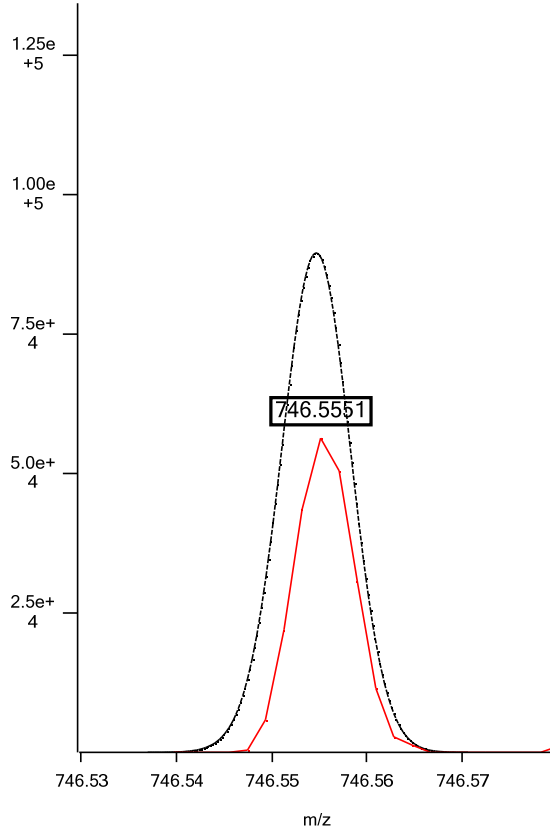
Isotope 1



Isotope 2

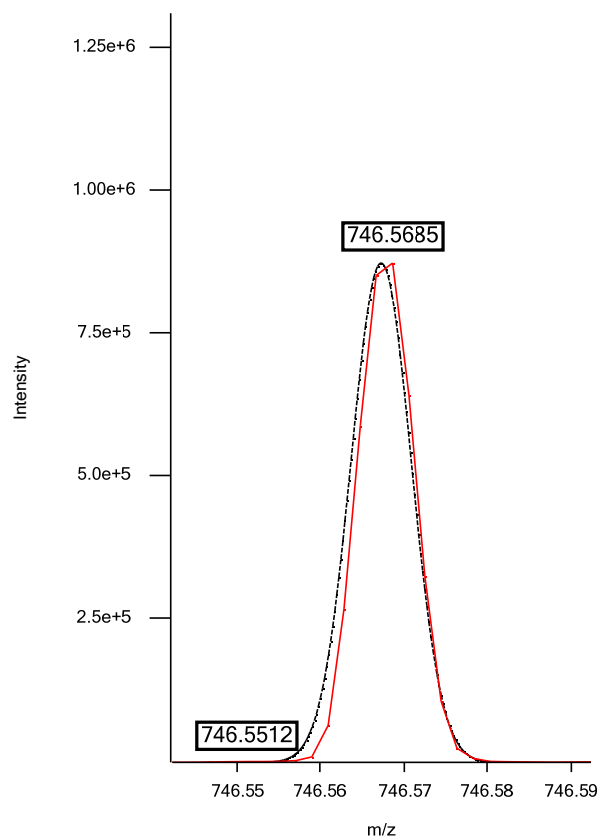


Isotope 3

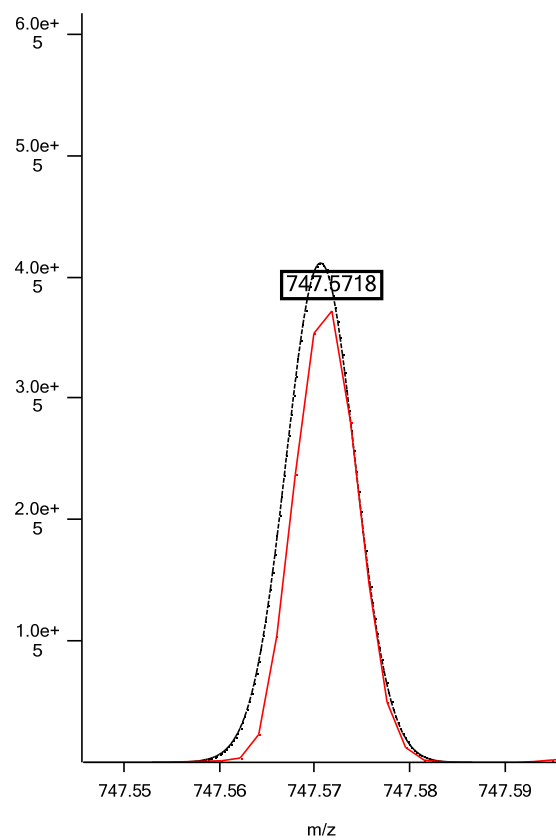


Positive ESI: PC 33:1; C₄₁H₈₁NO₈P; theoretical *m/z* 746.5699, (M+H)⁺; isotopic fit 0.0075

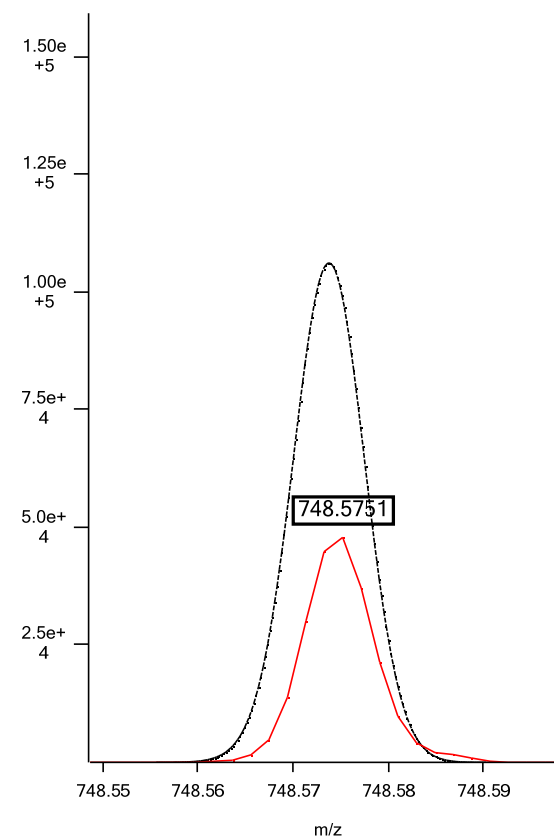
Isotope 1



Isotope 2

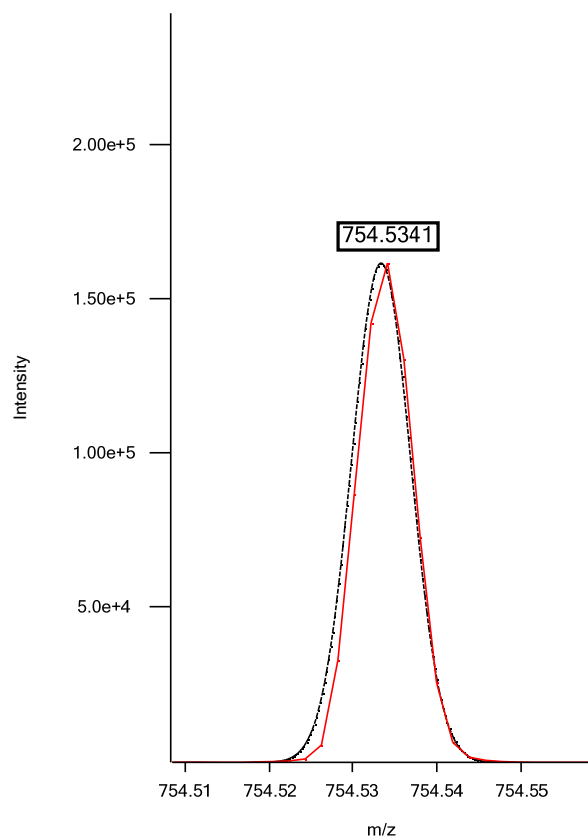


Isotope 3

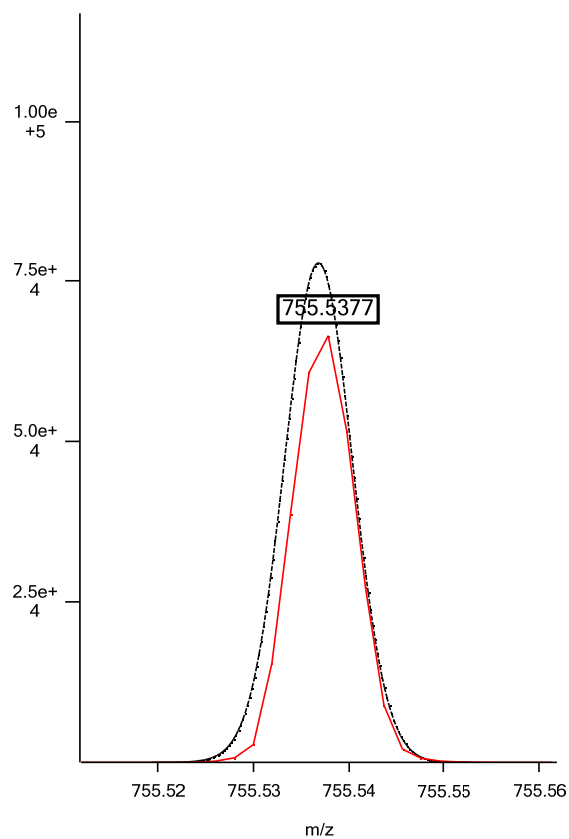


Positive ESI: PC 34:4; C₄₂H₇₇NO₈P; theoretical *m/z* 754.5387, (M+H)⁺; isotopic fit 0.0066

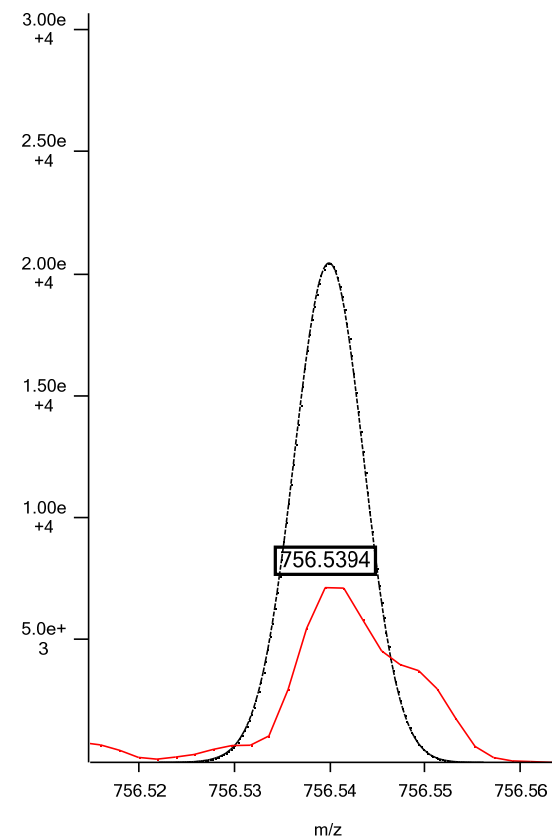
Isotope 1



Isotope 2

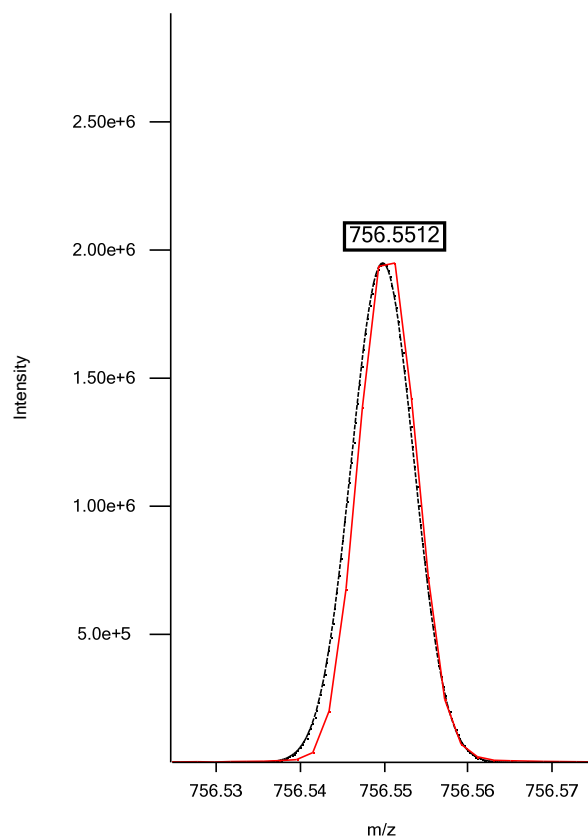


Isotope 3

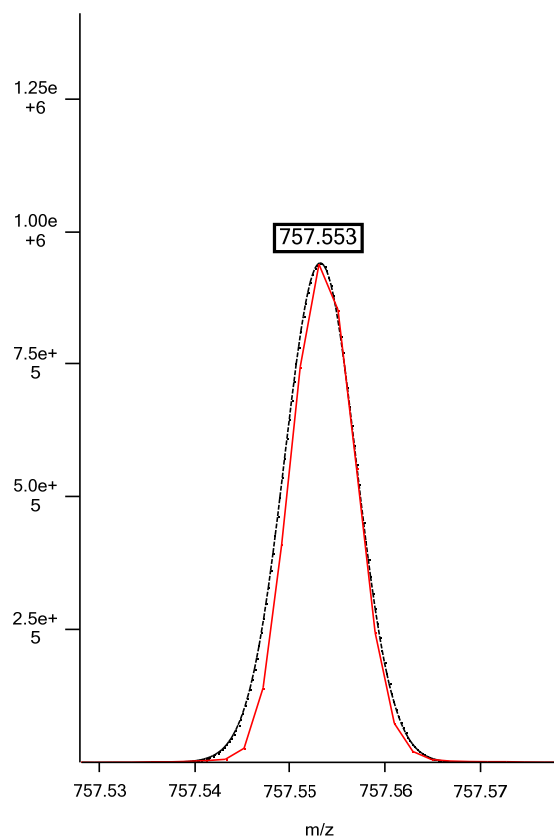


Positive ESI: PC 34:3; C₄₂H₇₉NO₈P; theoretical *m/z* 756.5543, (M+H)⁺; isotopic fit 0.0025

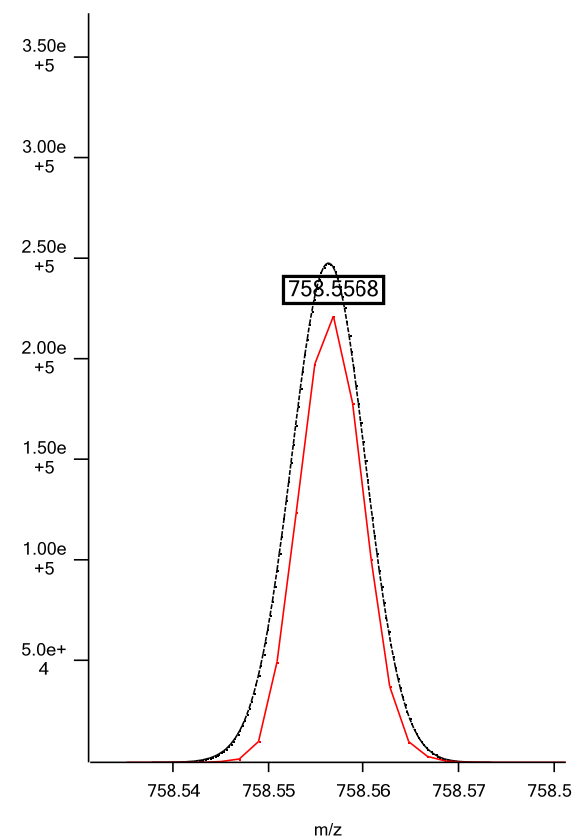
Isotope 1



Isotope 2

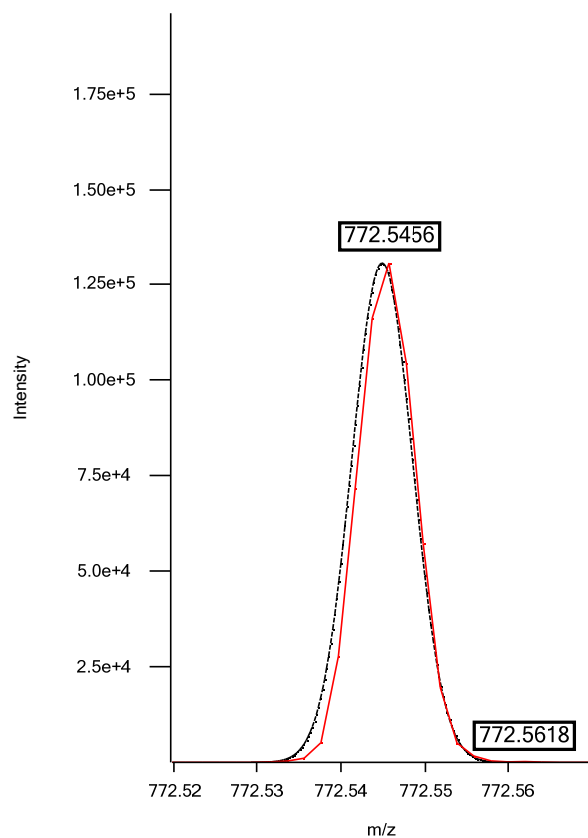


Isotope 3

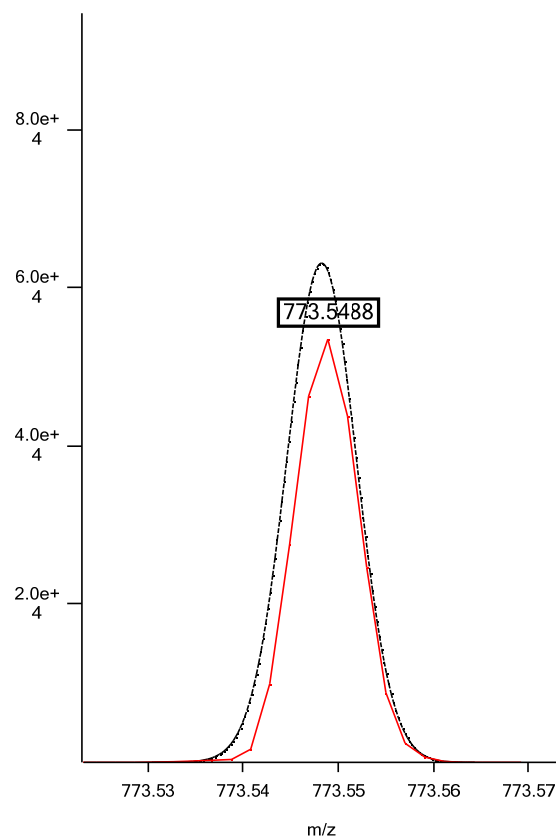


Positive ESI: Oxidized PC 18:0/Hydroxy-16:3; $C_{42}H_{79}NO_9P$; theoretical m/z 772.5492, $(M+H)^+$; isotopic fit 0.0106

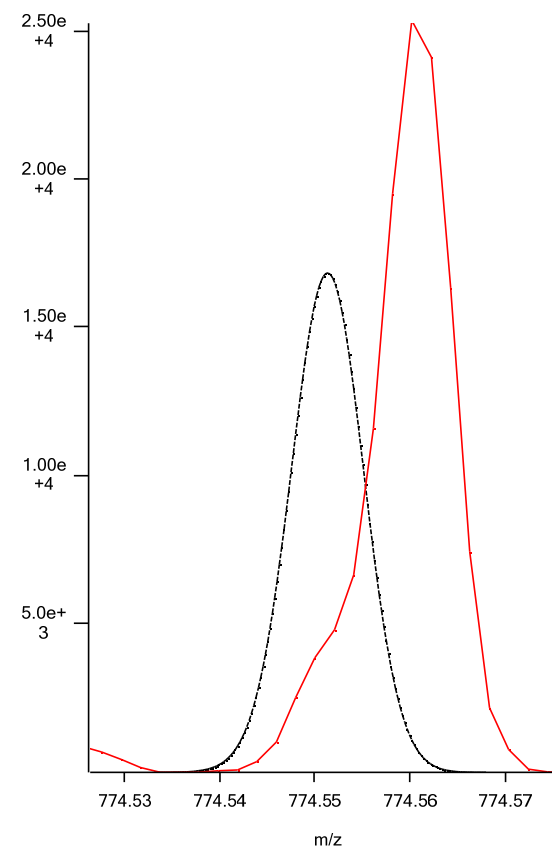
Isotope 1



Isotope 2

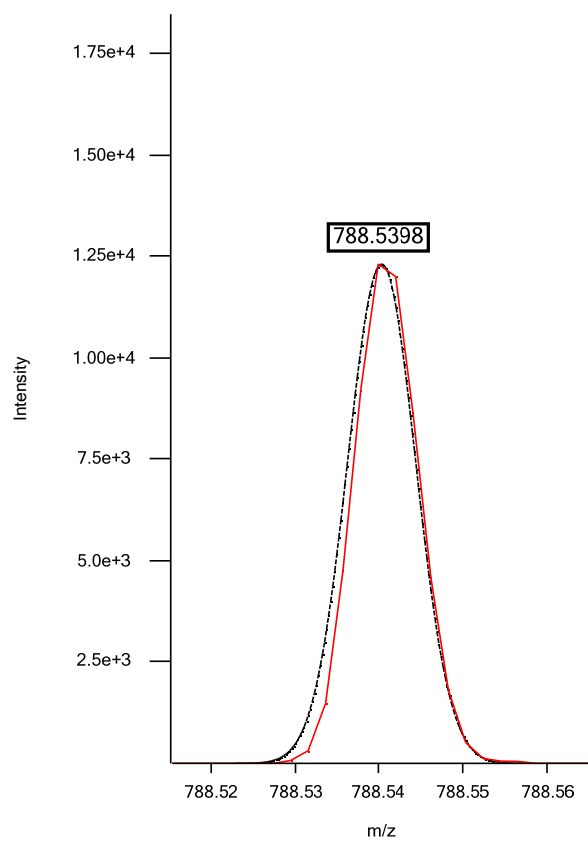


Isotope 3

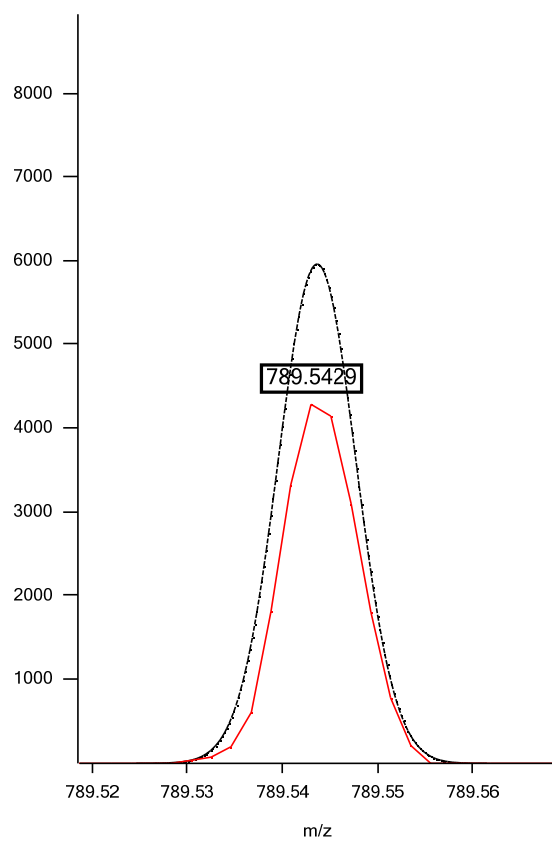


Positive ESI: Oxidized PC 16:0/Hydroperoxy-18:3; $C_{42}H_{79}NO_{10}P$; theoretical m/z 788.5441, (M+H)⁺; isotopic fit 0.0190

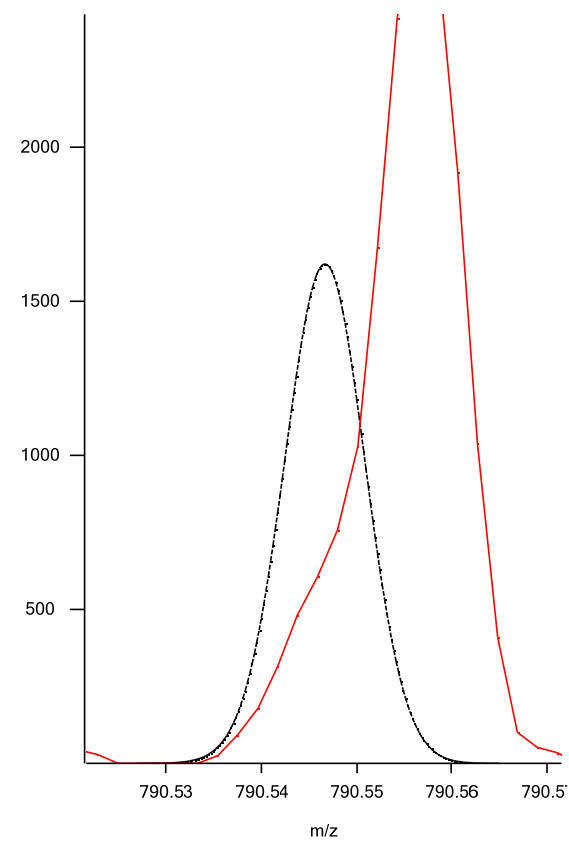
Isotope 1



Isotope 2

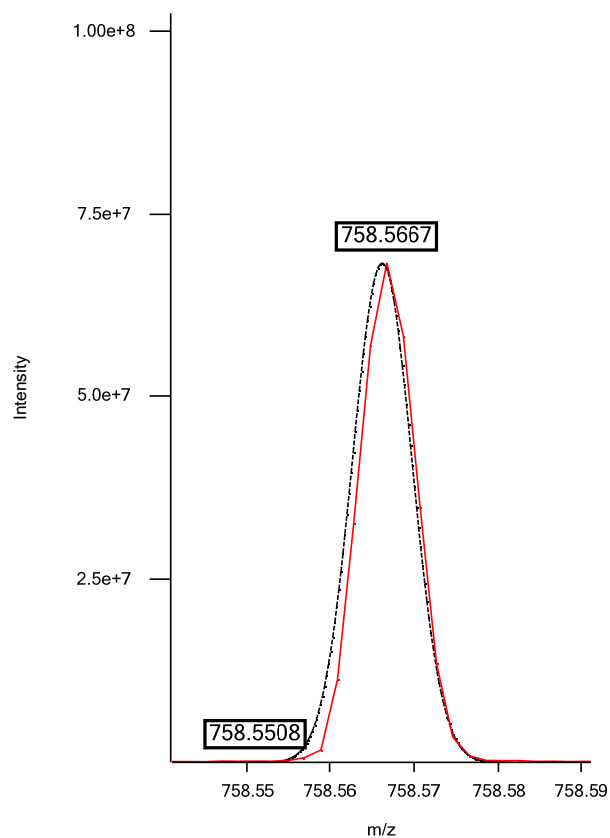


Isotope 3

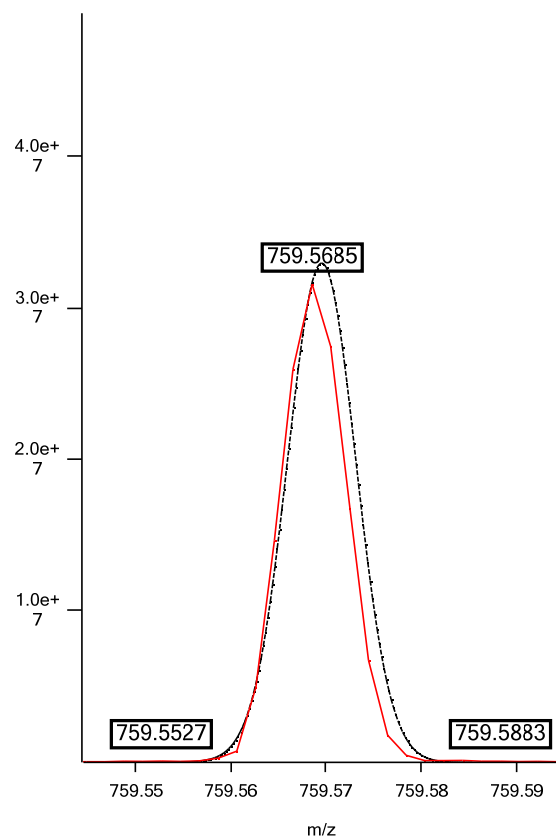


Positive ESI: PC 34:2; C₄₂H₈₁NO₈P; theoretical *m/z* 758.5699, (M+H)⁺; isotopic fit 0.0126

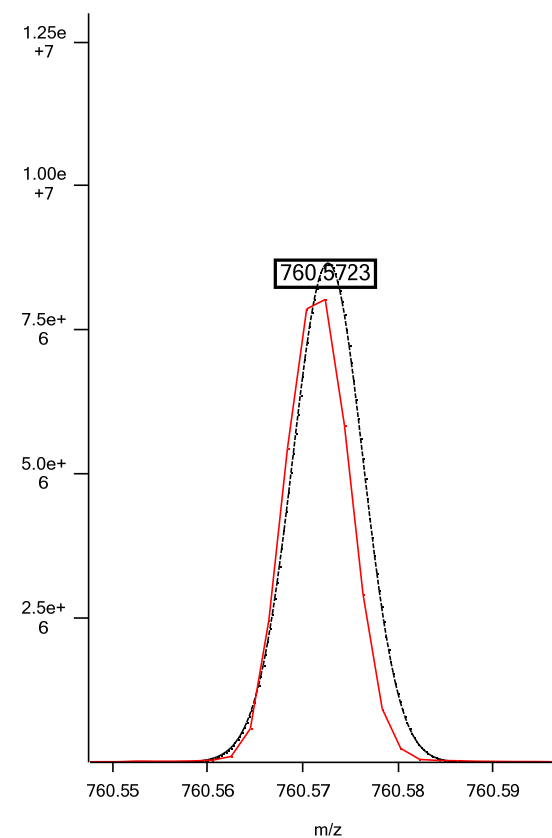
Isotope 1



Isotope 2

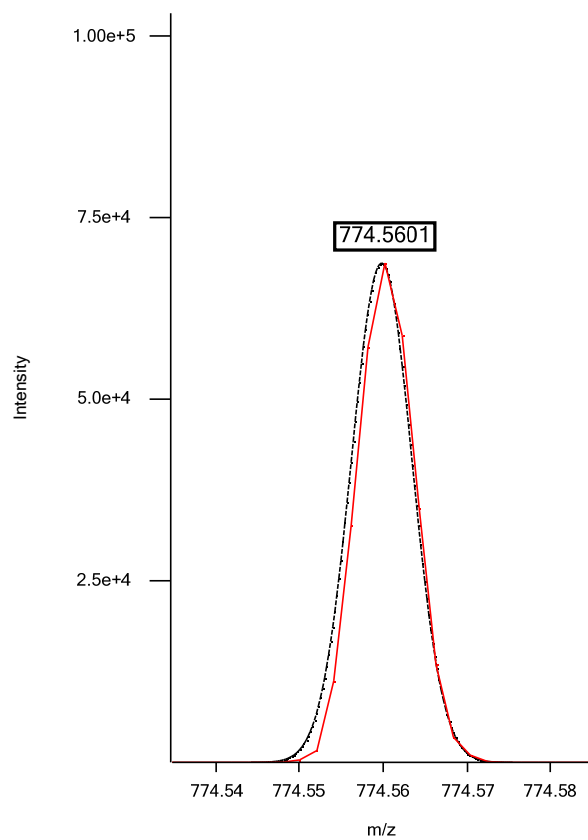


Isotope 3

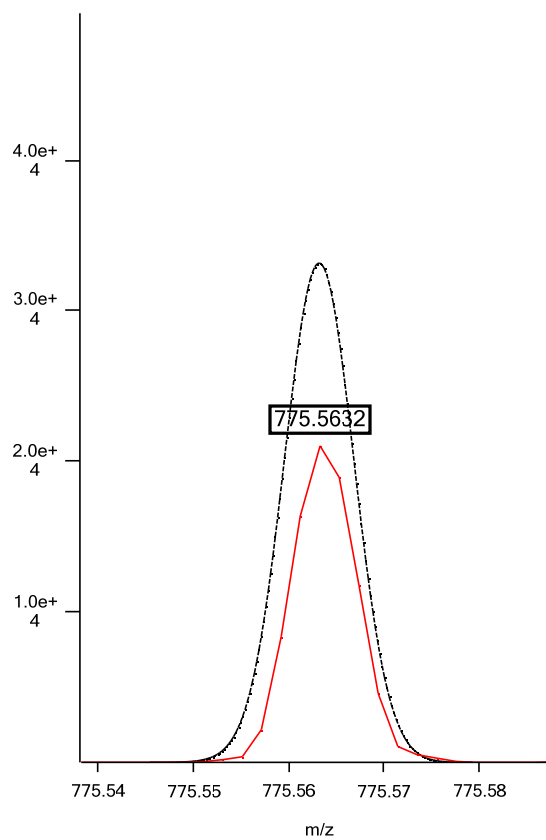


Positive ESI: Oxidized PC 16:0/Hydroxy-18:2; C₄₂H₈₁NO₉P; theoretical *m/z* 774.5649, (M+H)⁺; isotopic fit 0.0328

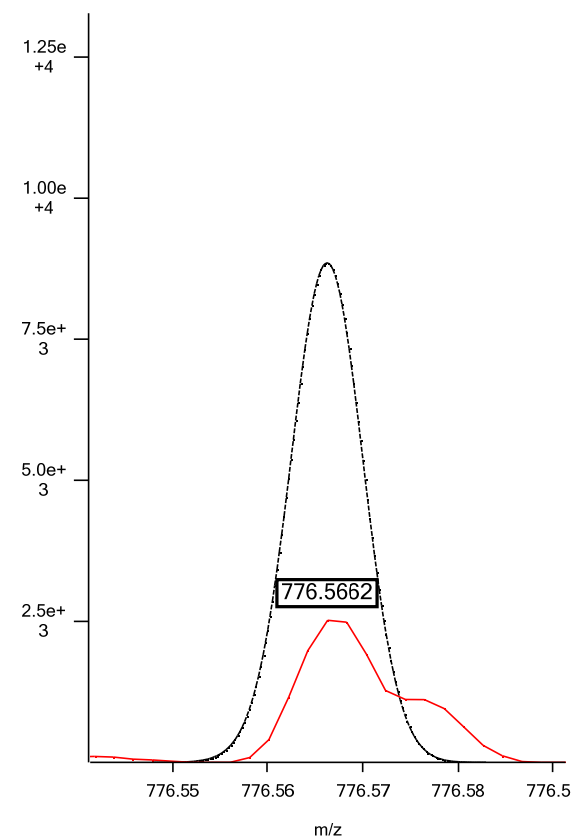
Isotope 1



Isotope 2

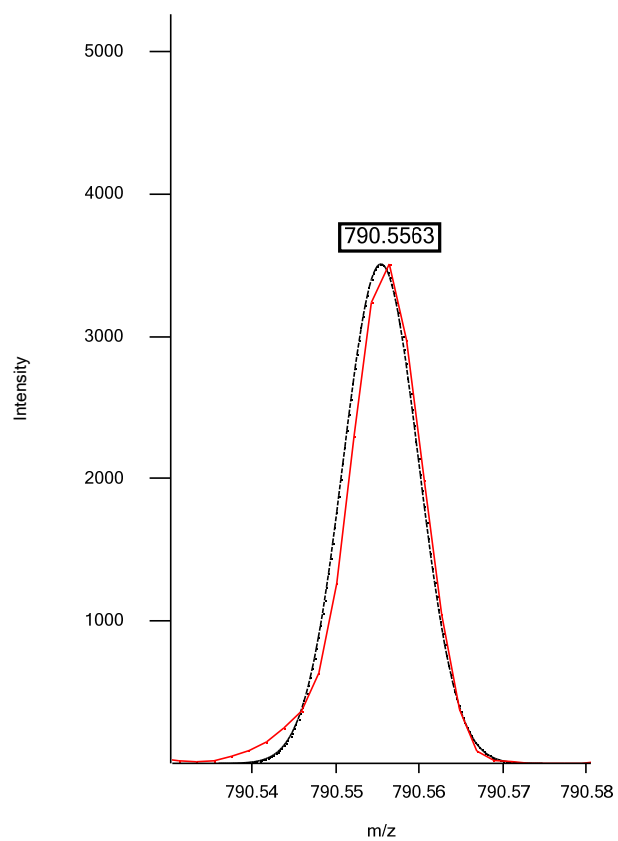


Isotope 3

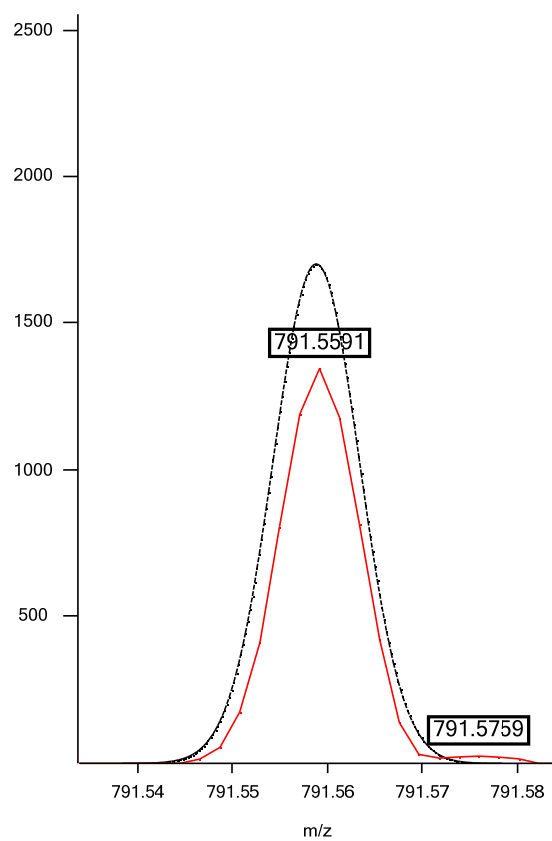


Positive ESI: Oxidized PC 16:0/Hydroperoxy-18:2; $C_{42}H_{81}NO_{10}P$; theoretical m/z 790.5598, (M+H)⁺; isotopic fit 0.0126

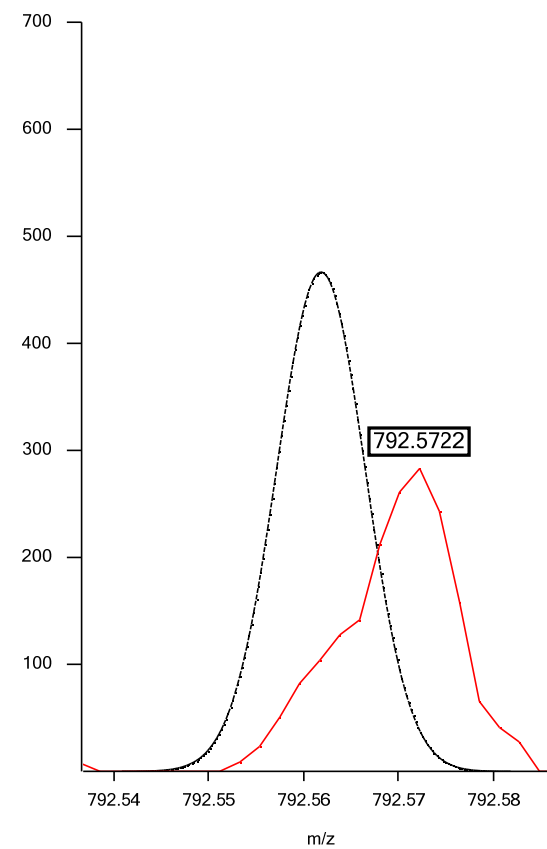
Isotope 1



Isotope 2

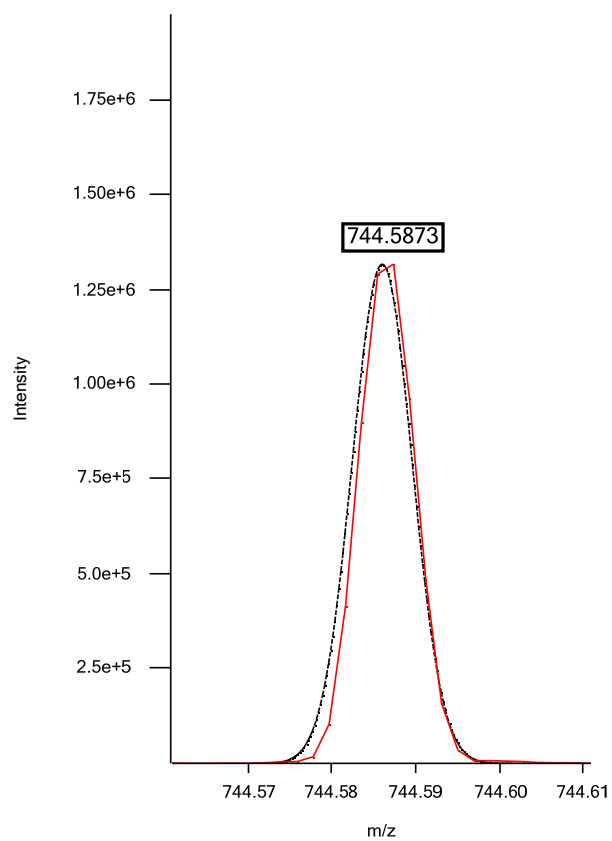


Isotope 3

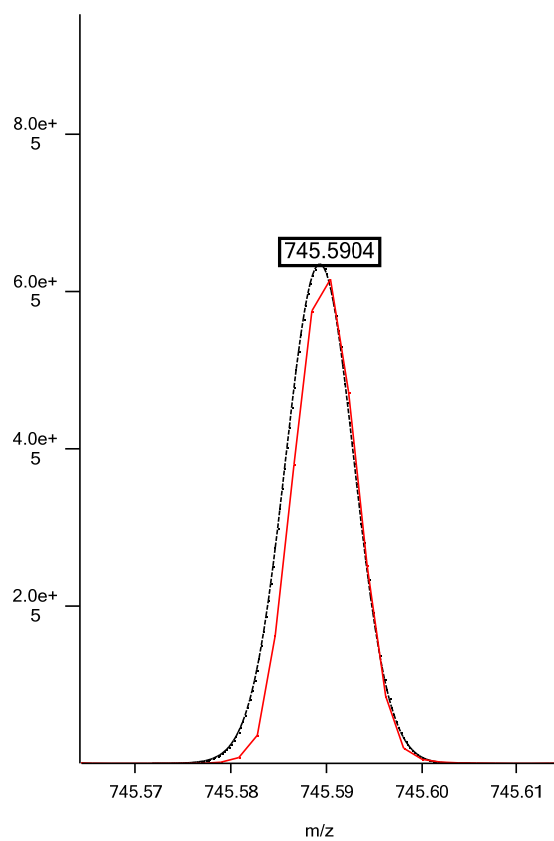


Positive ESI: PC 16:0e/18:2 or 16:1p/18:1; C₄₂H₈₃NO₇P; theoretical *m/z* 744.5907, (M+H)⁺; isotopic fit 0.0024

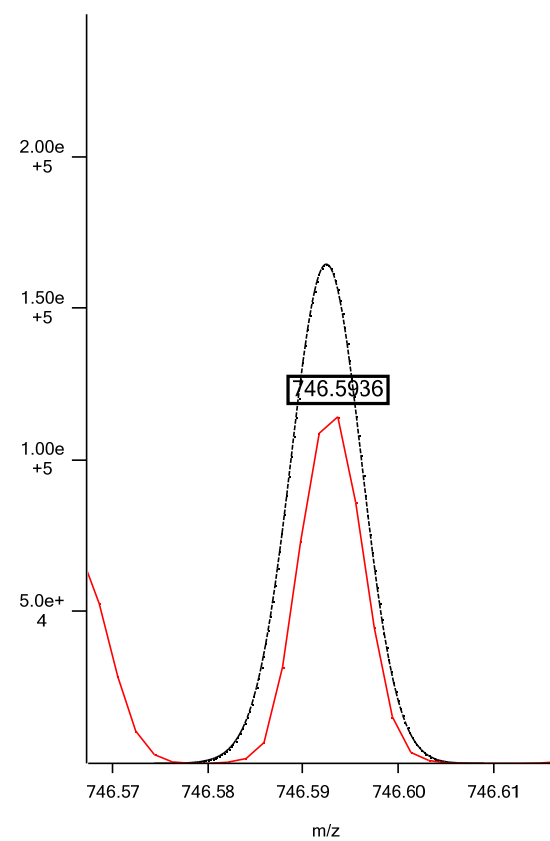
Isotope 1



Isotope 2

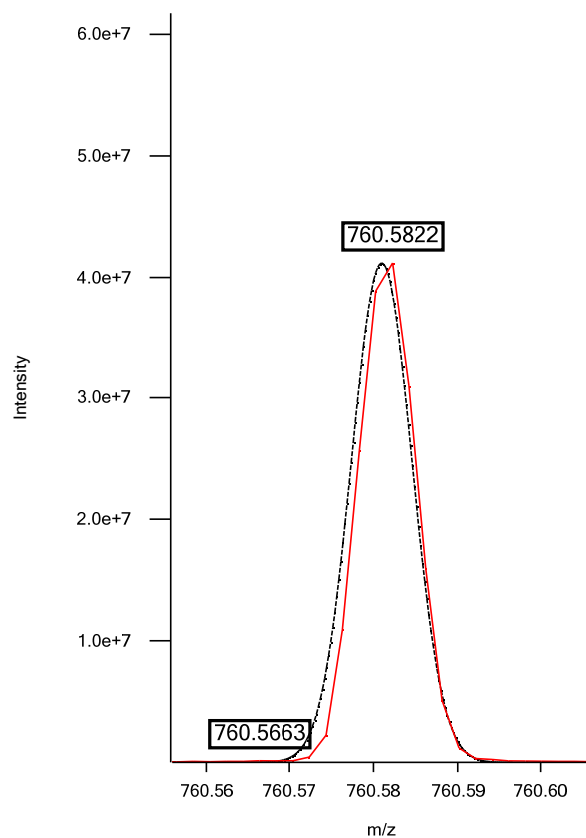


Isotope 3

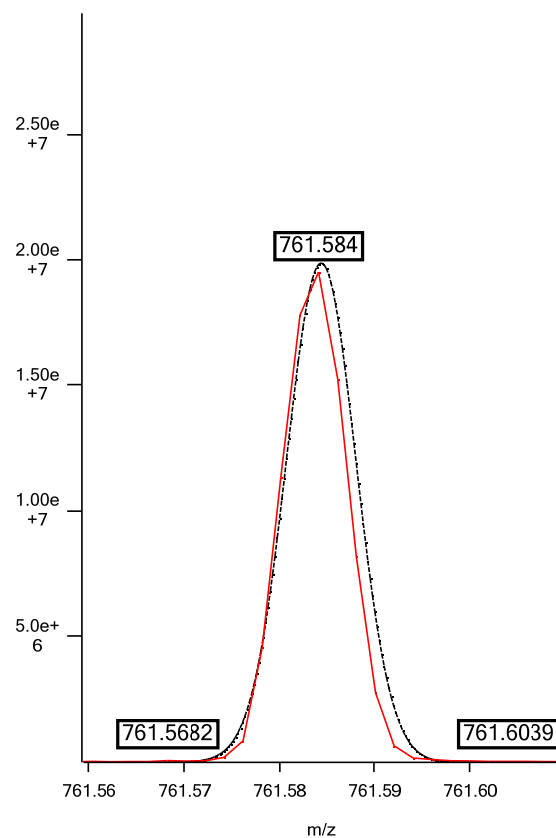


Positive ESI: PC 34:1; C₄₂H₈₃NO₈P; theoretical m/z 760.5856, (M+H)⁺; isotopic fit 0.0117

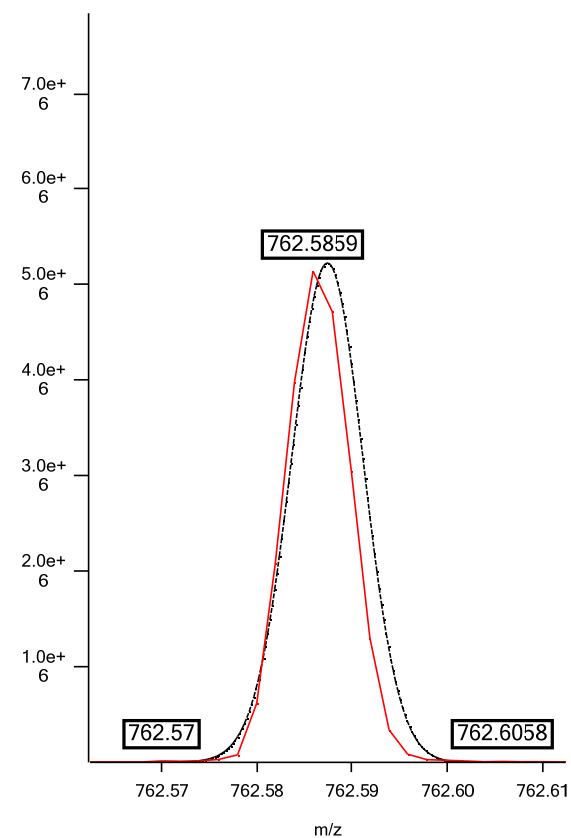
Isotope 1



Isotope 2

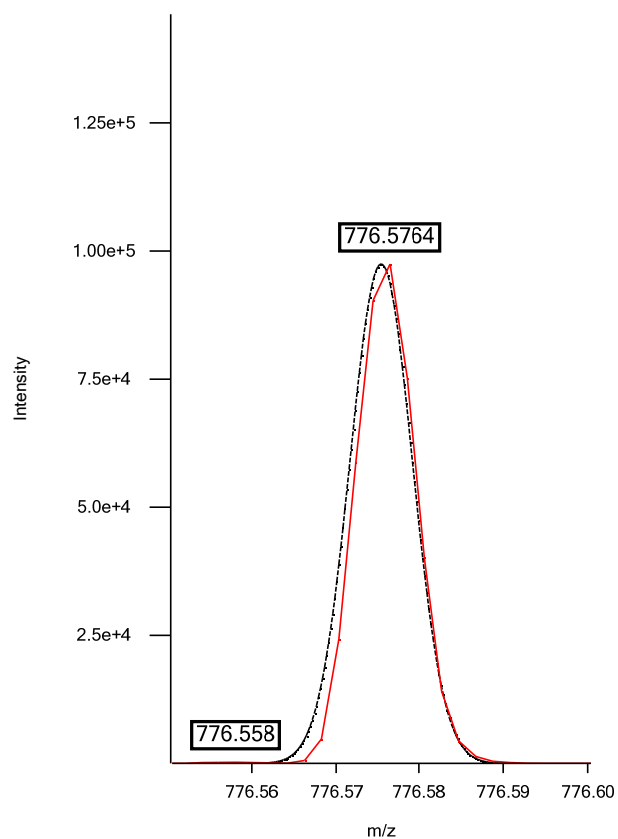


Isotope 3

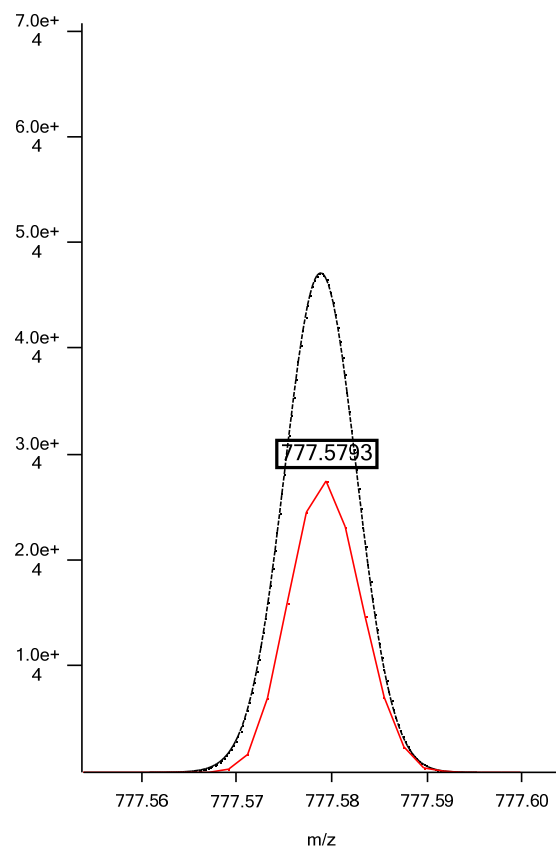


Positive ESI: Oxidized PC 16:0/Hydroxy-18:1; $C_{42}H_{83}NO_9P$; theoretical m/z 776.5805, $(M+H)^+$; isotopic fit 0.0366

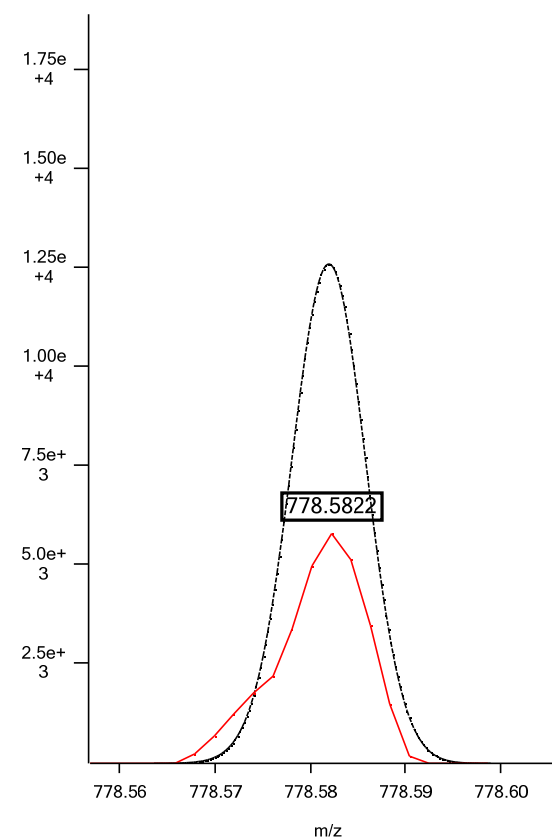
Isotope 1



Isotope 2

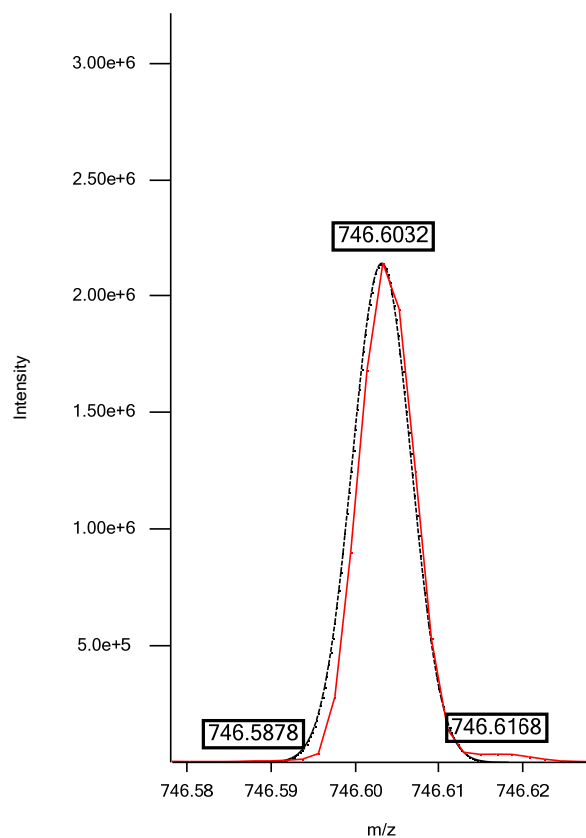


Isotope 3

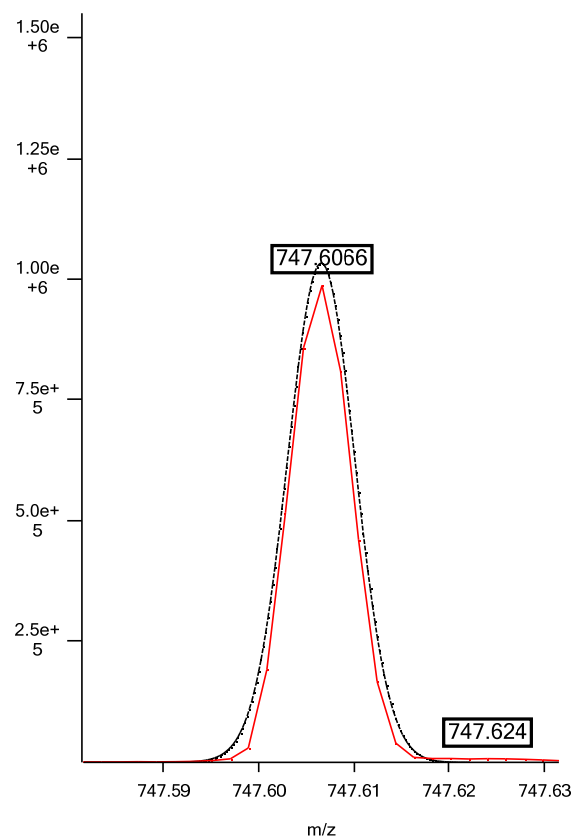


Positive ESI: PC 16:0e/18:1 or 16:1p/18:0; C₄₂H₈₅NO₇P; theoretical *m/z* 746.6063, (M+H)⁺; isotopic fit 0.0070

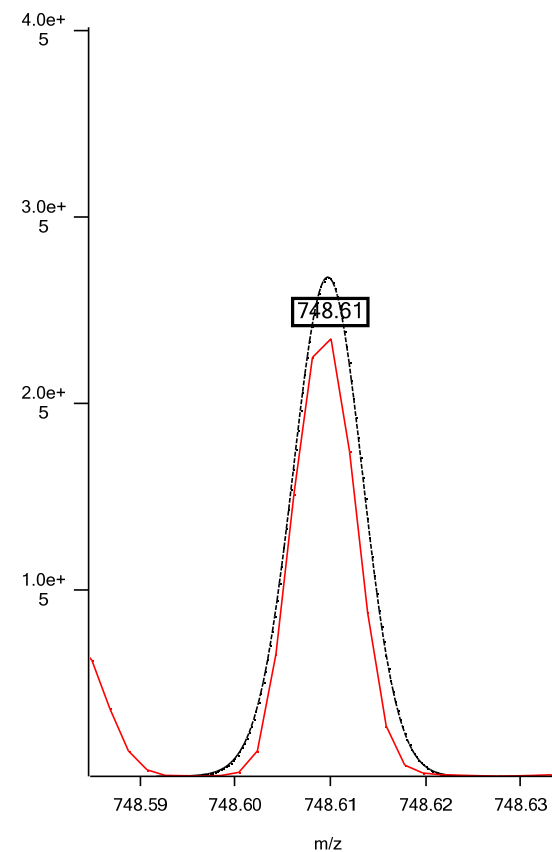
Isotope 1



Isotope 2

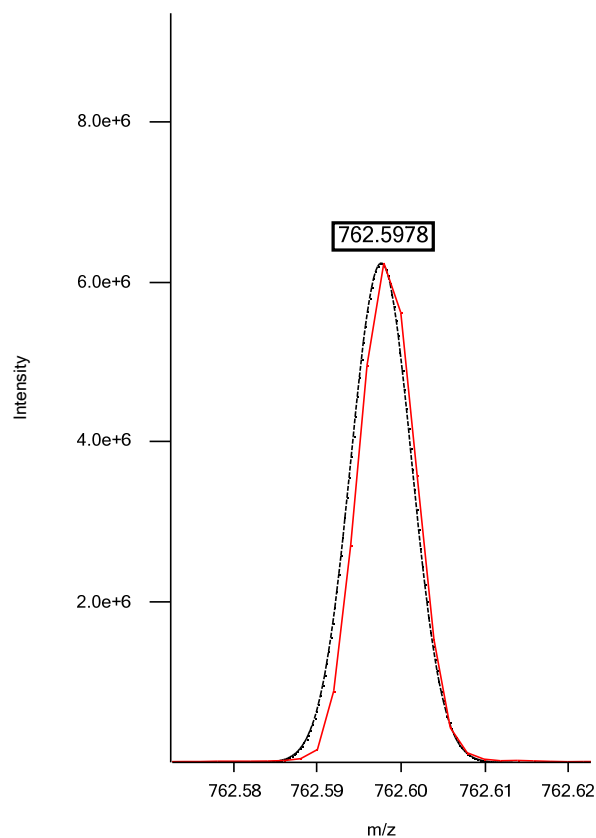


Isotope 3

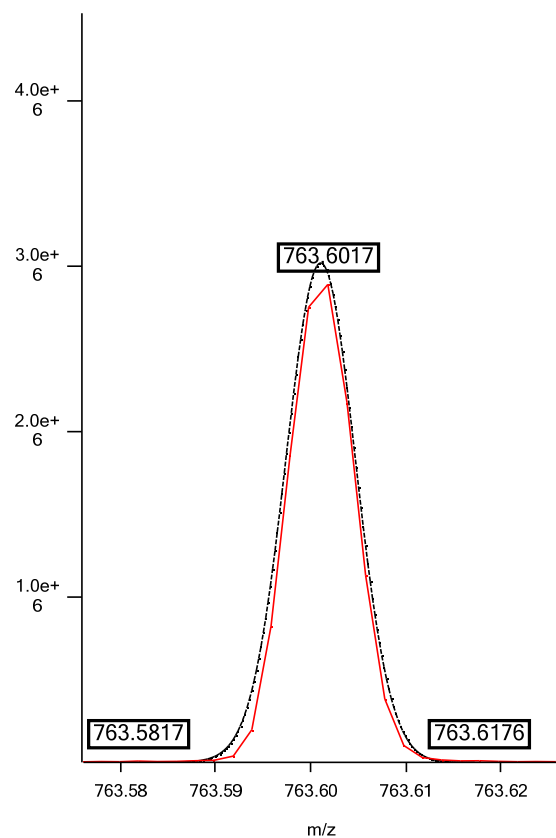


Positive ESI: PC 34:0; C₄₂H₈₅NO₈P; theoretical *m/z* 762.6012, (M+H)⁺; isotopic fit 0.0079

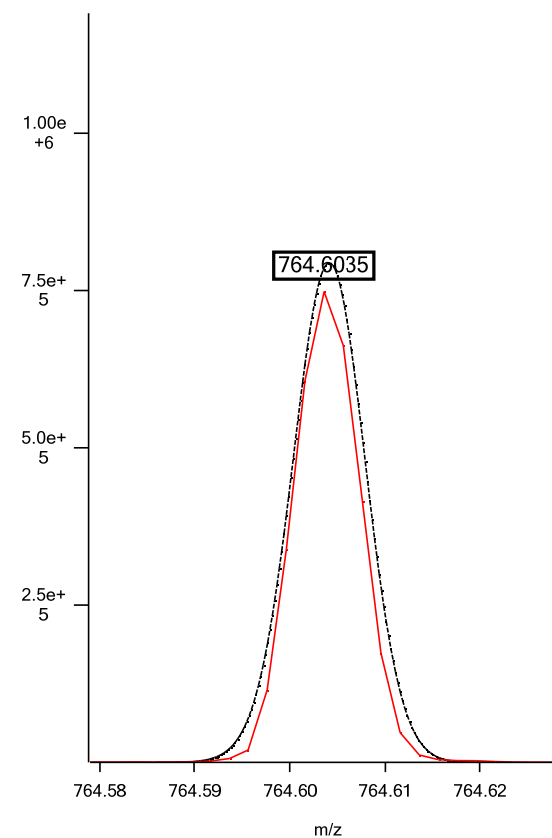
Isotope 1



Isotope 2

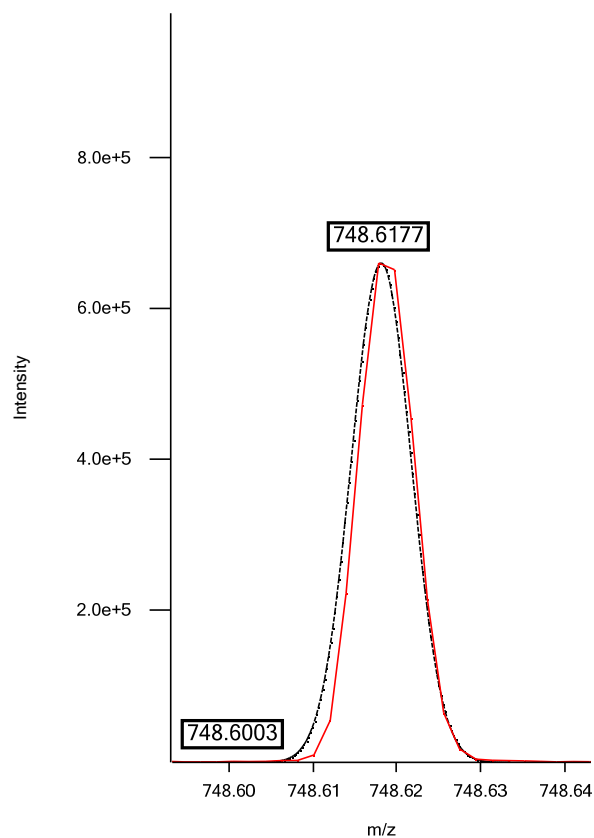


Isotope 3

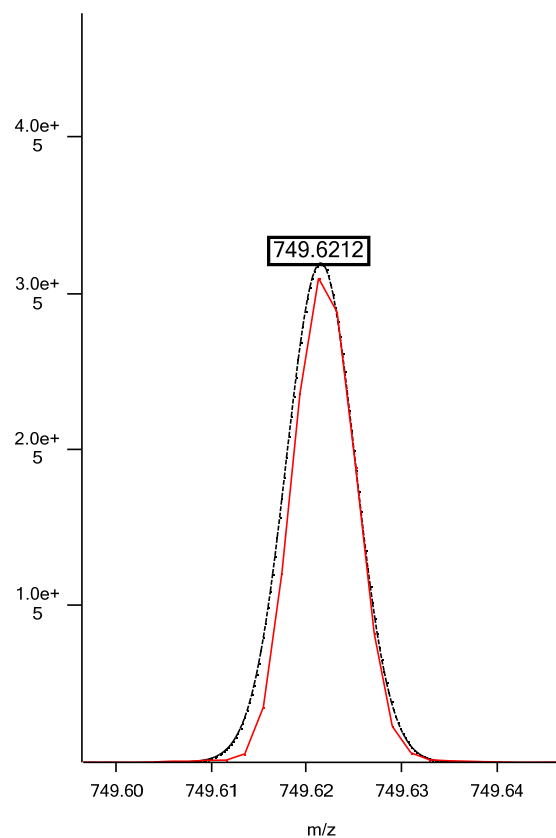


Positive ESI: PC 16:0e/18:0; C₄₂H₈₇NO₇P; theoretical *m/z* 748.6220, (M+H)⁺; isotopic fit 0.0046

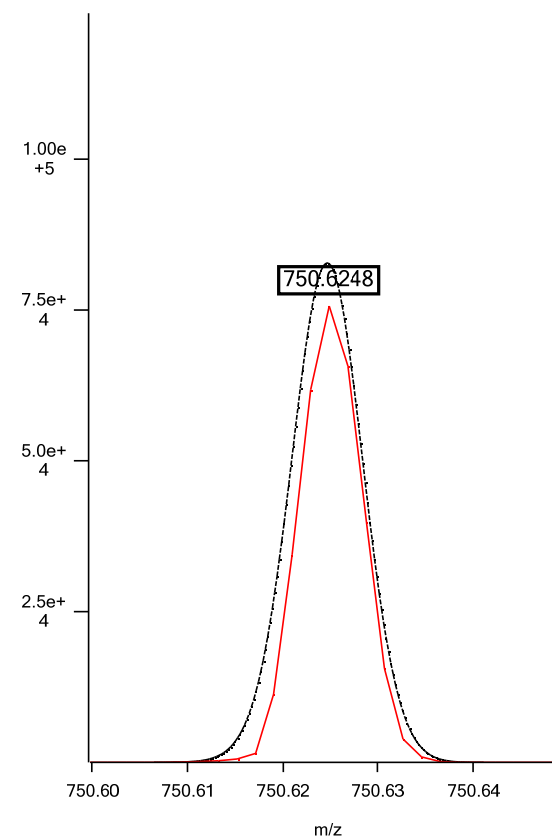
Isotope 1



Isotope 2

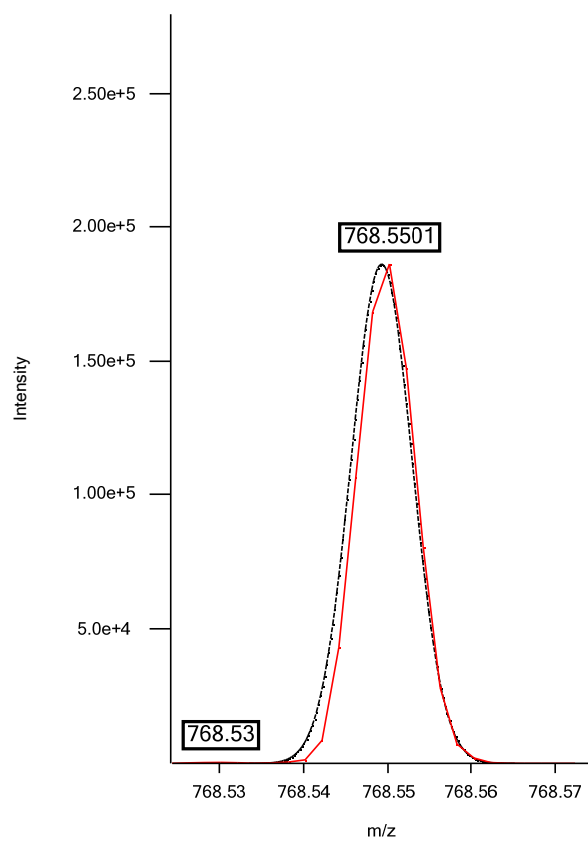


Isotope 3

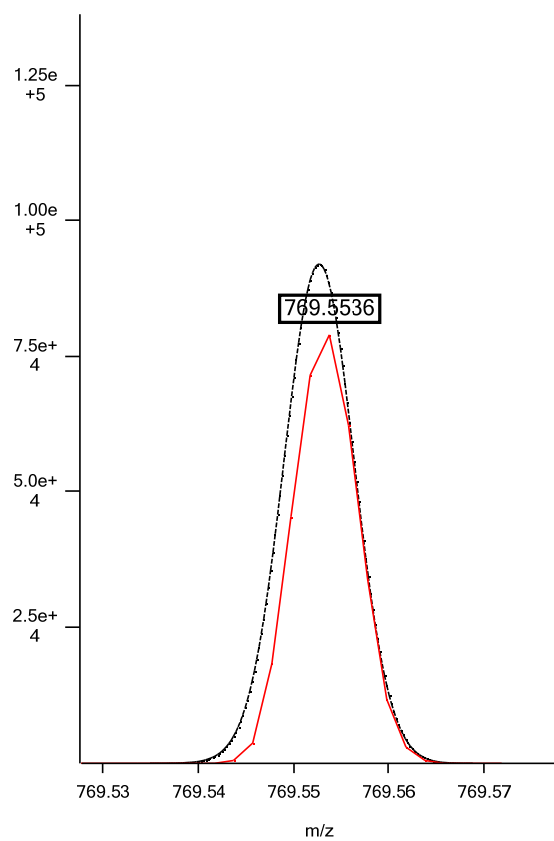


Positive ESI: PC 35:4; C₄₃H₇₉NO₈P; theoretical m/z 768.5543, (M+H)⁺; isotopic fit 0.0089

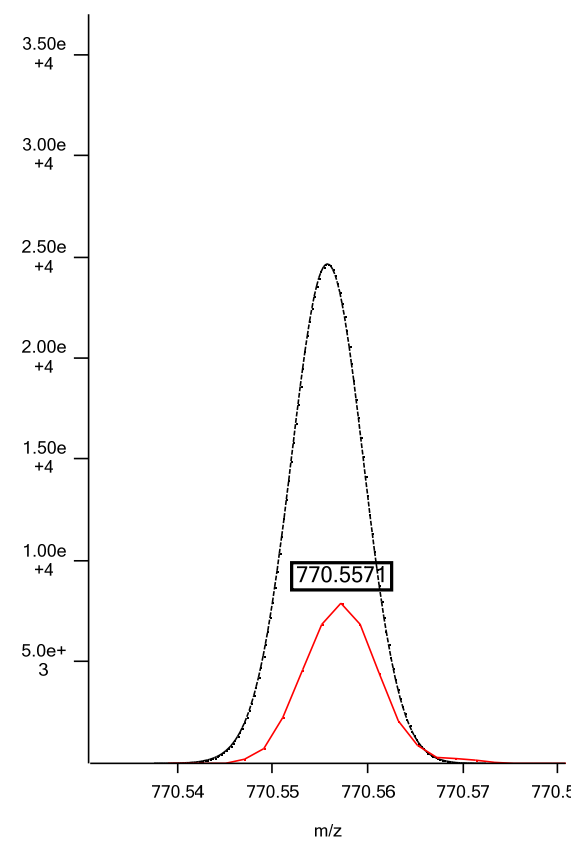
Isotope 1



Isotope 2

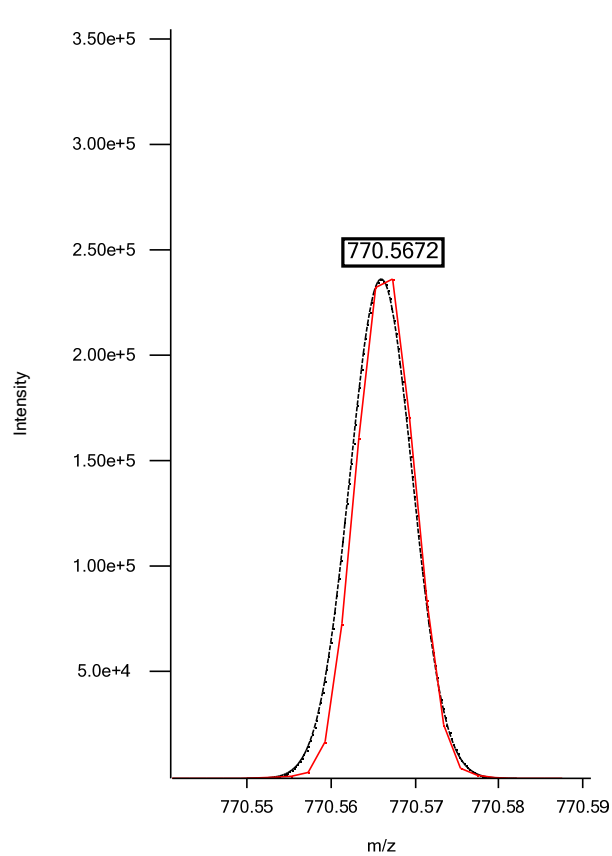


Isotope 3

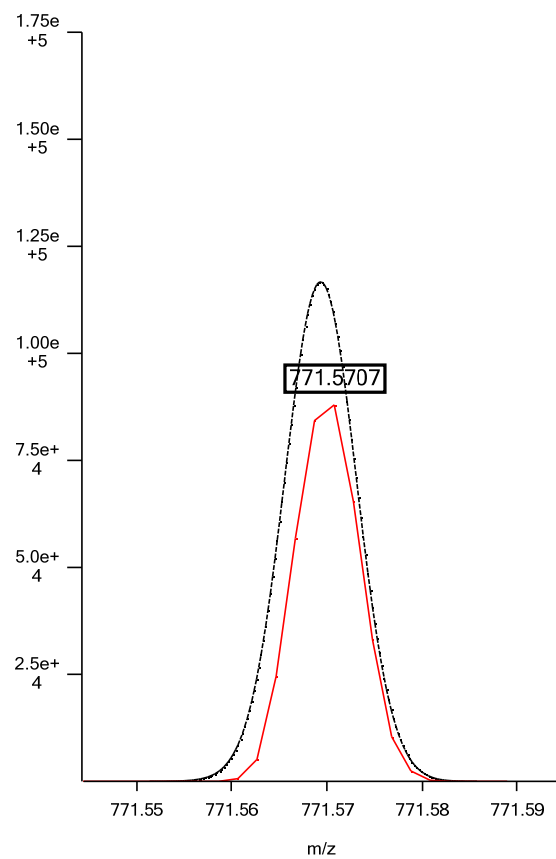


Positive ESI: PC 35:3; C₄₃H₈₁NO₈P; theoretical m/z 770.5699, (M+H)⁺; isotopic fit 0.0159

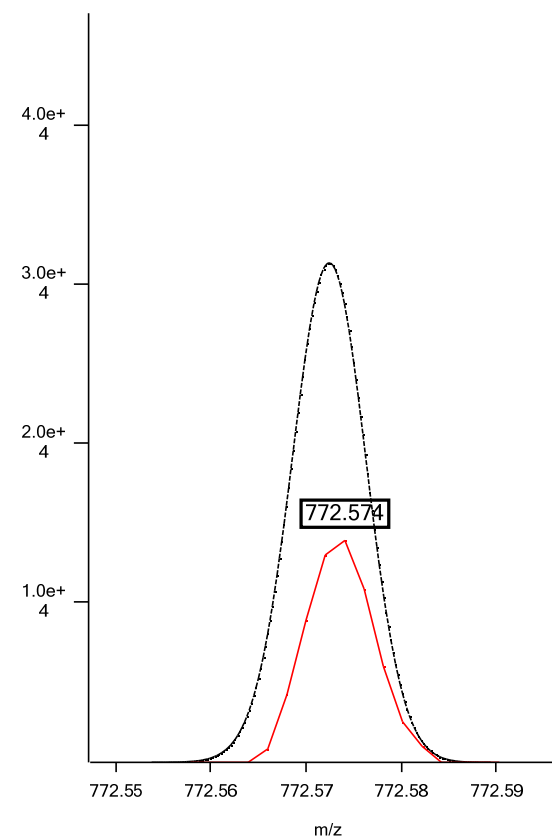
Isotope 1



Isotope 2

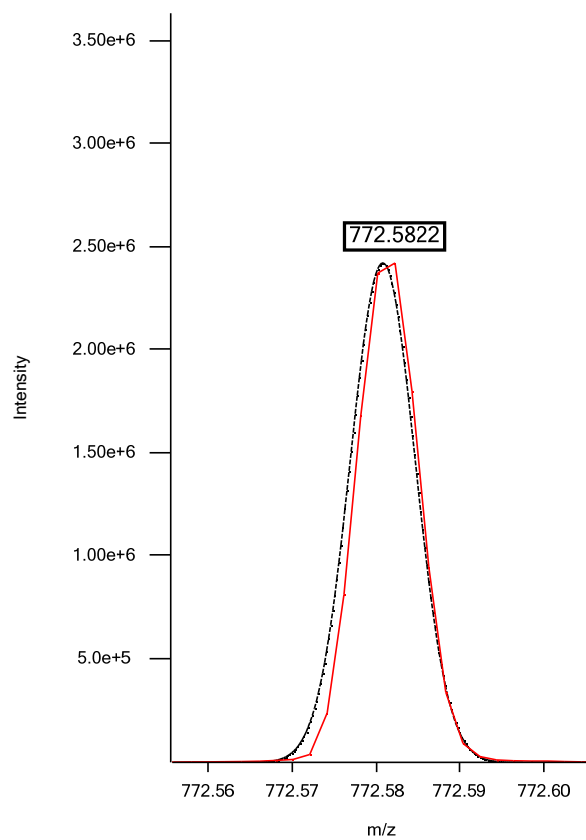


Isotope 3

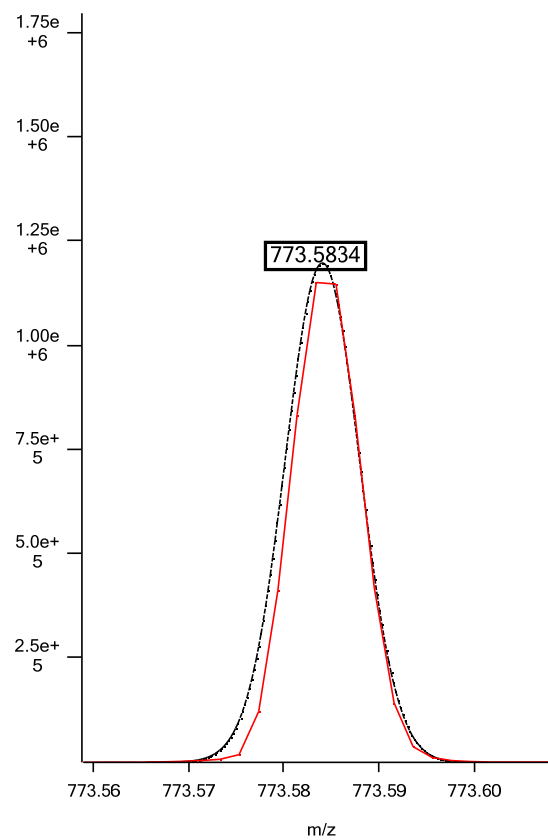


Positive ESI: PC 35:2; C₄₃H₈₃NO₈P; theoretical m/z 772.5856, (M+H)⁺; isotopic fit 0.0029

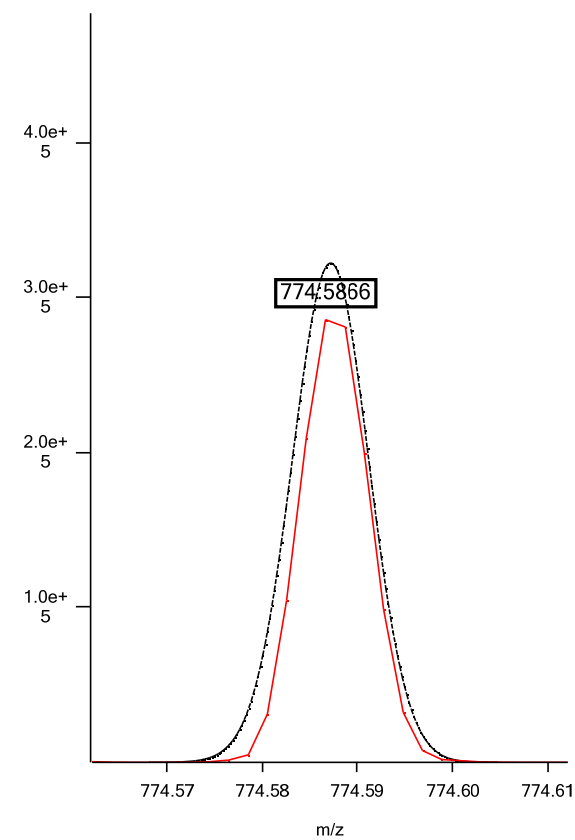
Isotope 1



Isotope 2

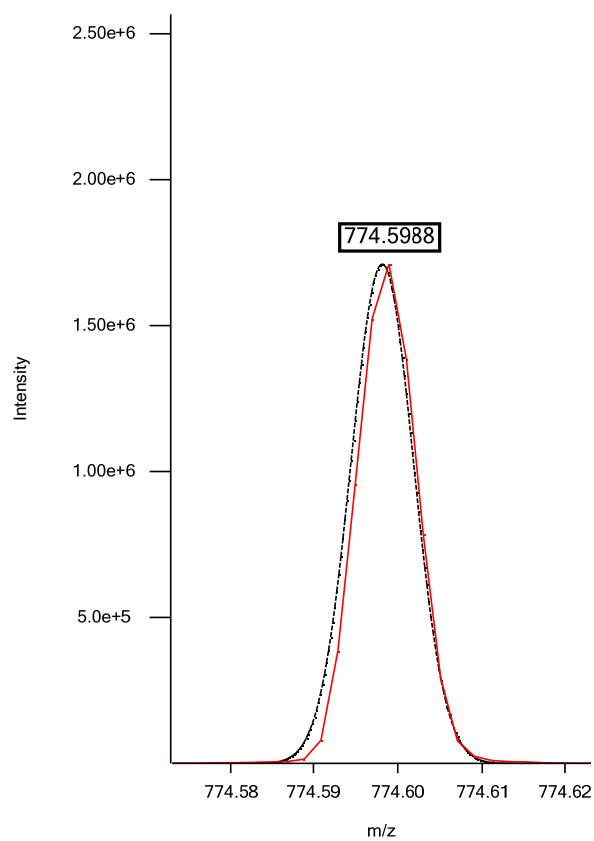


Isotope 3

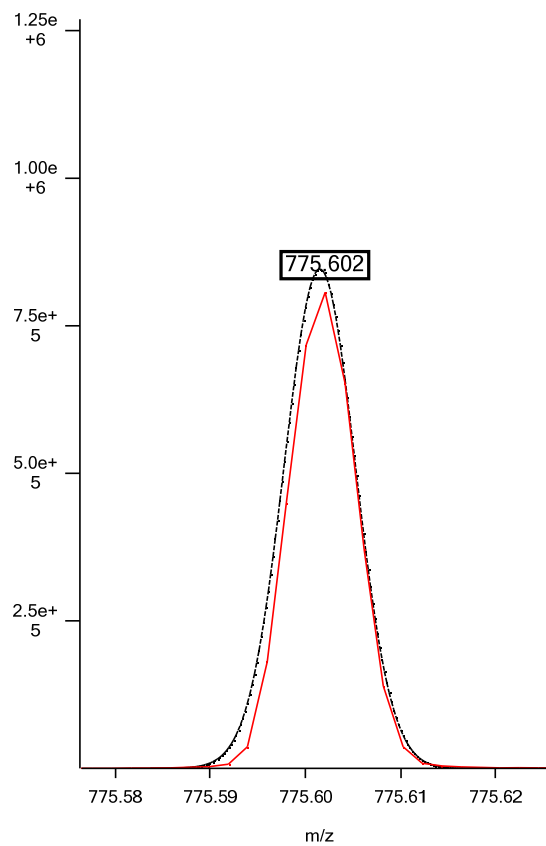


Positive ESI: PC 35:1; C₄₃H₈₅NO₈P; theoretical *m/z* 774.6012, (M+H)⁺; isotopic fit 0.0037

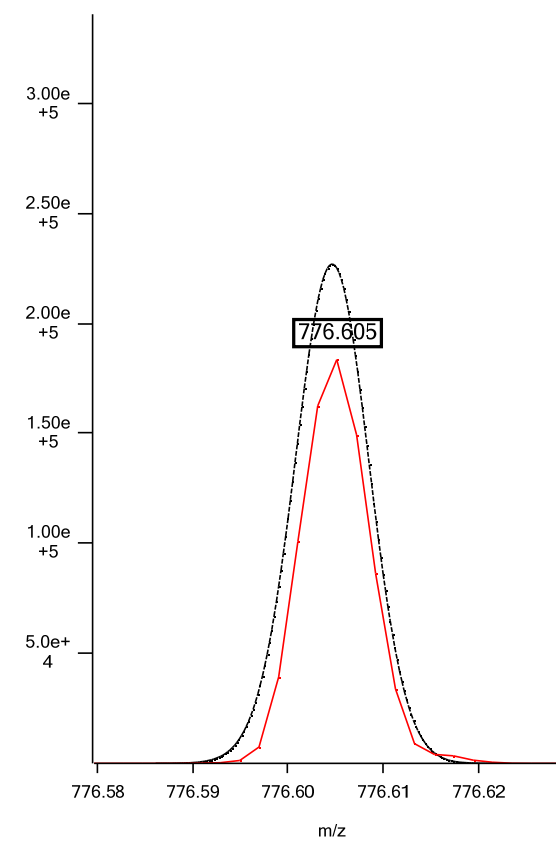
Isotope 1



Isotope 2

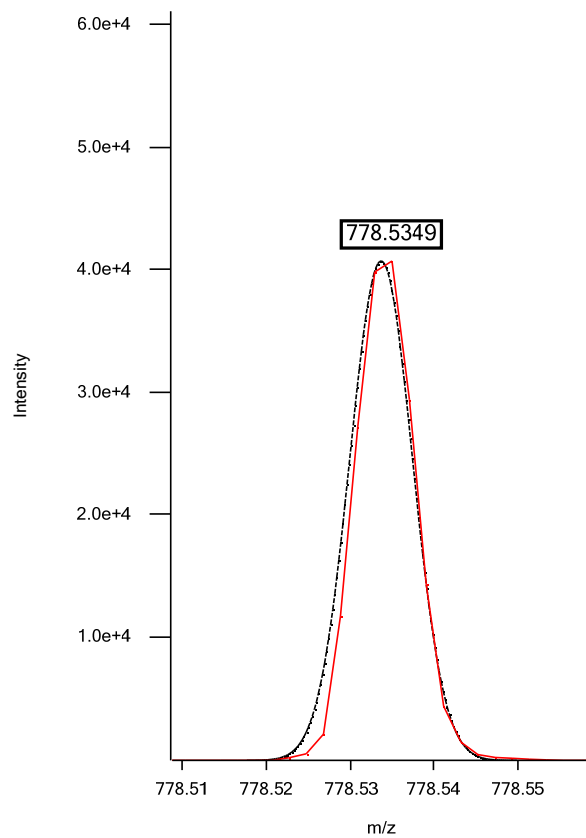


Isotope 3

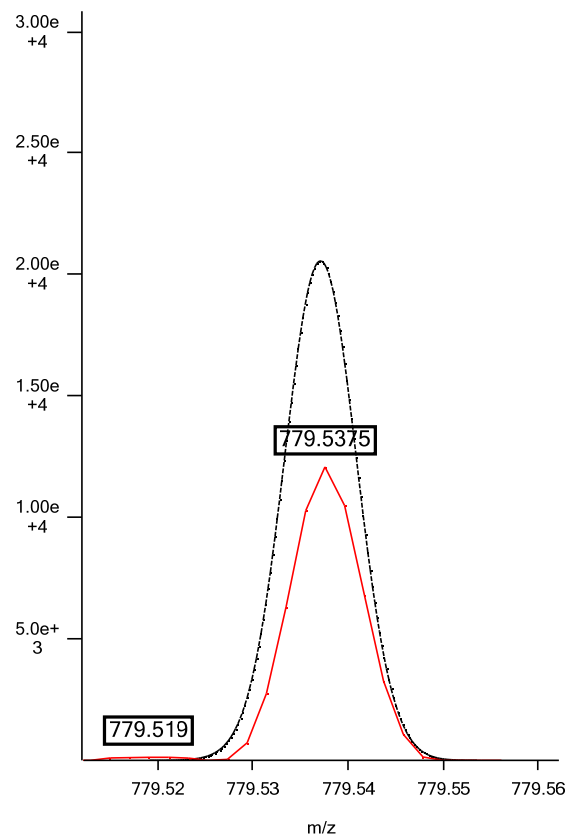


Positive ESI: PC 36:6; C₄₄H₇₇NO₈P; theoretical m/z 778.5387, (M+H)⁺; isotopic fit 0.0379

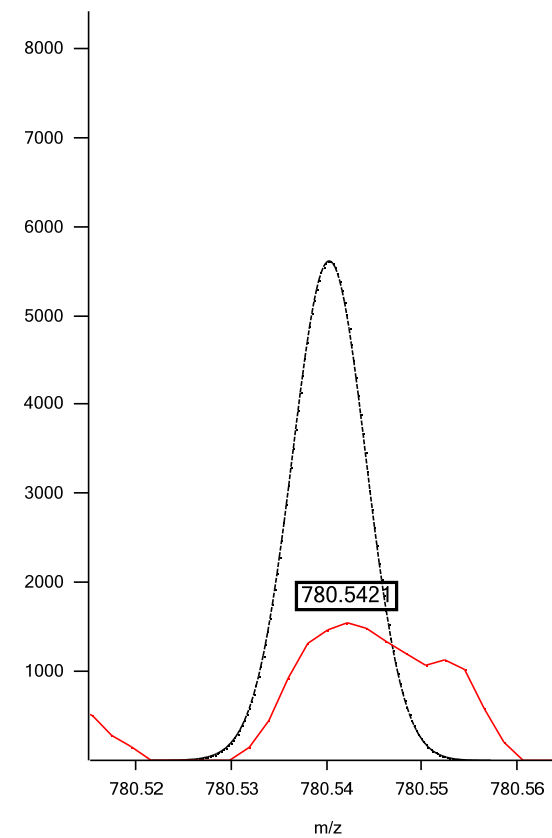
Isotope 1



Isotope 2

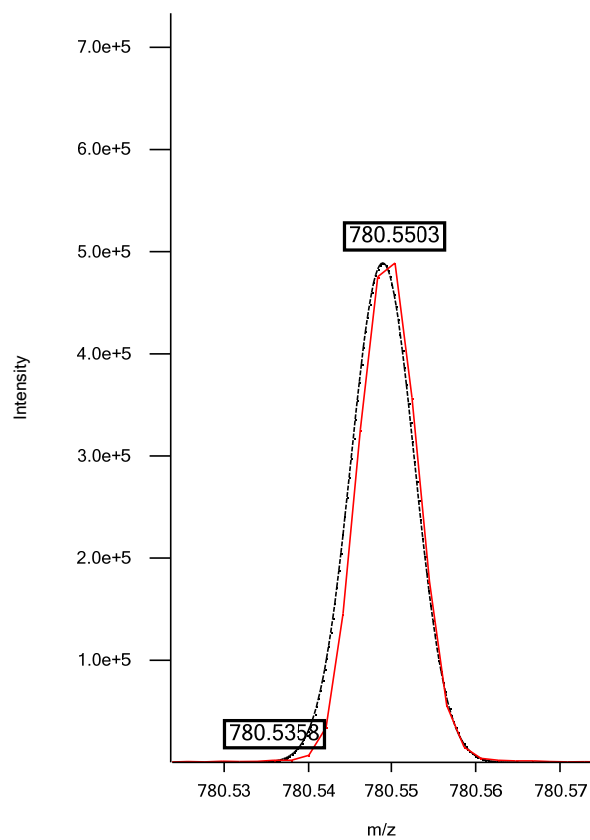


Isotope 3

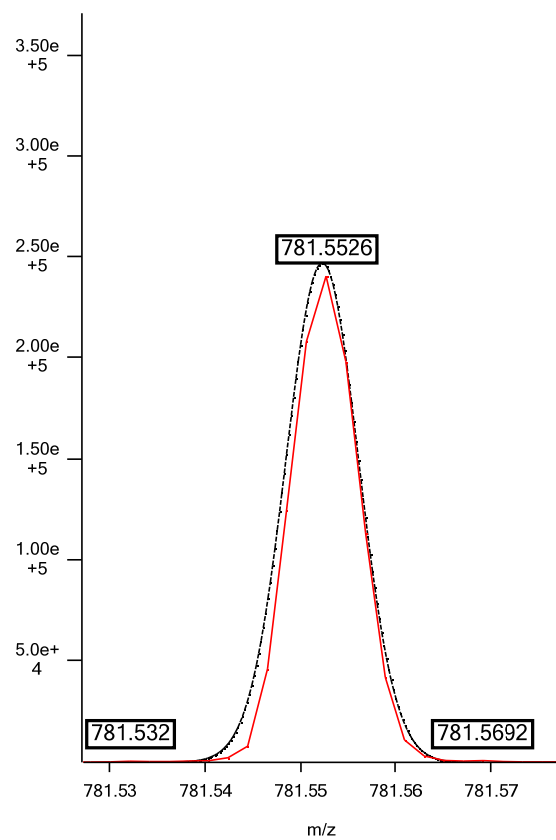


Positive ESI: PC 36:5; C₄₄H₇₉NO₈P; theoretical m/z 780.5543, (M+H)⁺; isotopic fit 0.0051

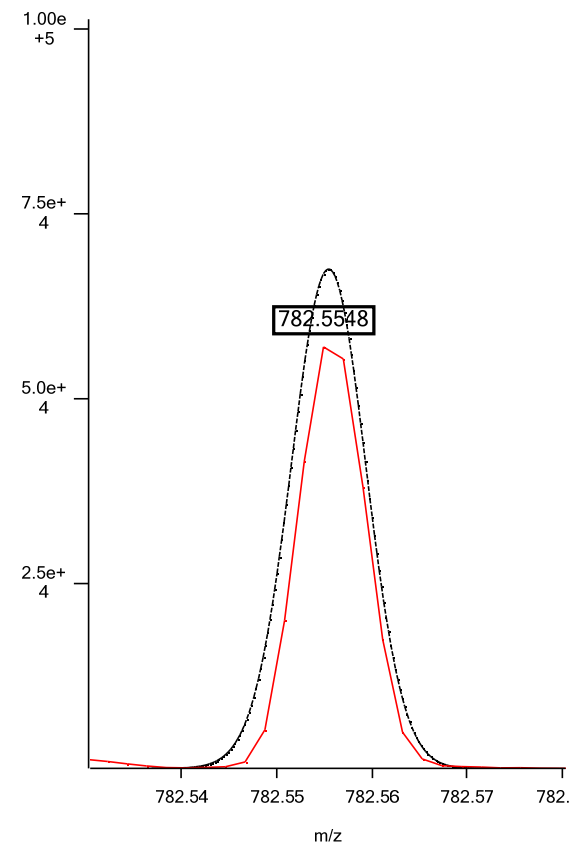
Isotope 1



Isotope 2

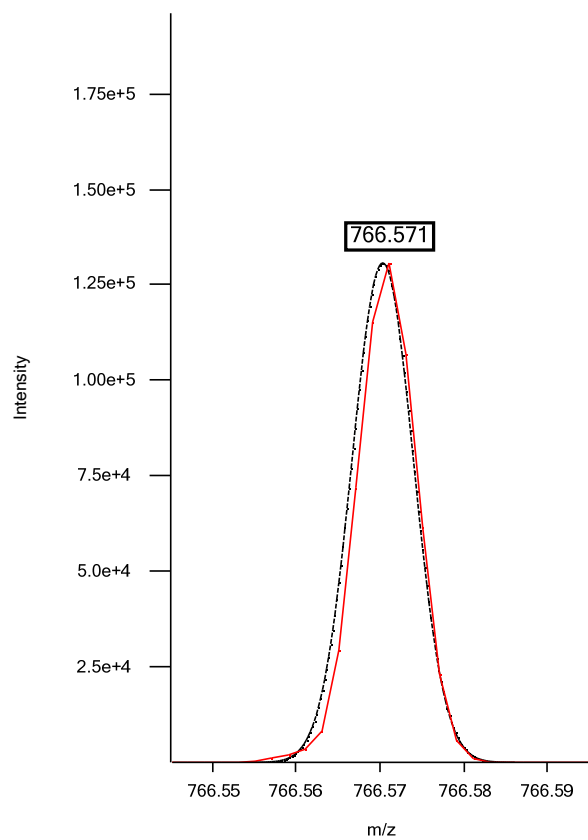


Isotope 3

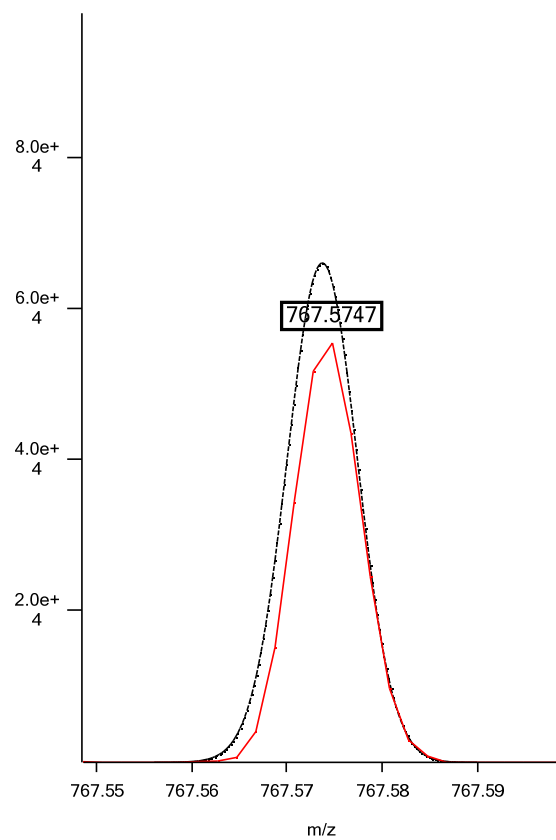


Positive ESI: PC 16:1p/20:4 or 16:0e/20:5; C₄₄H₈₁NO₇P; theoretical *m/z* 766.5750, (M+H)⁺; isotopic fit 0.0098

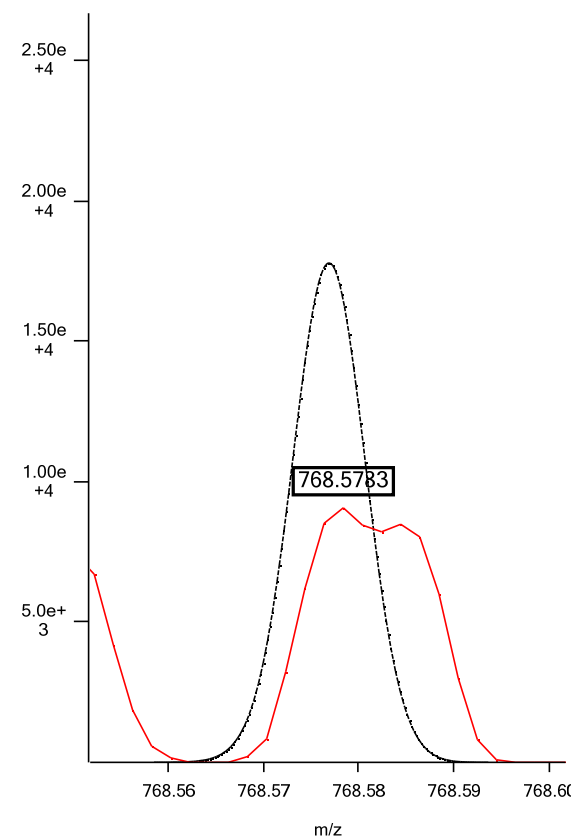
Isotope 1



Isotope 2

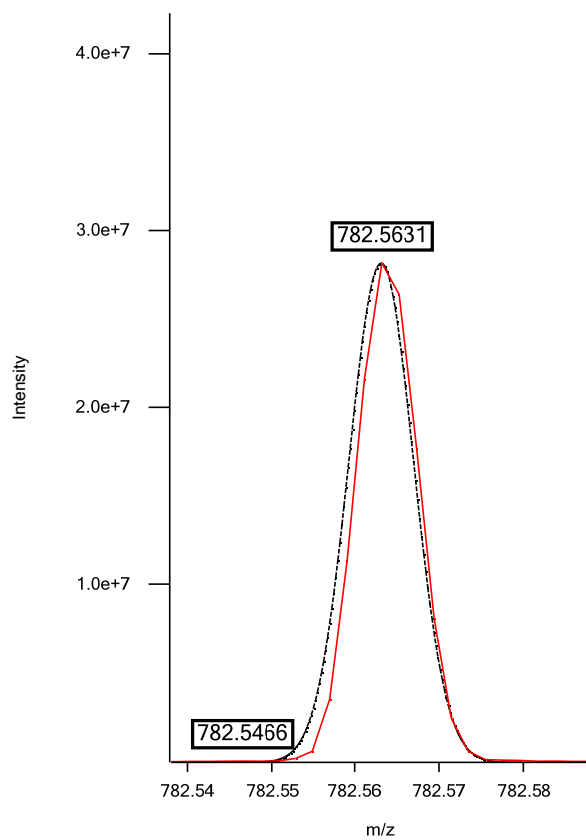


Isotope 3

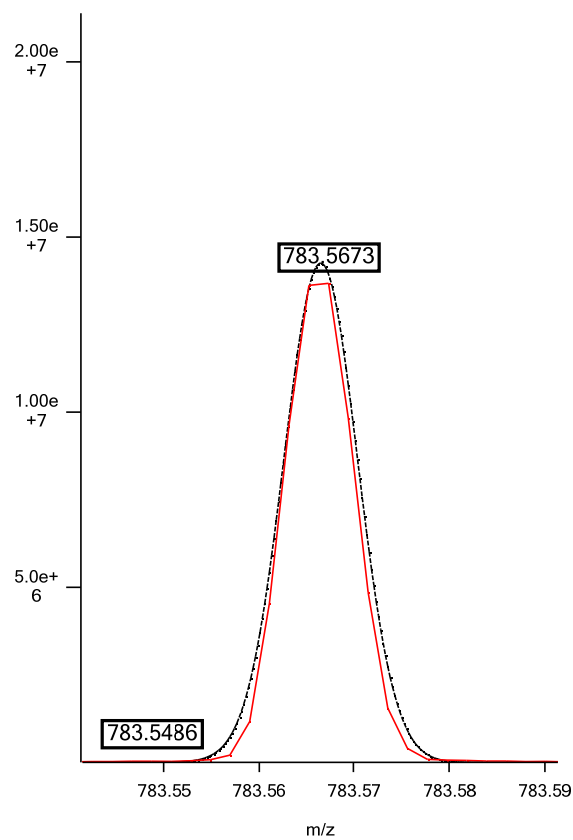


Positive ESI: PC 36:4; C₄₄H₈₁NO₈P; theoretical m/z 782.5699, (M+H)⁺; isotopic fit 0.0070

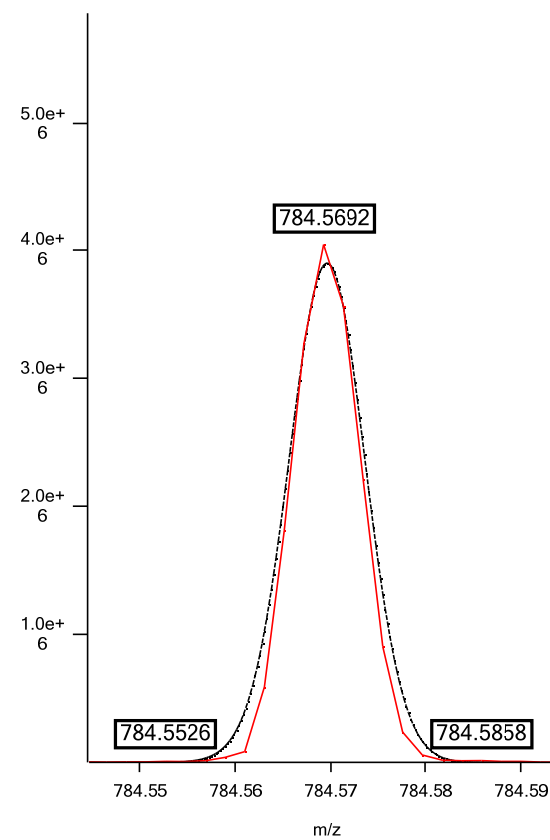
Isotope 1



Isotope 2

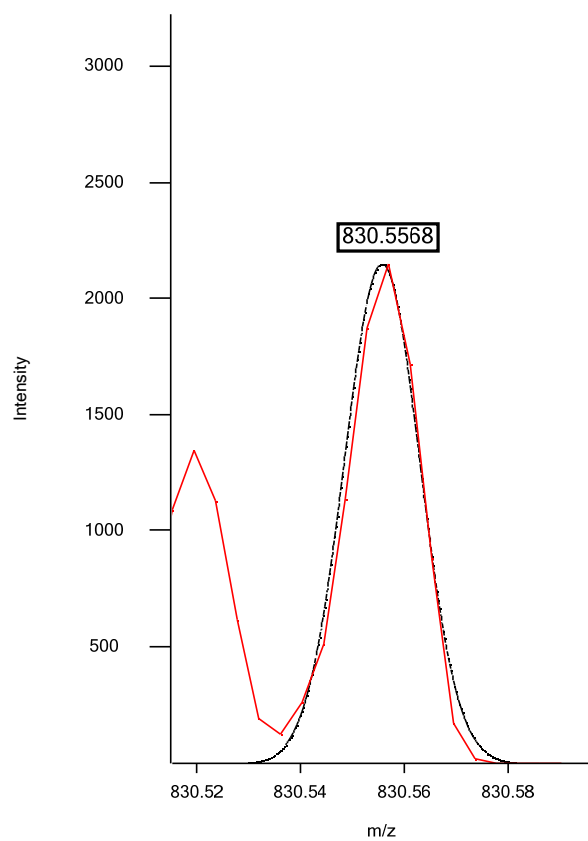


Isotope 3

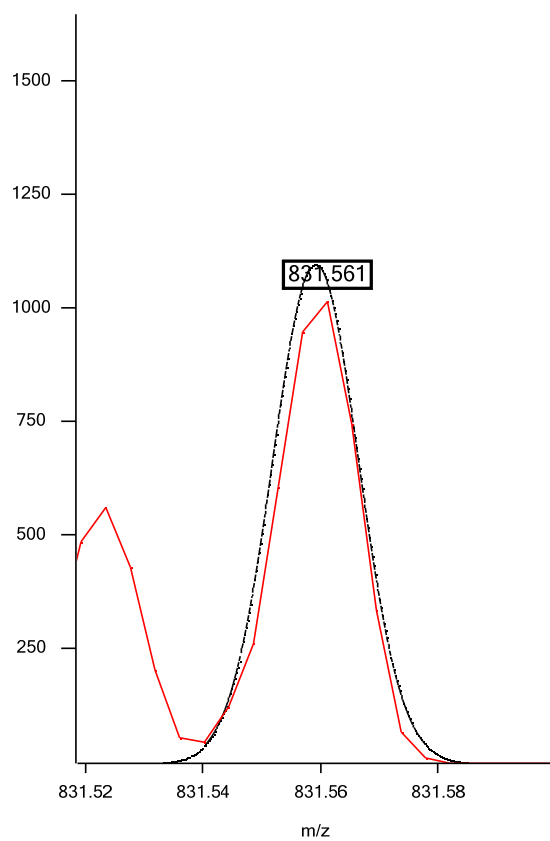


Negative ESI: Oxidized PC 16:0/Hydroxy-18:3; $C_{44}H_{81}NO_{11}P$; theoretical m/z 830.5547, (M-H)⁻; isotopic fit 0.0046

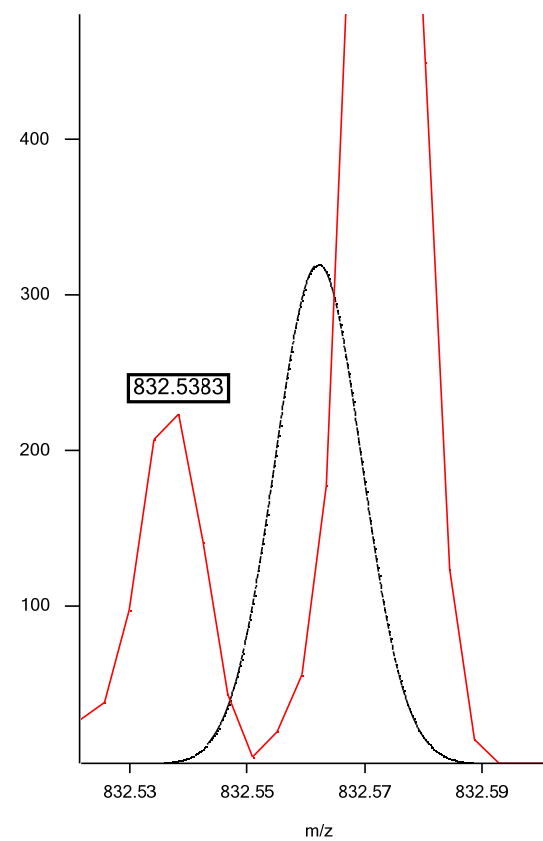
Isotope 1



Isotope 2

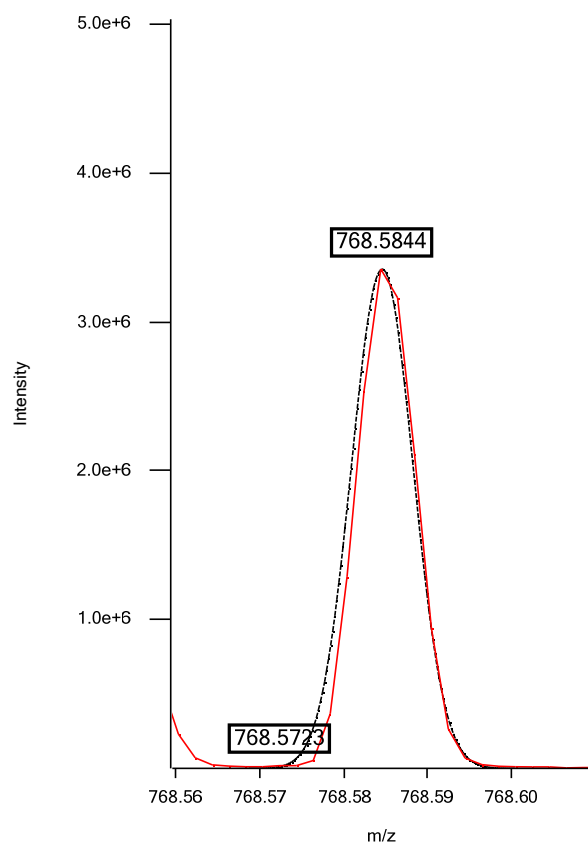


Isotope 3

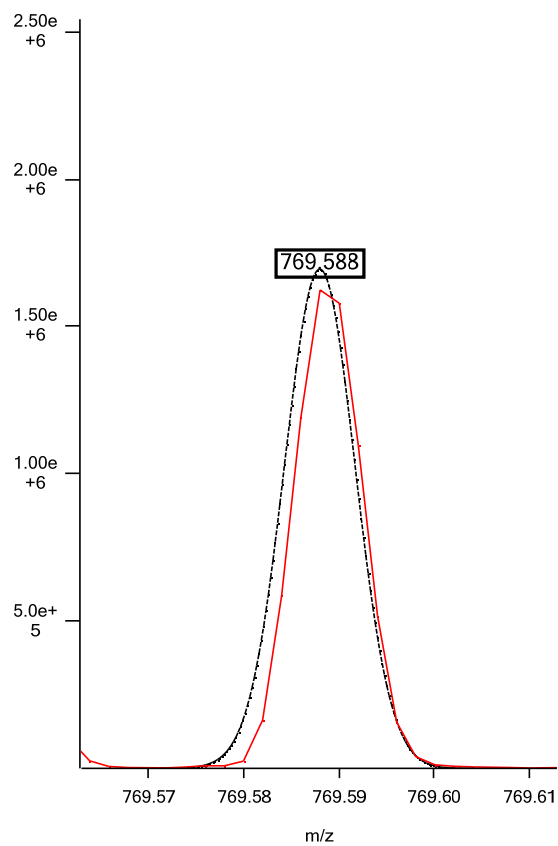


Positive ESI: PC 16:1p/20:3 or 16:0e/20:4; C₄₄H₈₃NO₇P; theoretical *m/z* 768.5907, (M+H)⁺; isotopic fit 0.0062

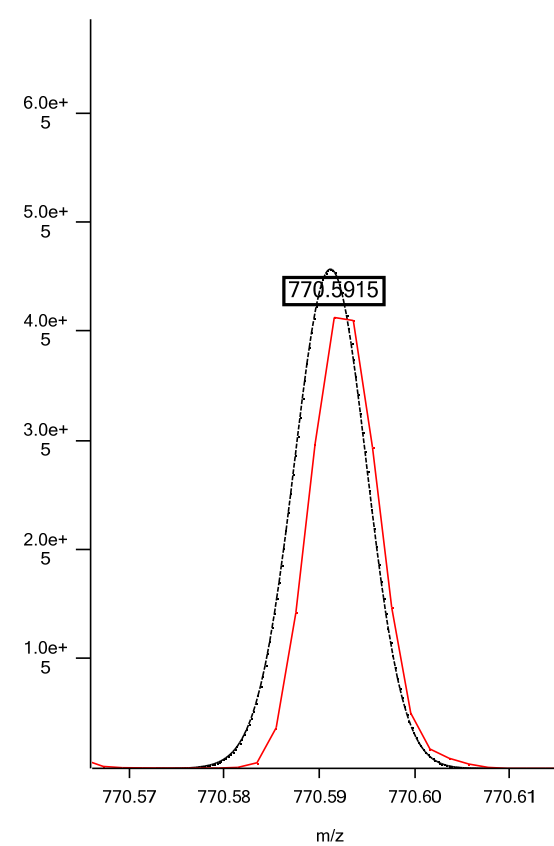
Isotope 1



Isotope 2

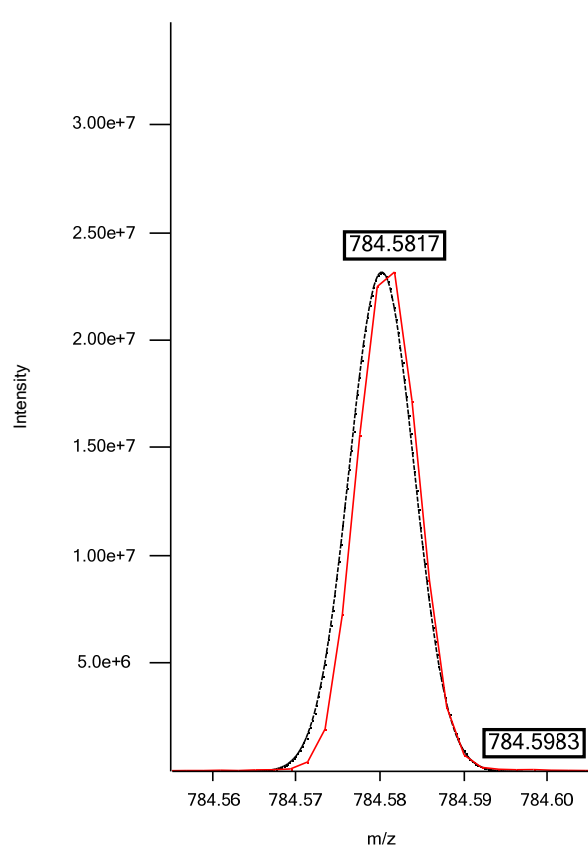


Isotope 3

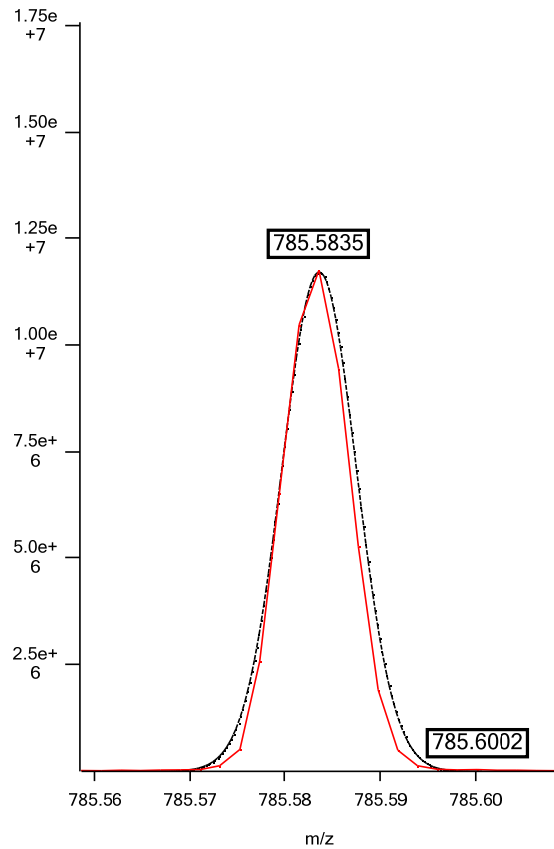


Positive ESI: PC 36:3; C₄₄H₈₃NO₈P; theoretical m/z 784.5856, (M+H)⁺; isotopic fit 0.0080

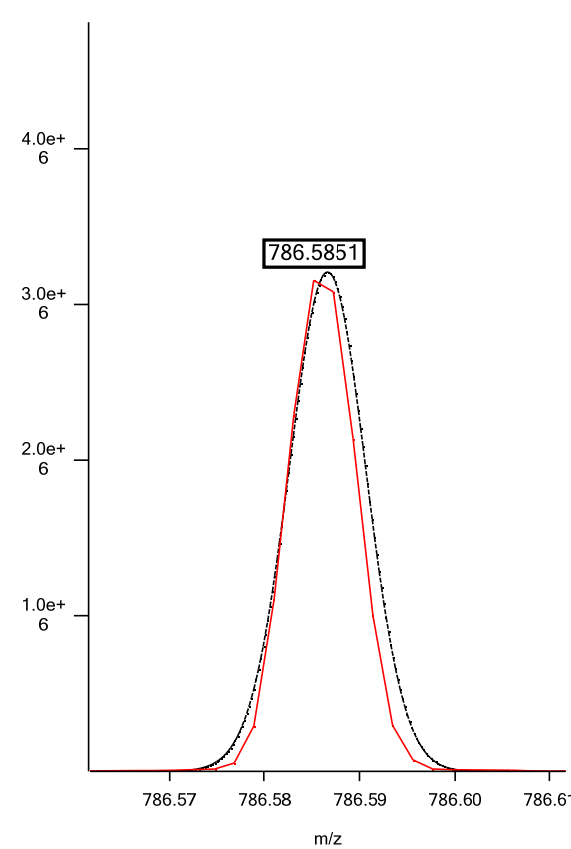
Isotope 1



Isotope 2

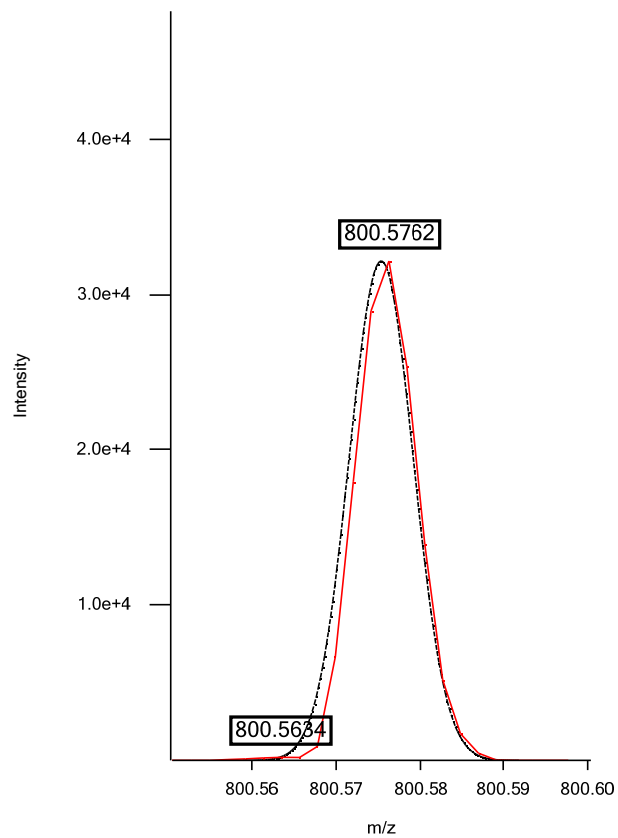


Isotope 3

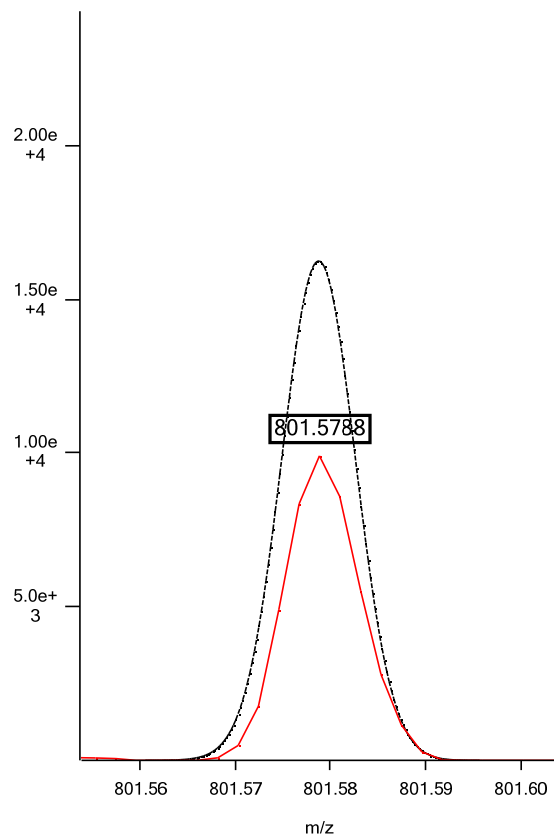


Positive ESI: Oxidized PC 18:0/Hydroxy-18:3; $C_{44}H_{83}NO_9P$; theoretical m/z 800.5805, $(M+H)^+$; isotopic fit 0.0350

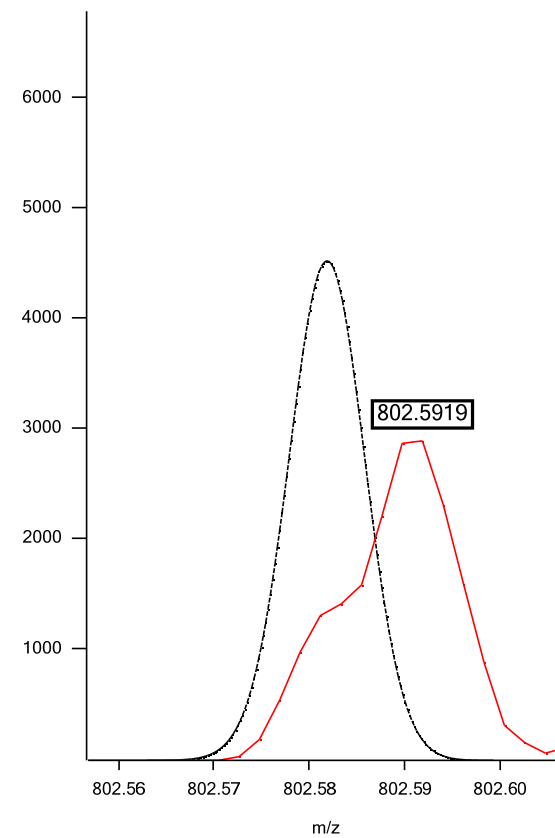
Isotope 1



Isotope 2

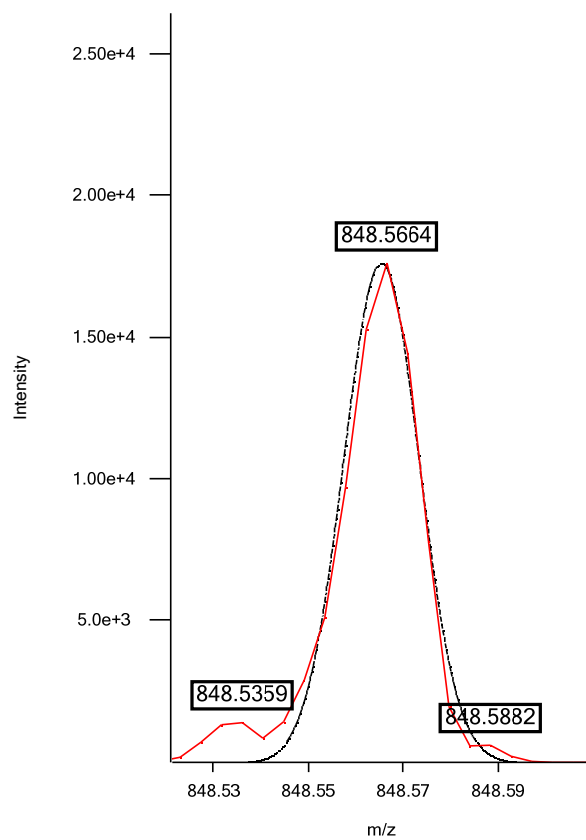


Isotope 3

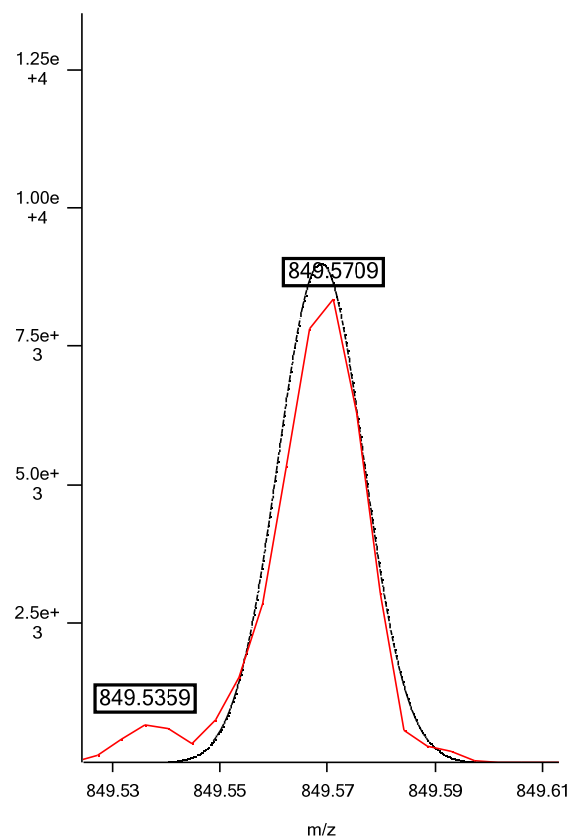


Negative ESI: Oxidized PC 16:0/Hydroperoxy-18:2; $C_{44}H_{83}NO_{12}P$; theoretical m/z 848.5653, (M-H)⁻; isotopic fit 0.0041

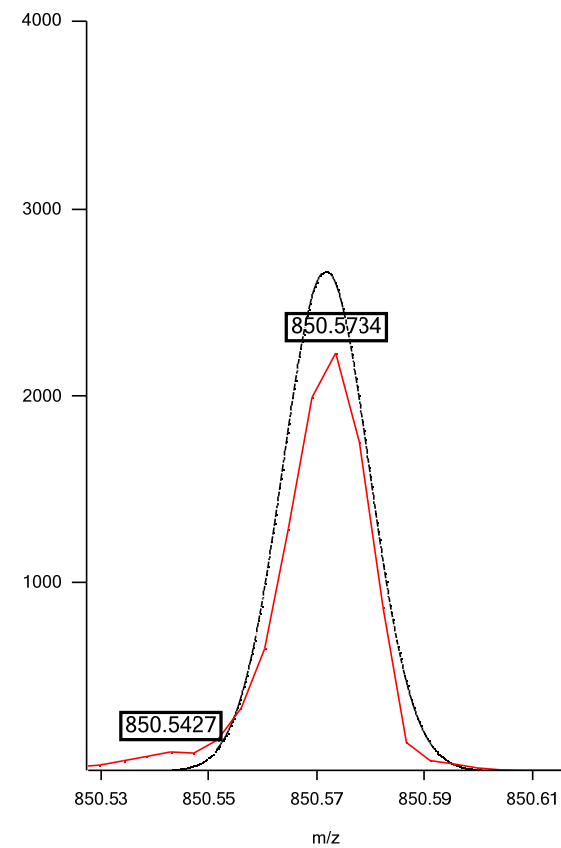
Isotope 1



Isotope 2

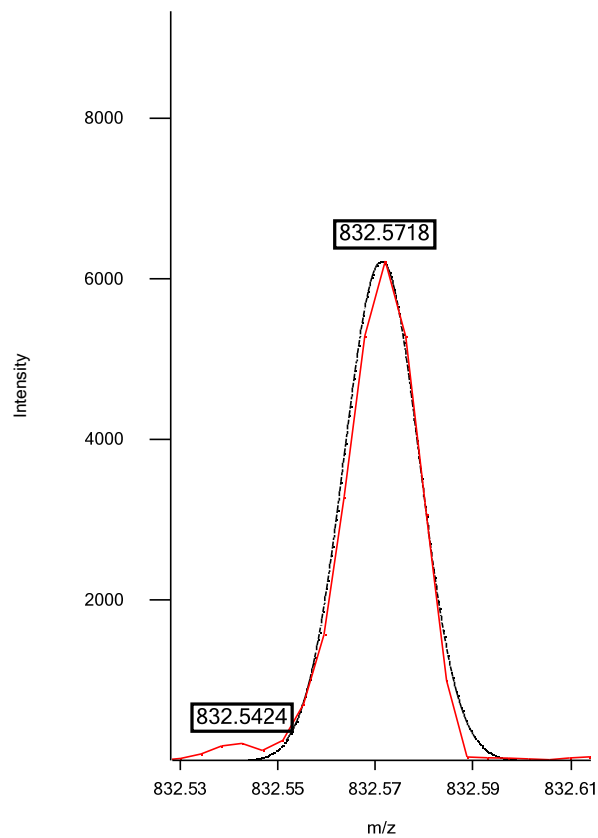


Isotope 3

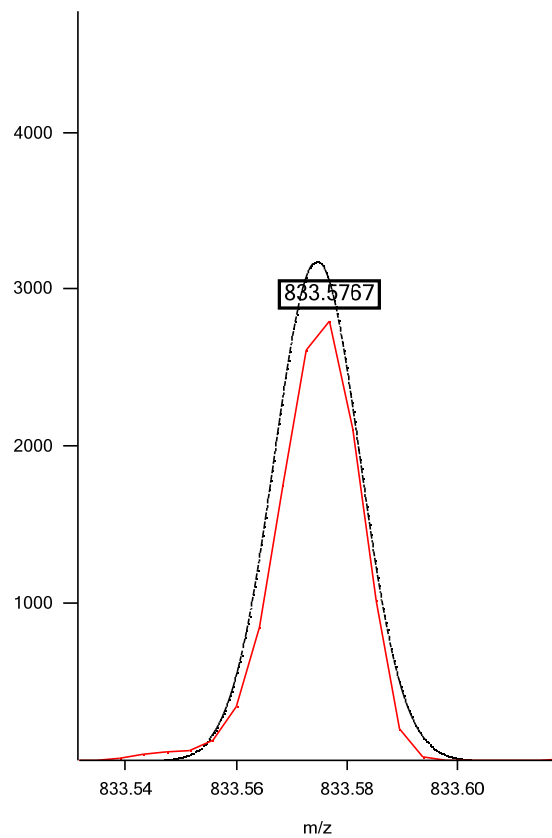


Negative ESI: Oxidized PC 16:0/Hydroxy-18:2; $C_{44}H_{83}NO_{11}P$; theoretical m/z 832.5703, (M-H)⁻; isotopic fit 0.0067

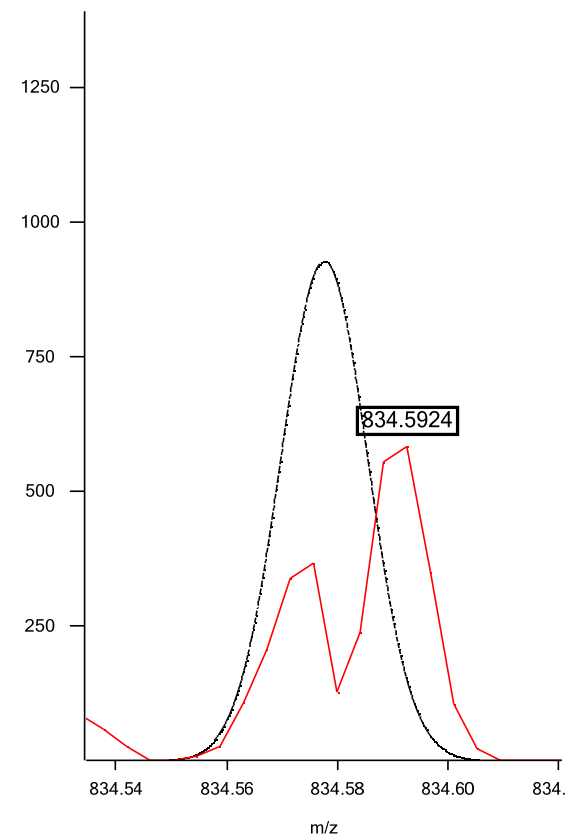
Isotope 1



Isotope 2

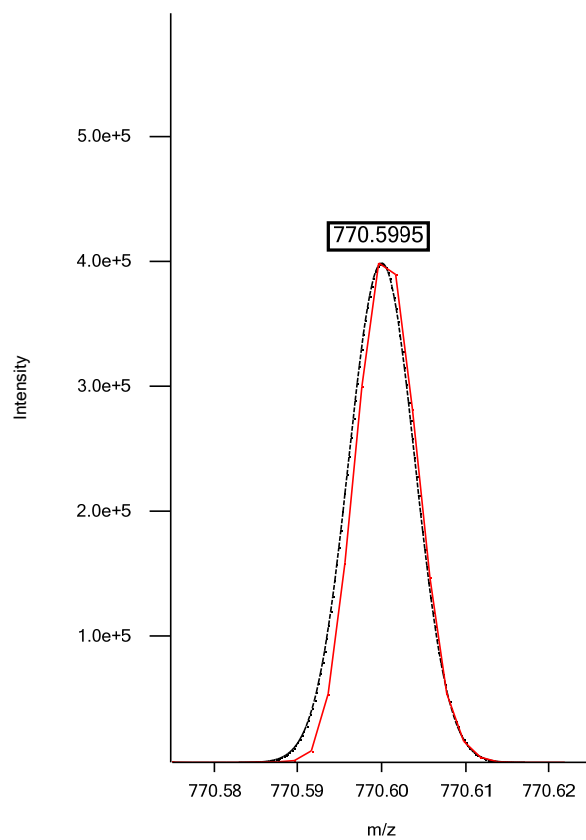


Isotope 3

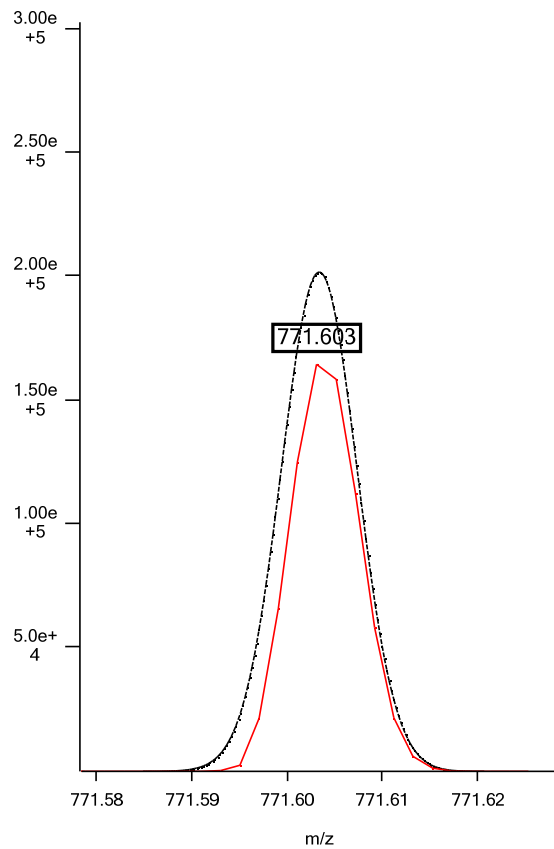


Positive ESI: PC 16:1p/20:2 or 16:0e/20:3; $C_{44}H_{85}NO_7P$; theoretical m/z 770.6063, (M+H)⁺; isotopic fit 0.0125

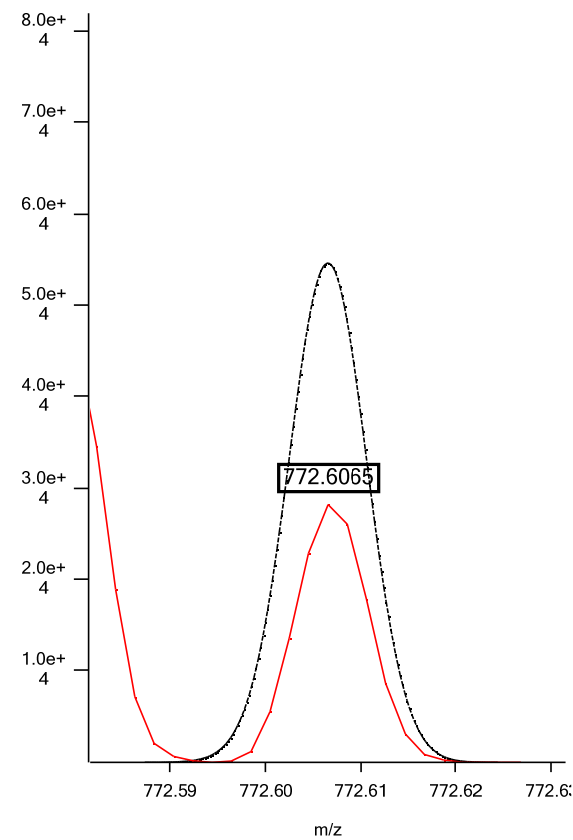
Isotope 1



Isotope 2

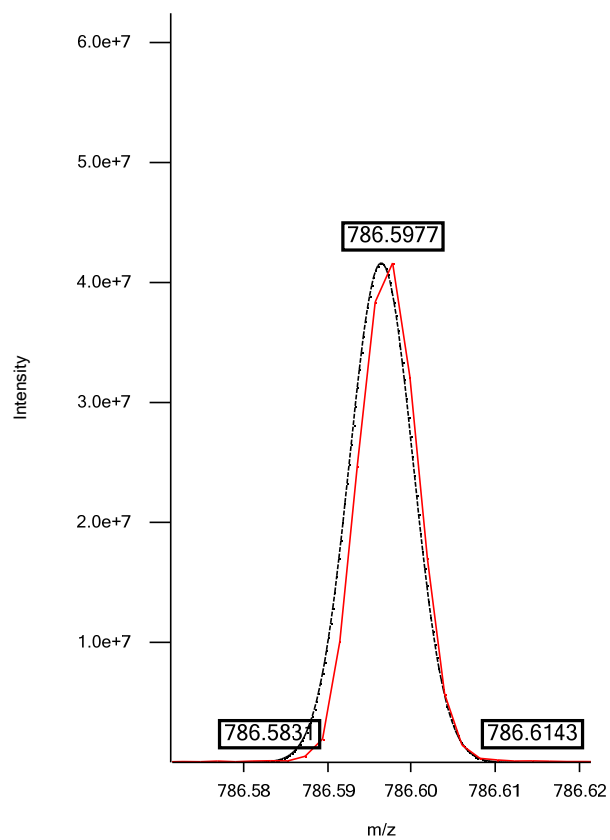


Isotope 3

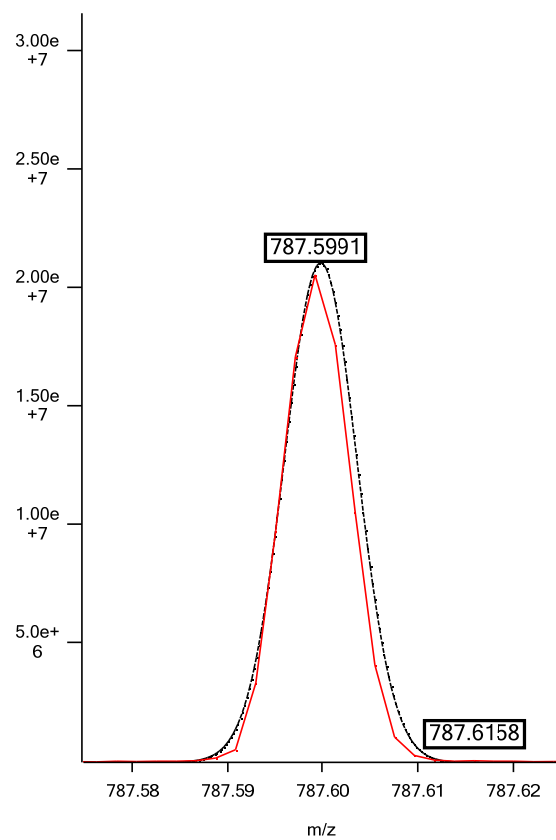


Positive ESI: PC 36:2; C₄₄H₈₅NO₈P; theoretical m/z 786.6013, (M+H)⁺; isotopic fit 0.0114

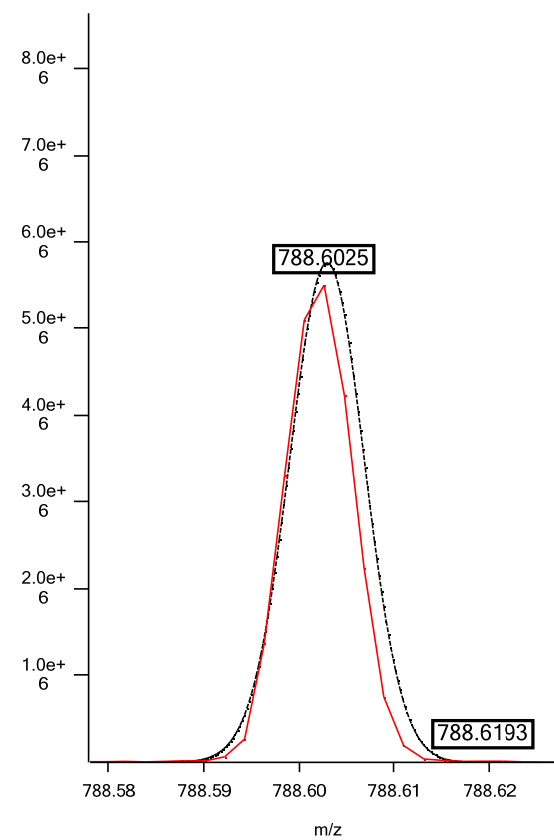
Isotope 1



Isotope 2

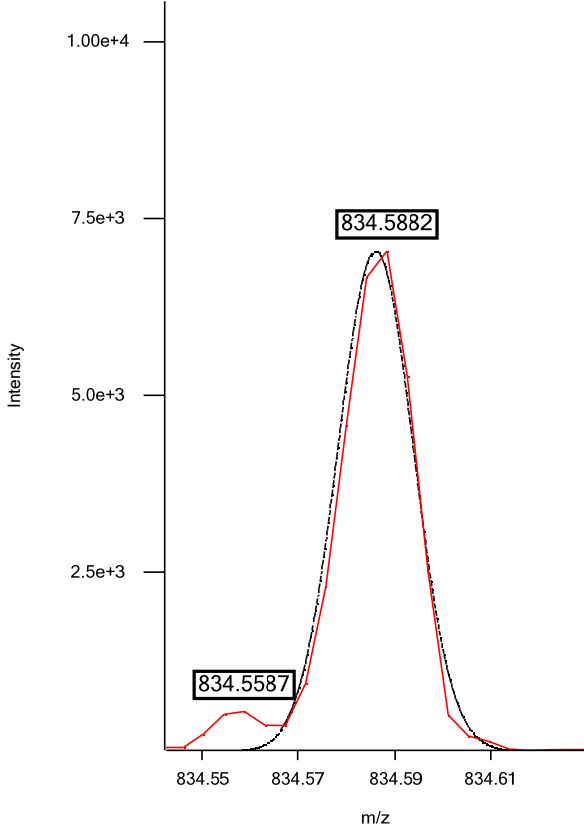


Isotope 3

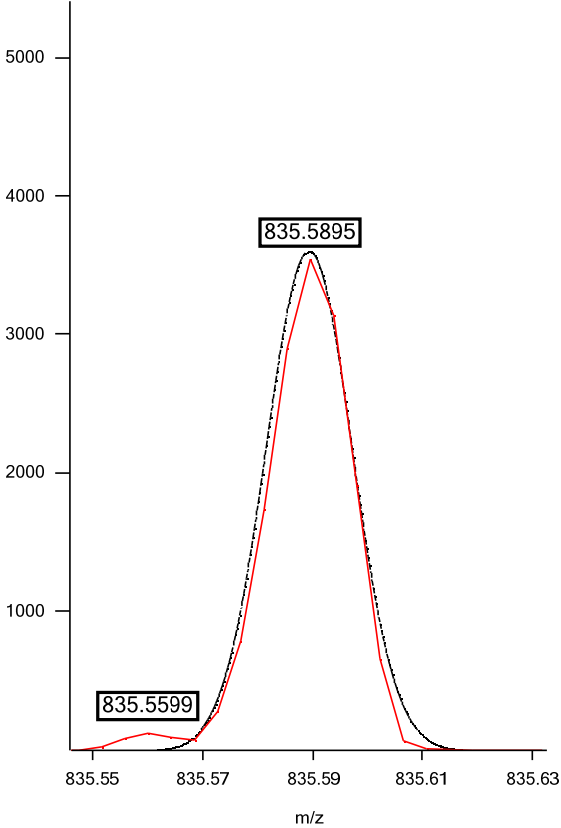


Negative ESI: Oxidized PC 18:0/Hydroxy-16:1 or 16:0/Hydroxy-18:1; $C_{44}H_{85}NO_{11}P$; theoretical m/z 834.5860, (M-H)⁻; isotopic fit 0.0025

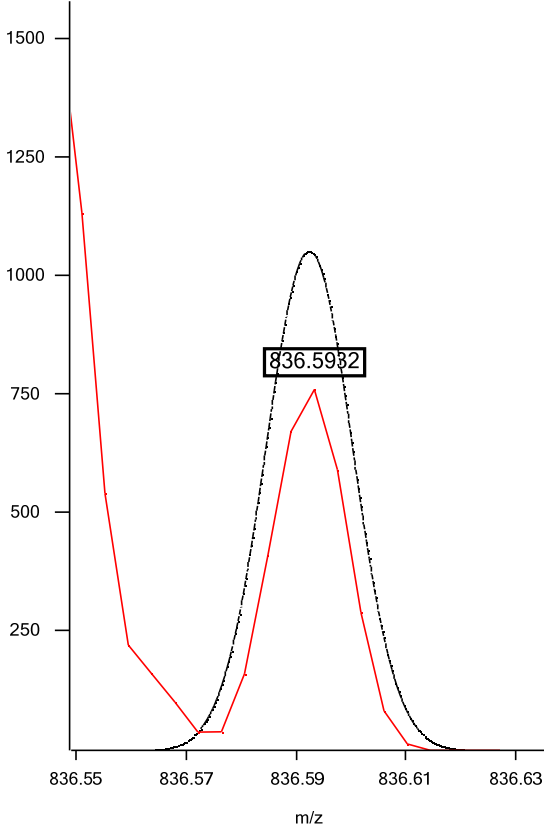
Isotope 1



Isotope 2

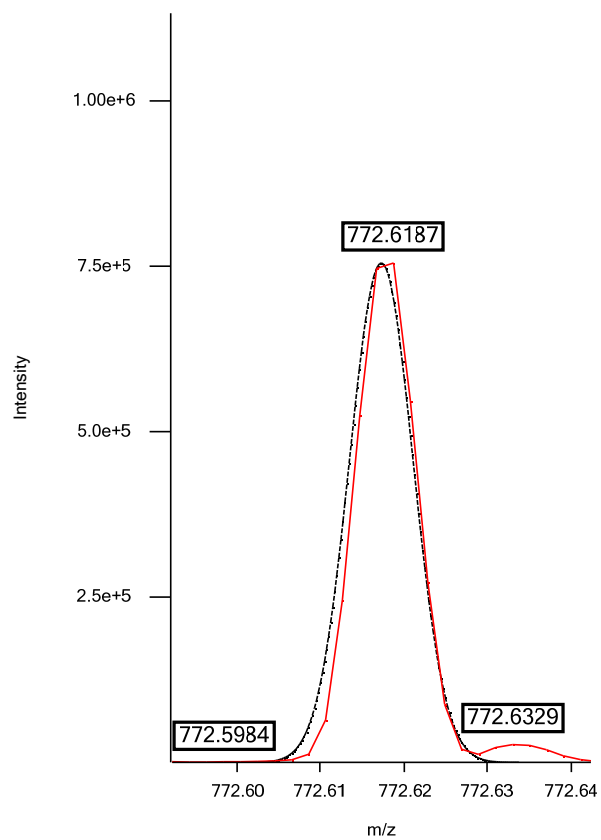


Isotope 3

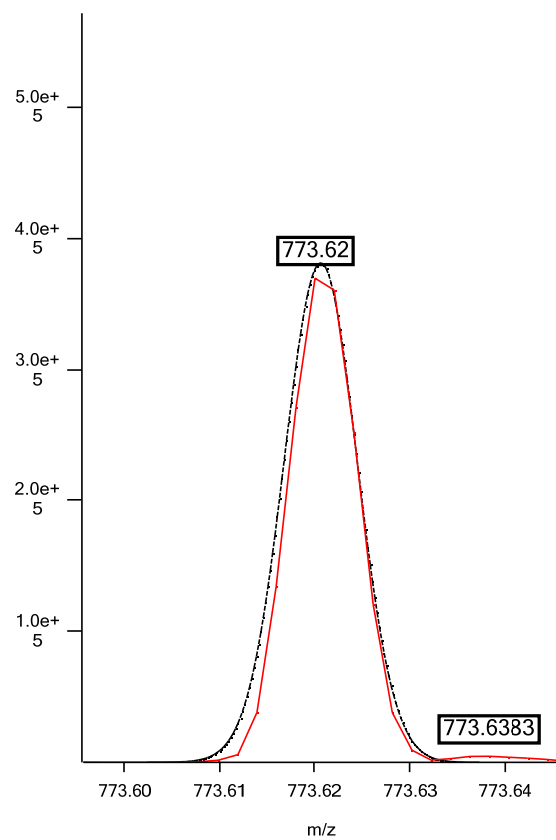


Positive ESI: PC 16:1p/20:1 or 16:0e/20:2; $C_{44}H_{87}NO_7P$; theoretical m/z 772.6220, $(M+H)^+$; isotopic fit 0.0036

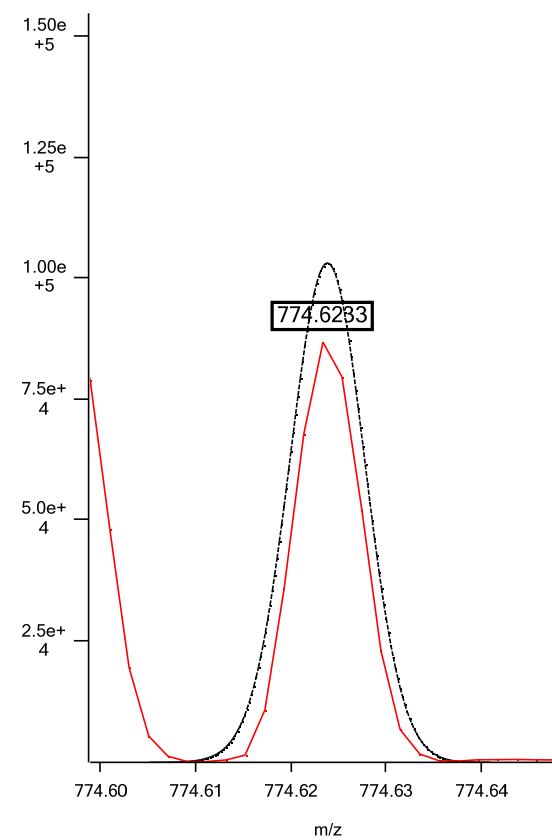
Isotope 1



Isotope 2

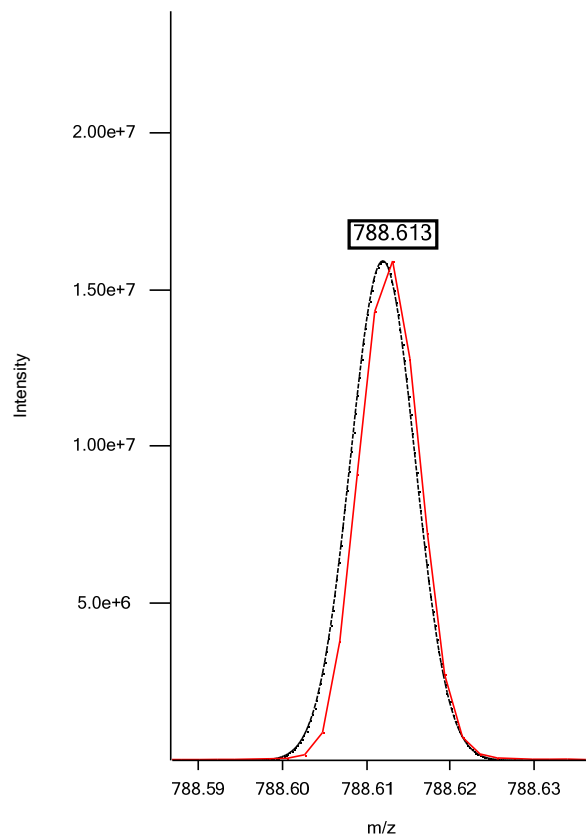


Isotope 3

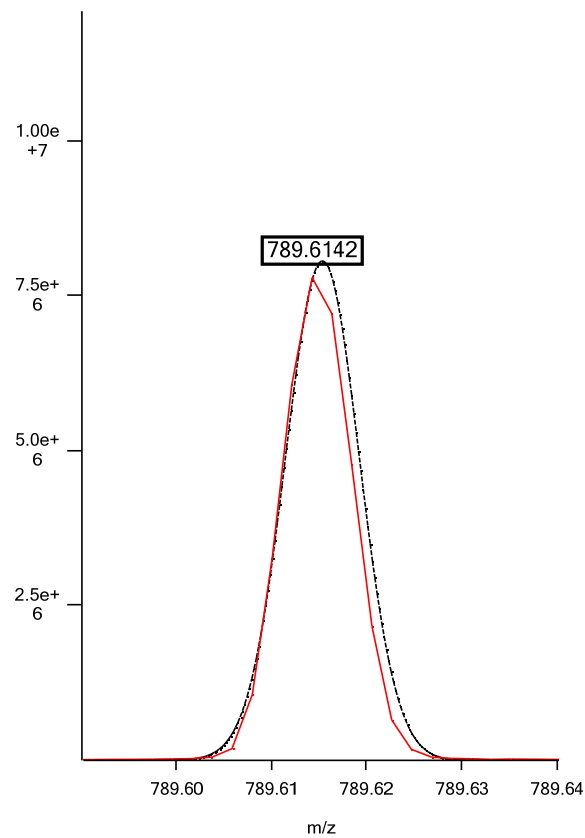


Positive ESI: PC 36:1; C₄₄H₈₇NO₈P; theoretical m/z 788.6169, (M+H)⁺; isotopic fit 0.0112

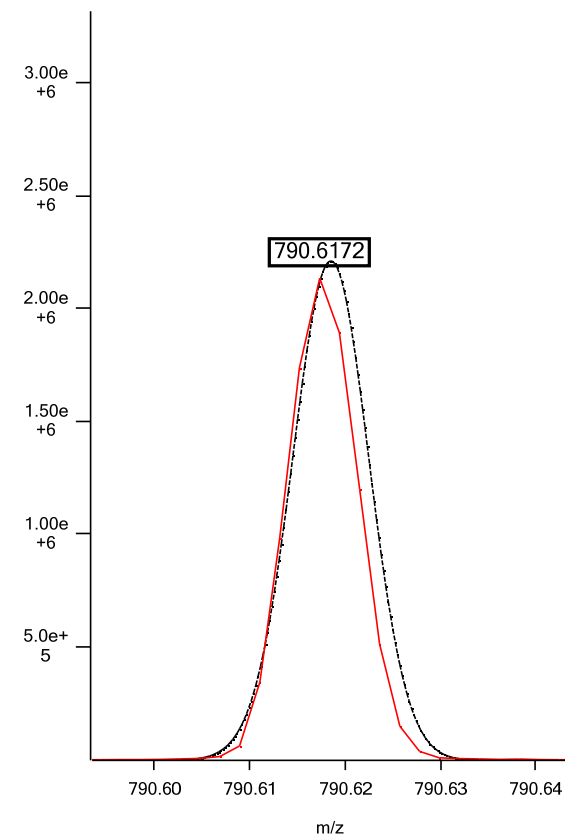
Isotope 1



Isotope 2

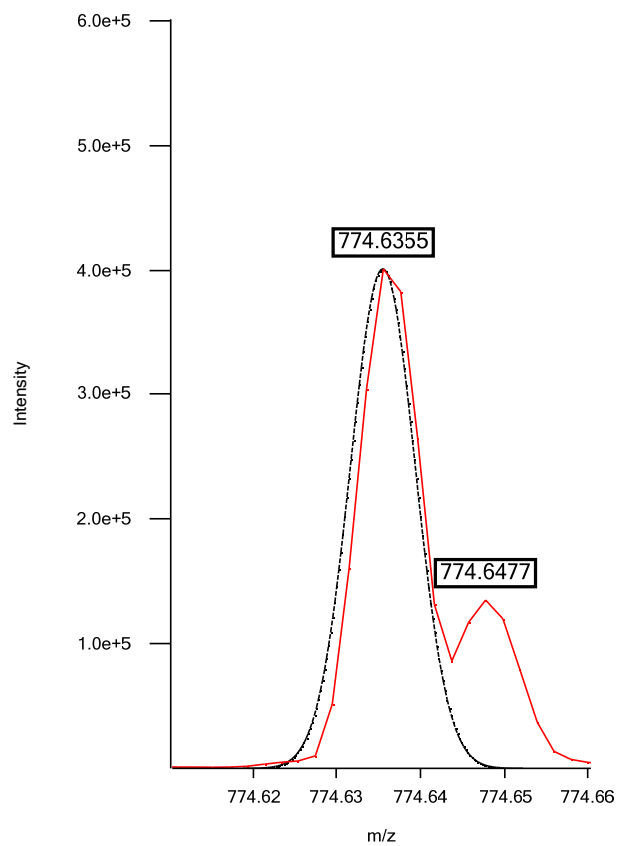


Isotope 3

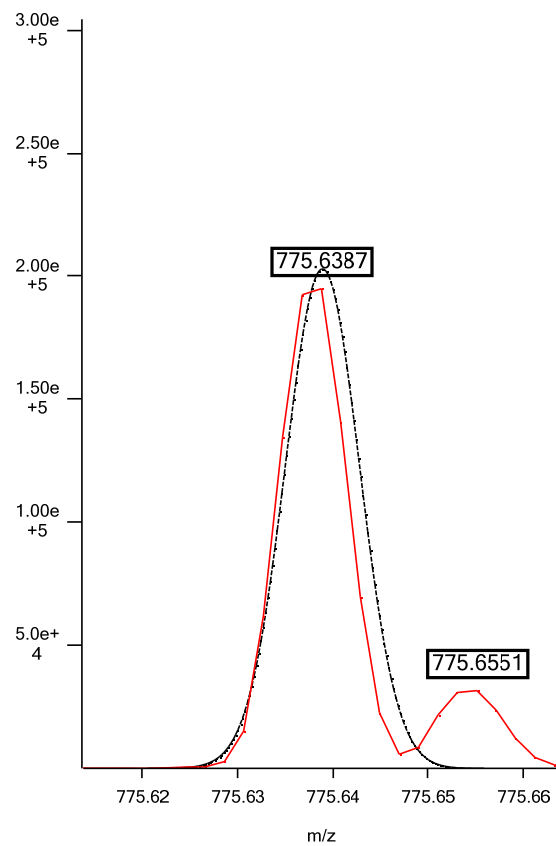


Positive ESI: PC 16:1p/20:0 or 16:0e/20:0; $C_{44}H_{89}NO_7P$; theoretical m/z 774.6376, $(M+H)^+$; isotopic fit 0.0190

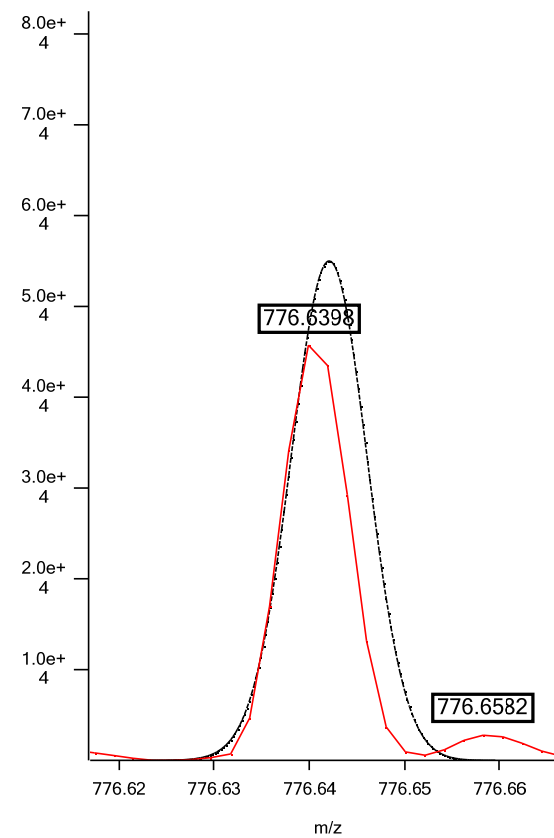
Isotope 1



Isotope 2

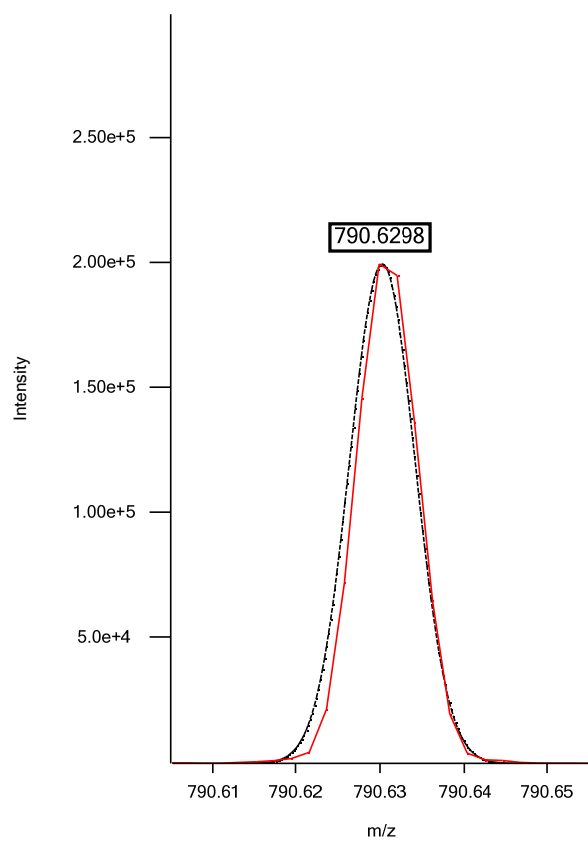


Isotope 3

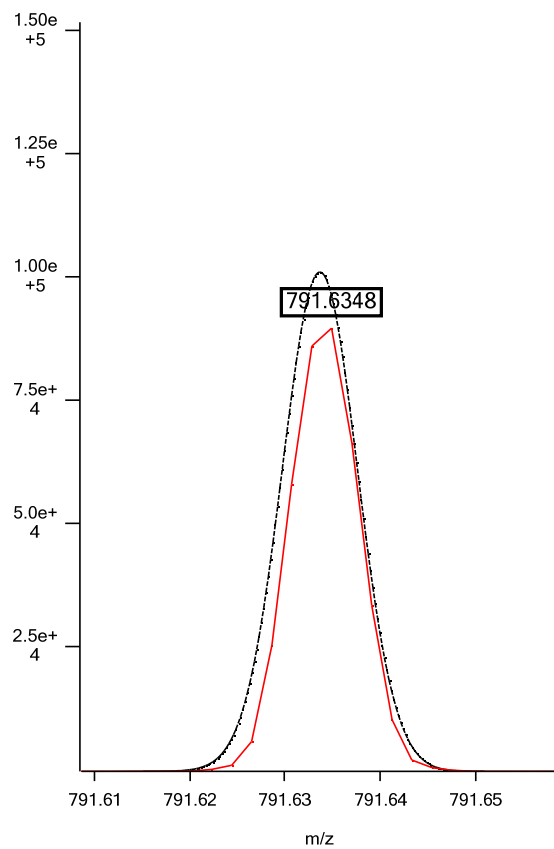


Positive ESI: PC 36:0; C₄₄H₈₉NO₈P; theoretical m/z 790.6325, (M+H)⁺; isotopic fit 0.0053

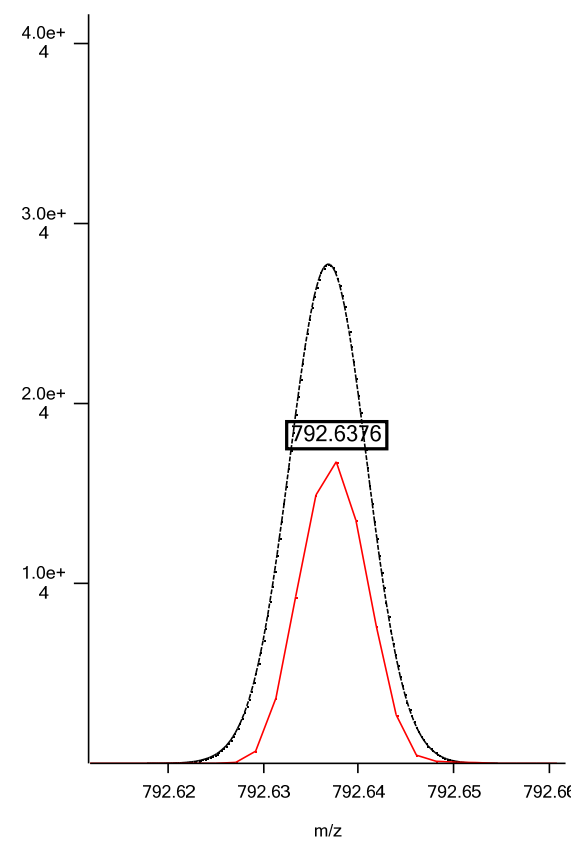
Isotope 1



Isotope 2

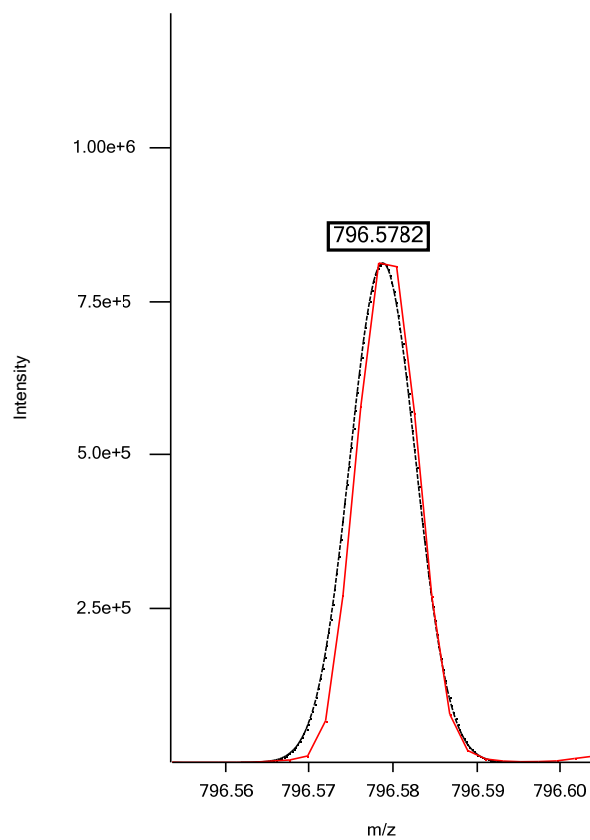


Isotope 3

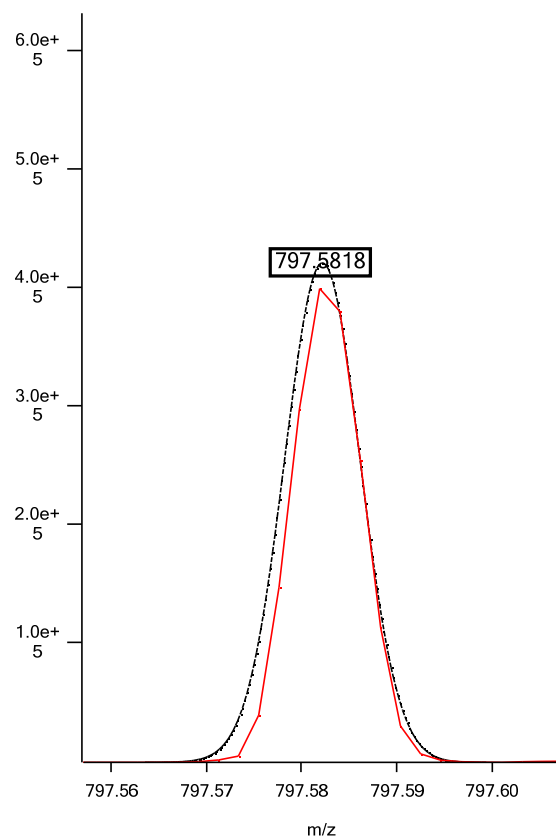


Positive ESI: PC 37:4; C₄₅H₈₃NO₈P; theoretical m/z 796.5856, (M+H)⁺; isotopic fit 0.0043

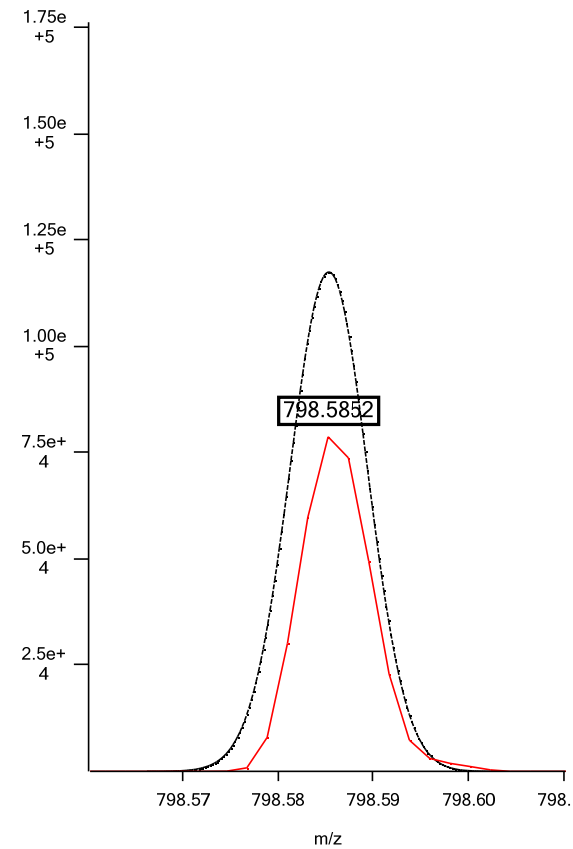
Isotope 1



Isotope 2

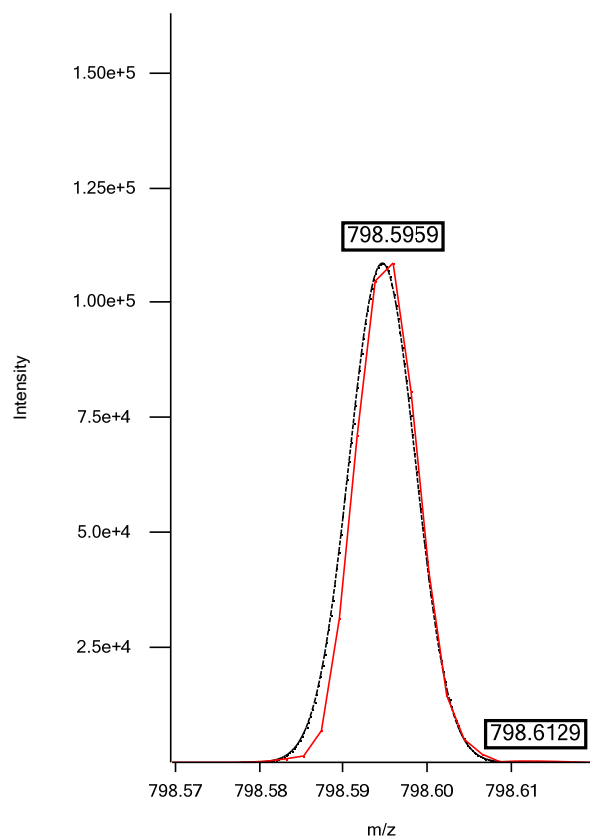


Isotope 3

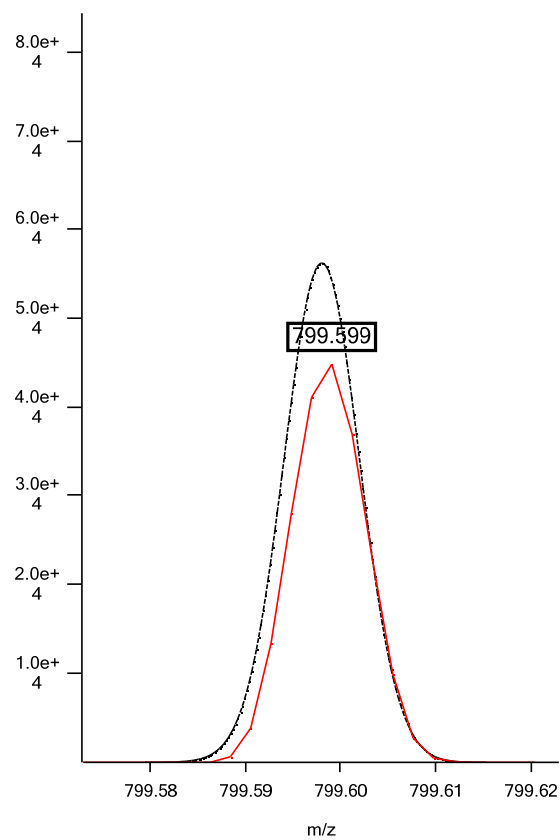


Positive ESI: PC 37:3; C₄₅H₈₅NO₈P; theoretical *m/z* 798.6013, (M+H)⁺; isotopic fit 0.0132

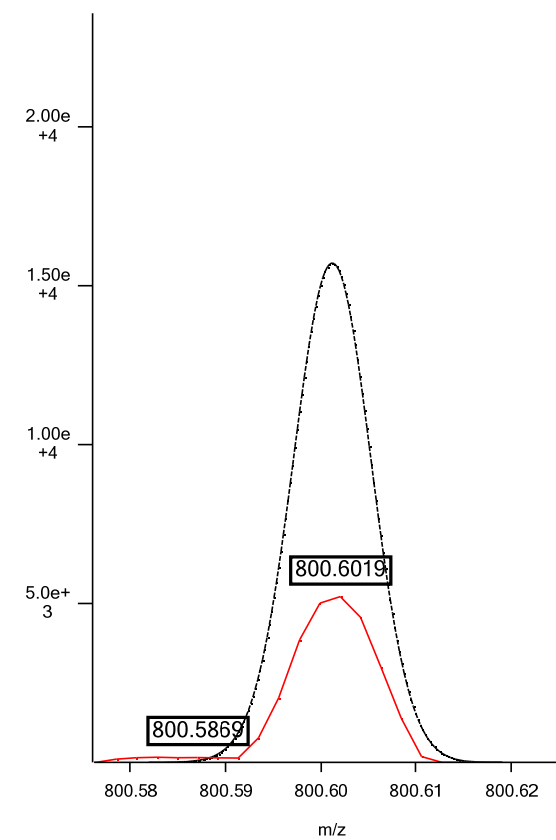
Isotope 1



Isotope 2

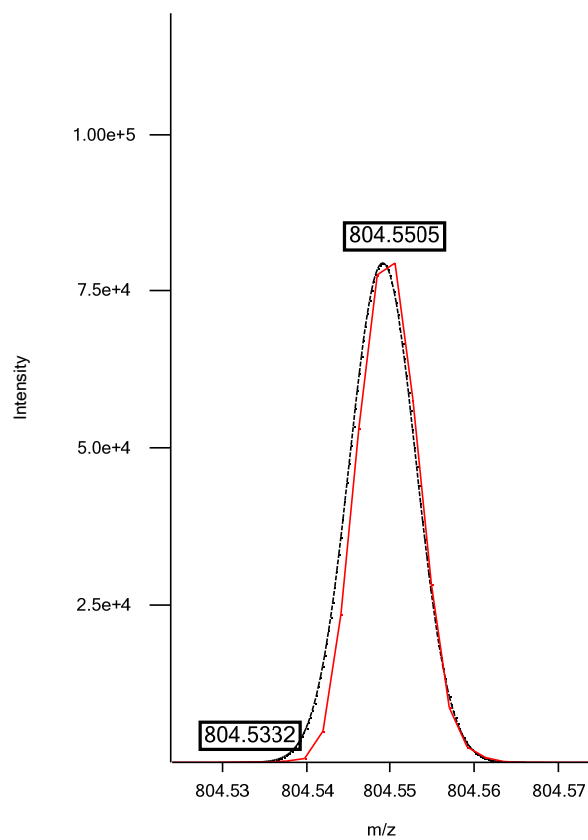


Isotope 3

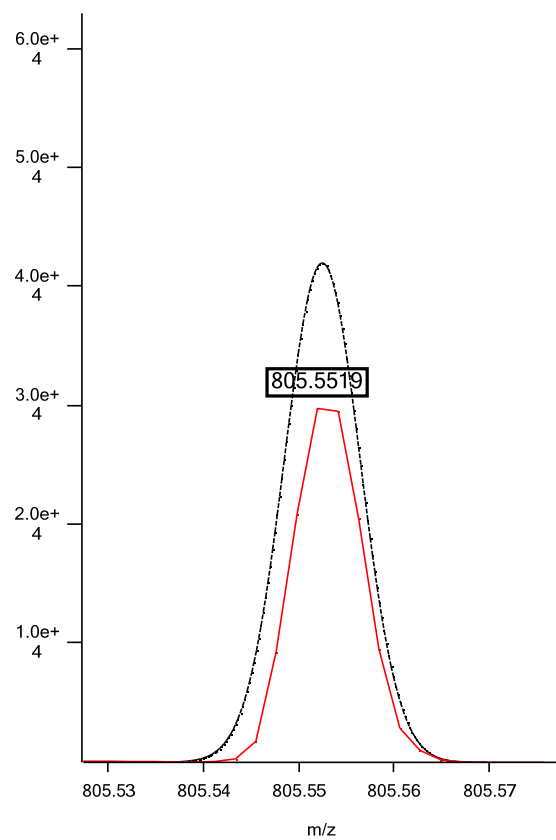


Positive ESI: PC 38:7; C₄₆H₇₉NO₈P; theoretical m/z 804.5543, (M+H)⁺; isotopic fit 0.0223

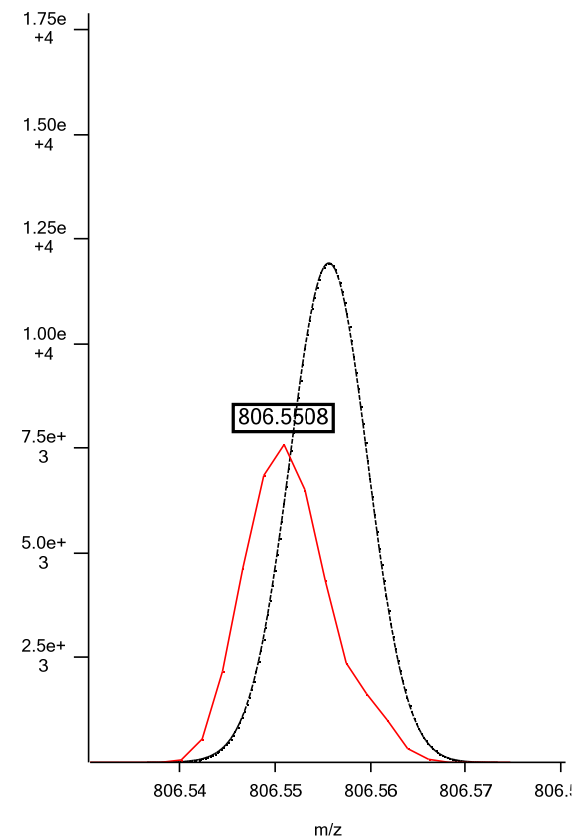
Isotope 1



Isotope 2

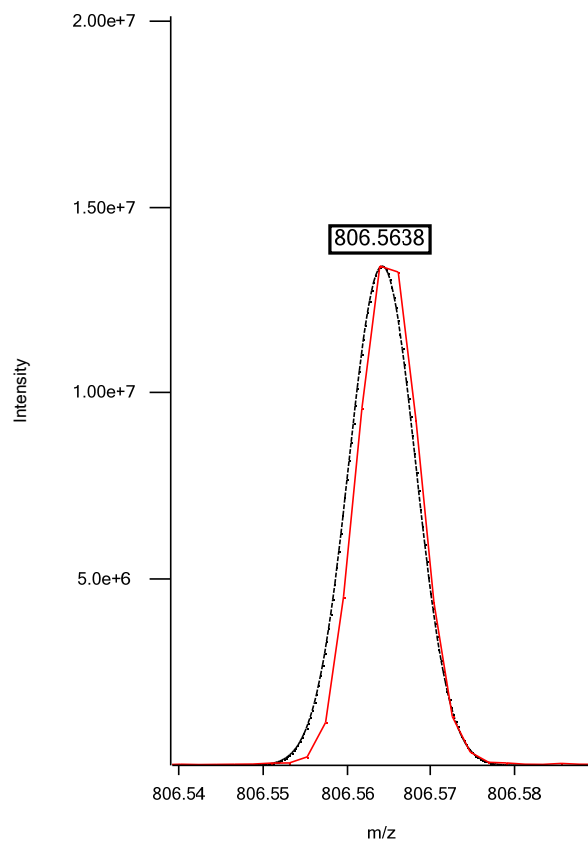


Isotope 3

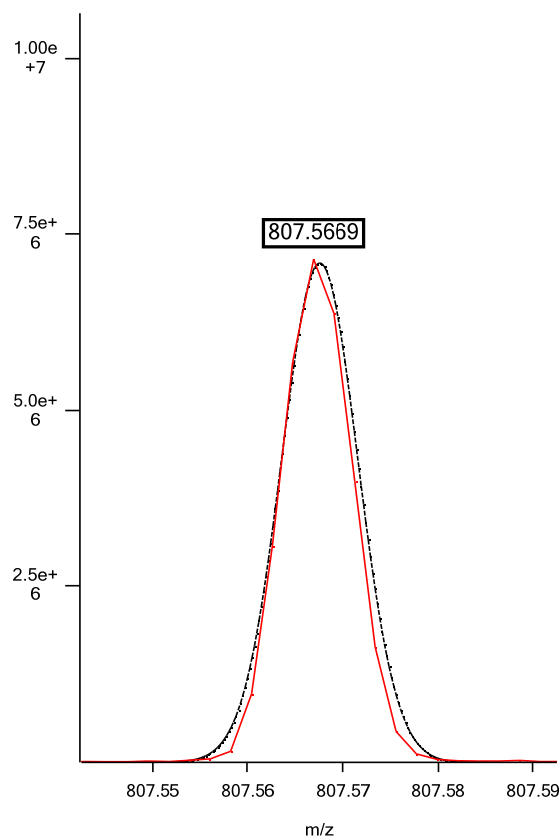


Positive ESI: PC 38:6; C₄₆H₈₁NO₈P; theoretical m/z 806.5699, (M+H)⁺; isotopic fit 0.0077

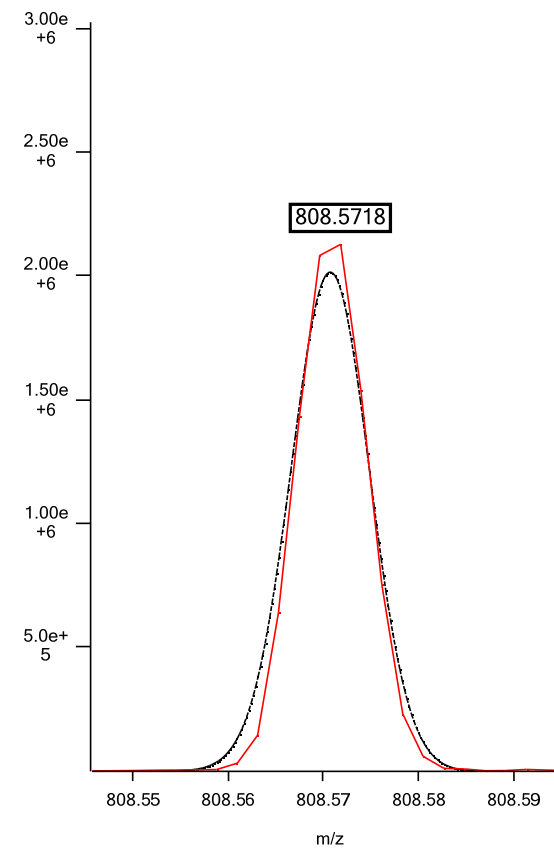
Isotope 1



Isotope 2

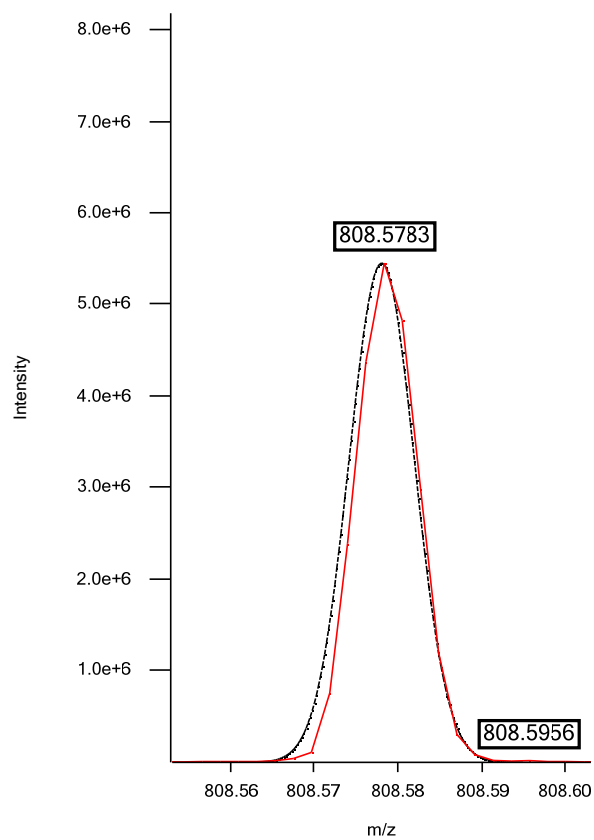


Isotope 3

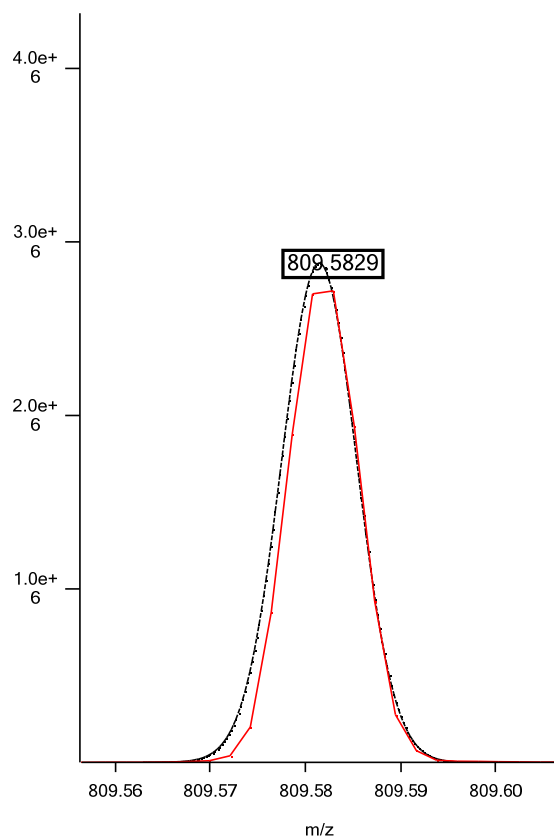


Positive ESI: PC 38:5; C₄₆H₈₃NO₈P; theoretical m/z 808.5856, (M+H)⁺; isotopic fit 0.0035

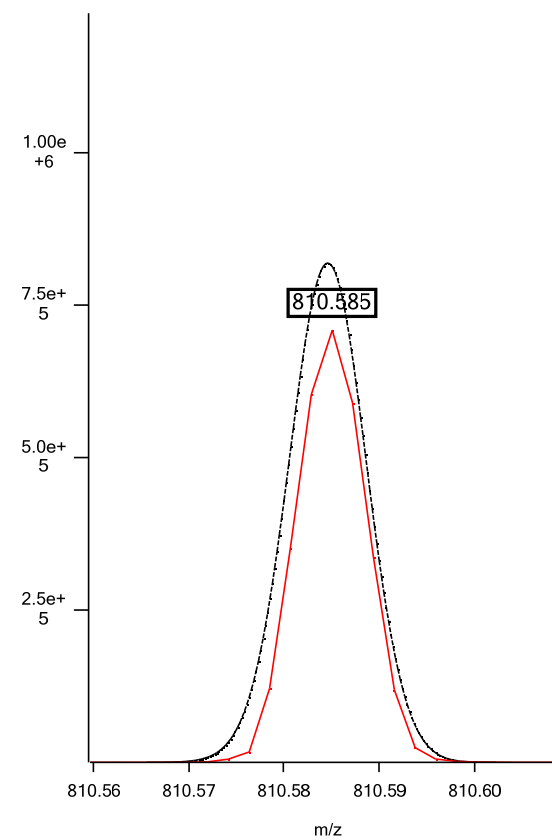
Isotope 1



Isotope 2

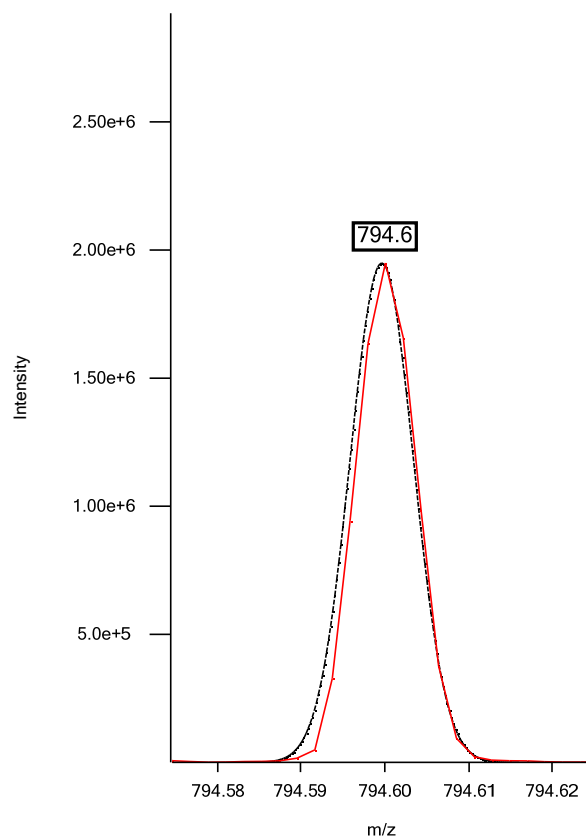


Isotope 3

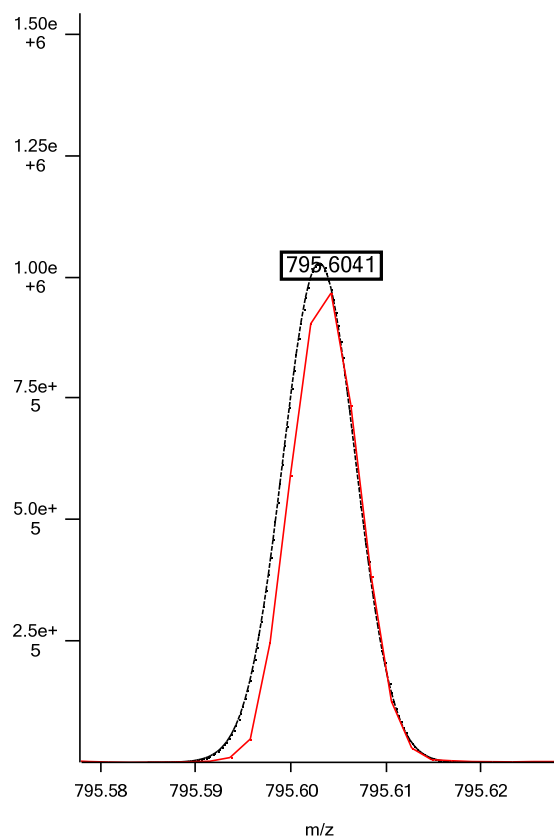


Positive ESI: PC 16:1p/22:4 or 16:0e/22:5; C₄₆H₈₅NO₇P; theoretical *m/z* 794.6063, (M+H)⁺; isotopic fit 0.0032

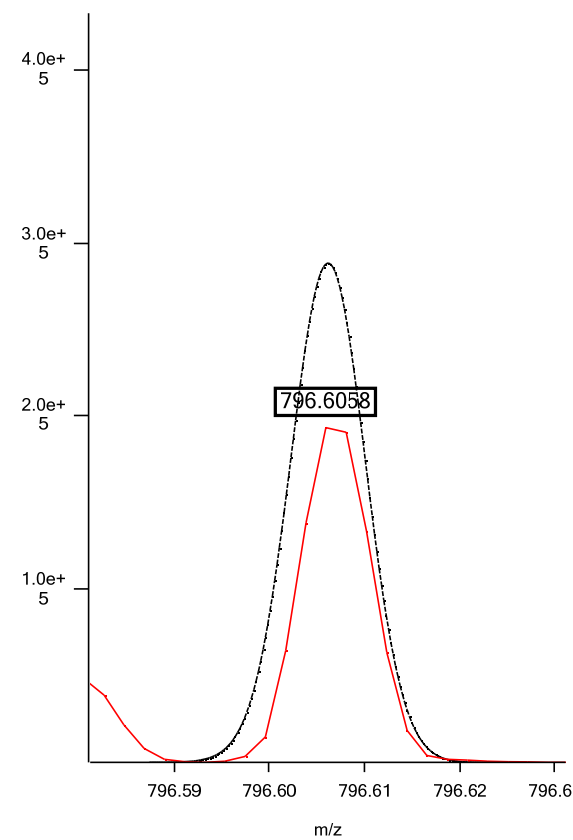
Isotope 1



Isotope 2

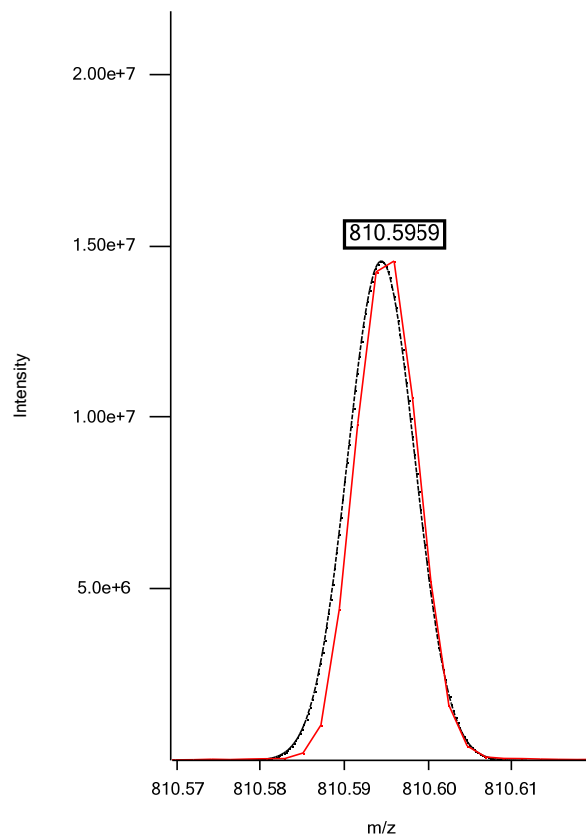


Isotope 3

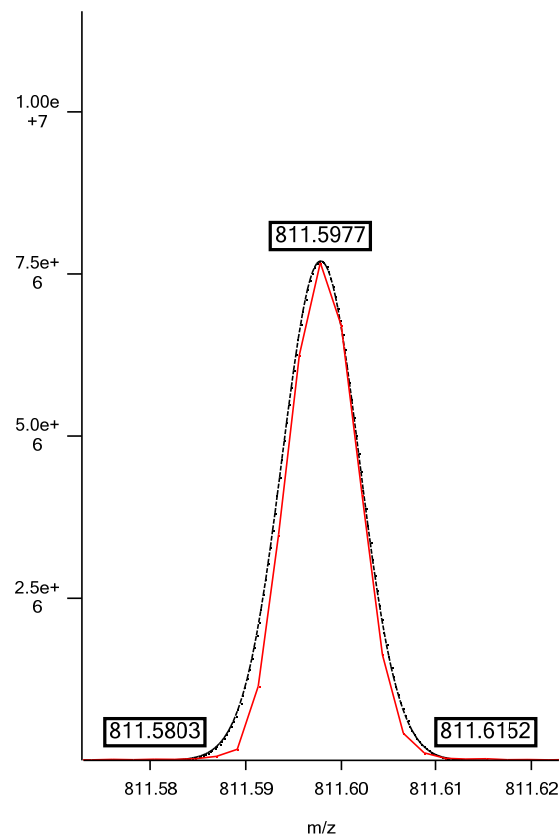


Positive ESI: PC 38:4; C₄₆H₈₅NO₈P; theoretical m/z 810.6013, (M+H)⁺; isotopic fit 0.0042

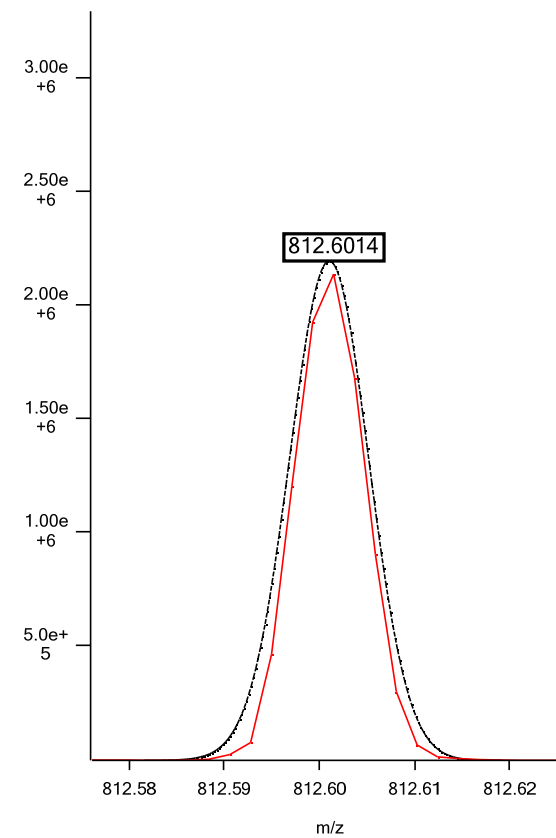
Isotope 1



Isotope 2

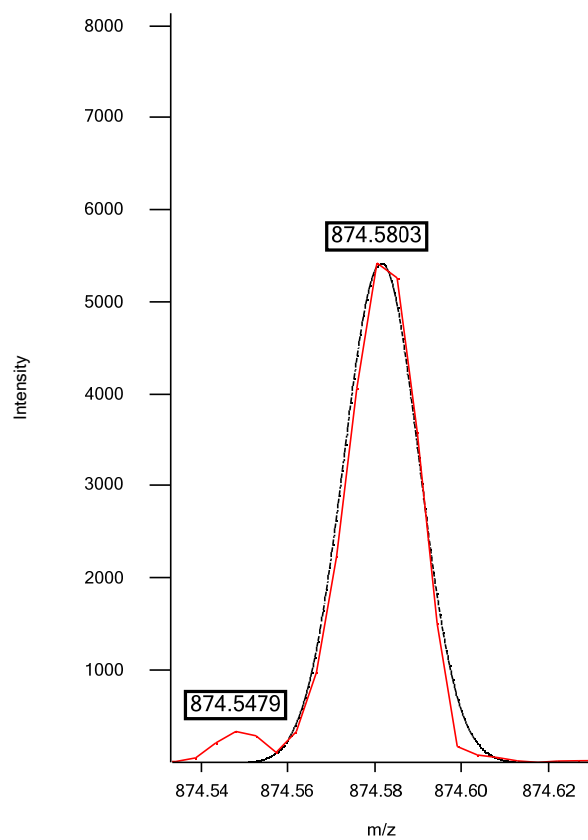


Isotope 3

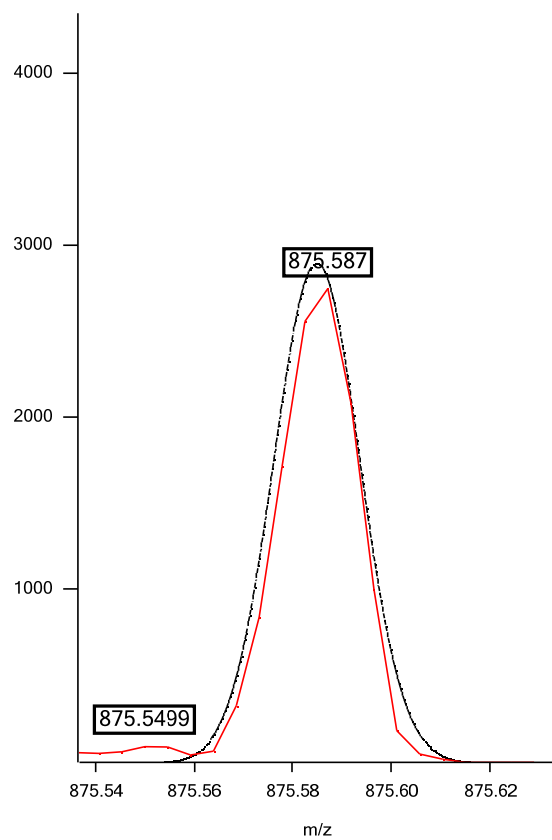


Negative ESI: Oxidized PC 18:1/Hydroperoxy-18:2; $C_{46}H_{85}NO_{12}P$; theoretical m/z 874.5809, (M-H)⁻; isotopic fit 0.0039

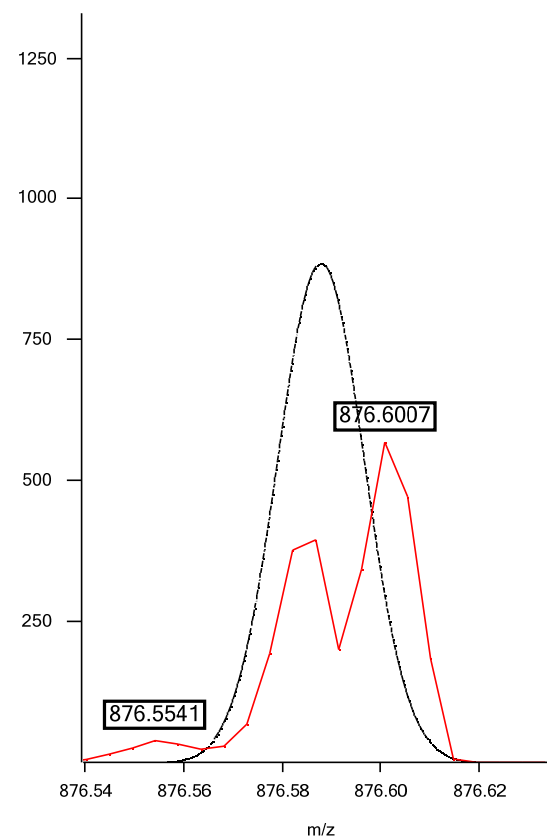
Isotope 1



Isotope 2

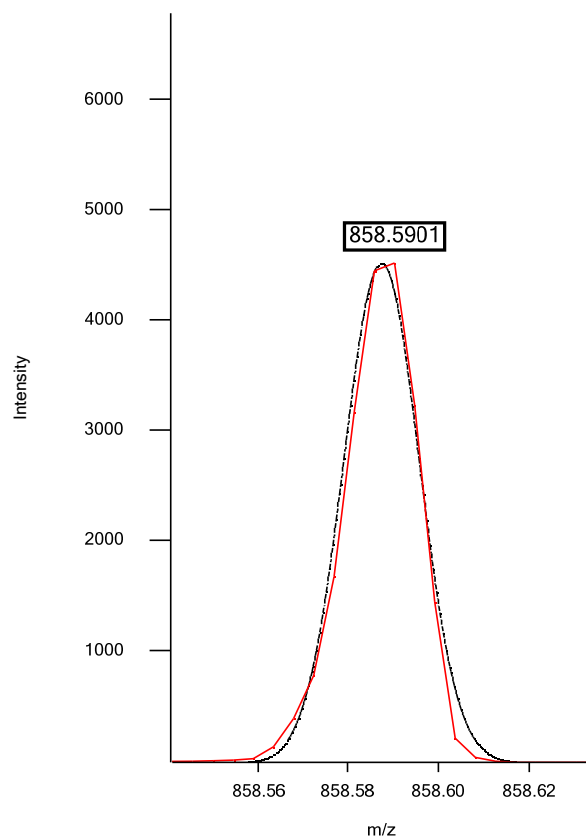


Isotope 3

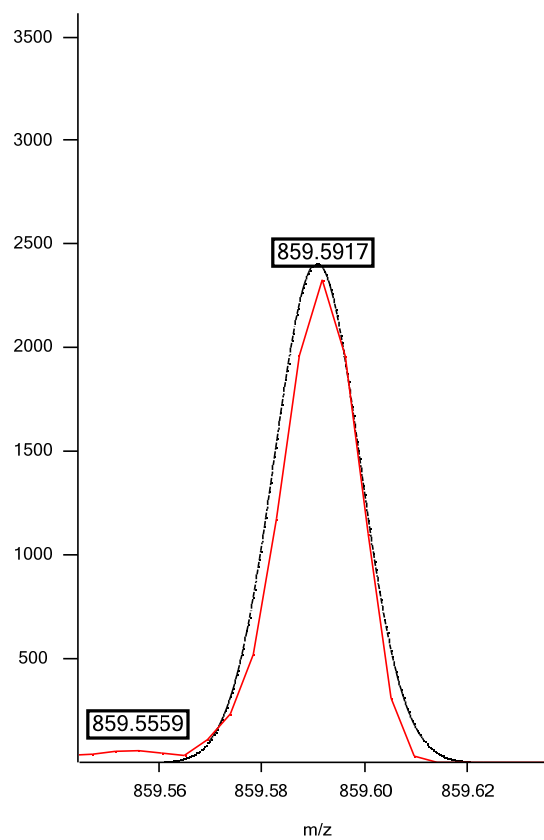


Negative ESI: Oxidized PC 16:0/Hydroxy-20:3; $C_{46}H_{85}NO_{11}P$; theoretical m/z 858.5860, (M-H)⁻; isotopic fit 0.0036

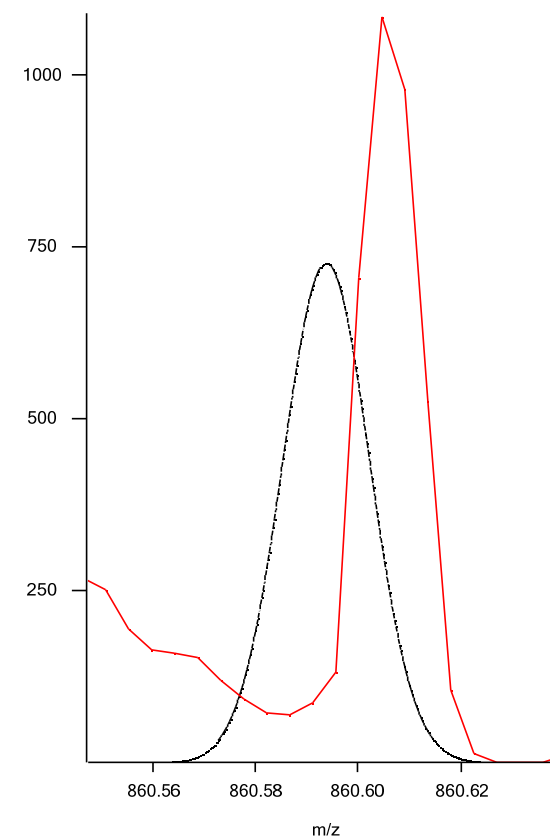
Isotope 1



Isotope 2

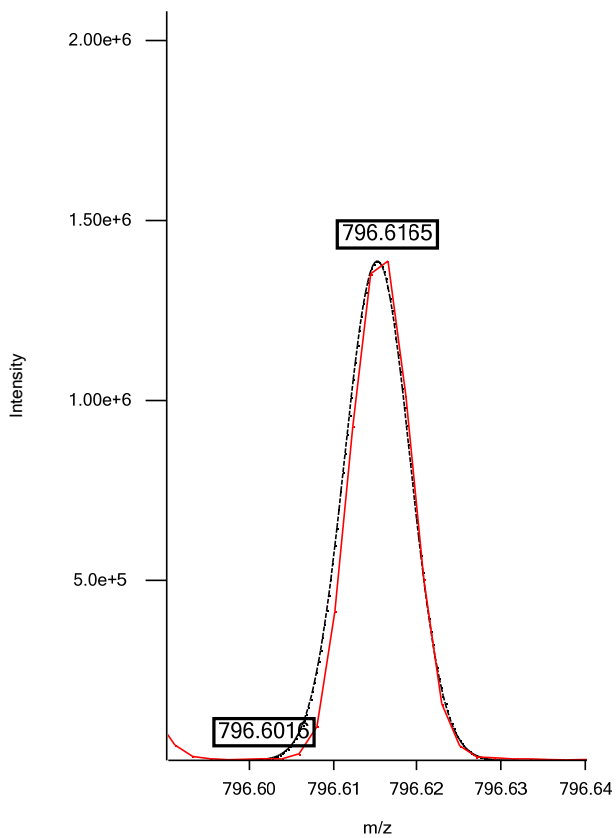


Isotope 3

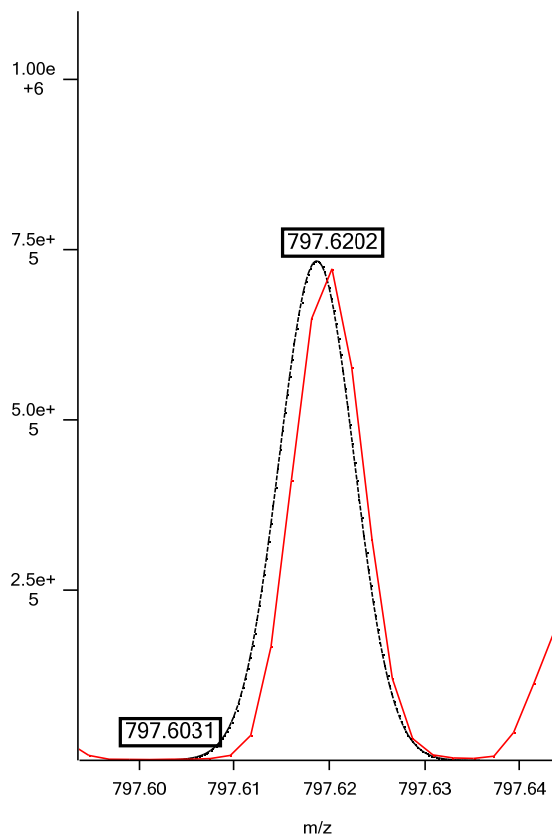


Positive ESI: PC 16:1p/22:3 or 16:0e/22:4; C₄₆H₈₇NO₇P; theoretical *m/z* 796.6220, (M+H)⁺; isotopic fit 0.0050

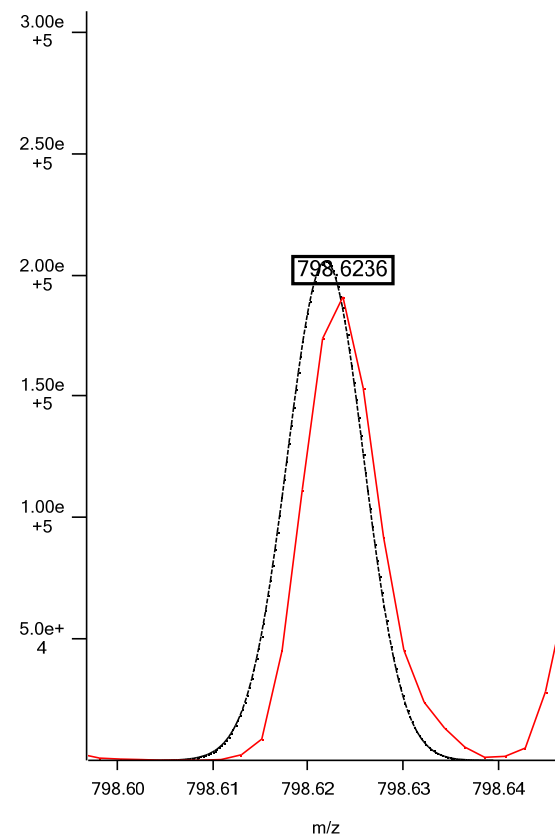
Isotope 1



Isotope 2

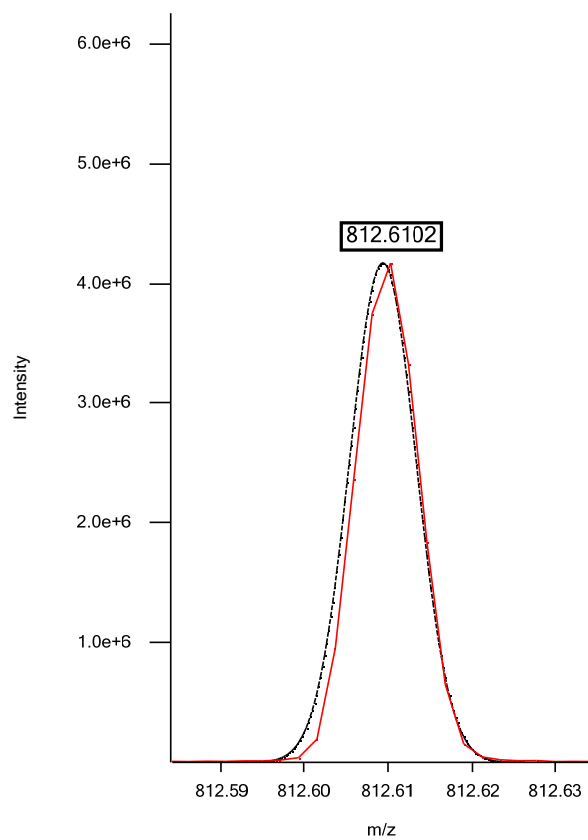


Isotope 3

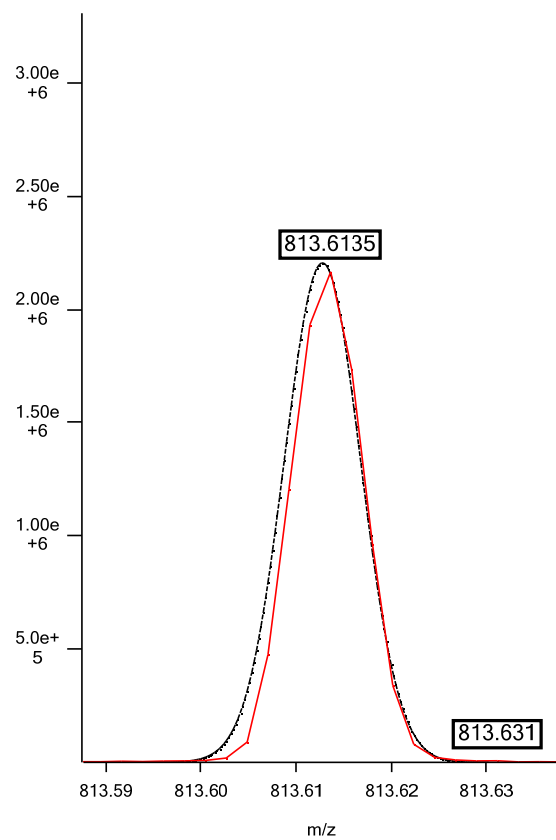


Positive ESI: PC 38:3; C₄₆H₈₇NO₈P; theoretical m/z 812.6169, (M+H)⁺; isotopic fit 0.0047

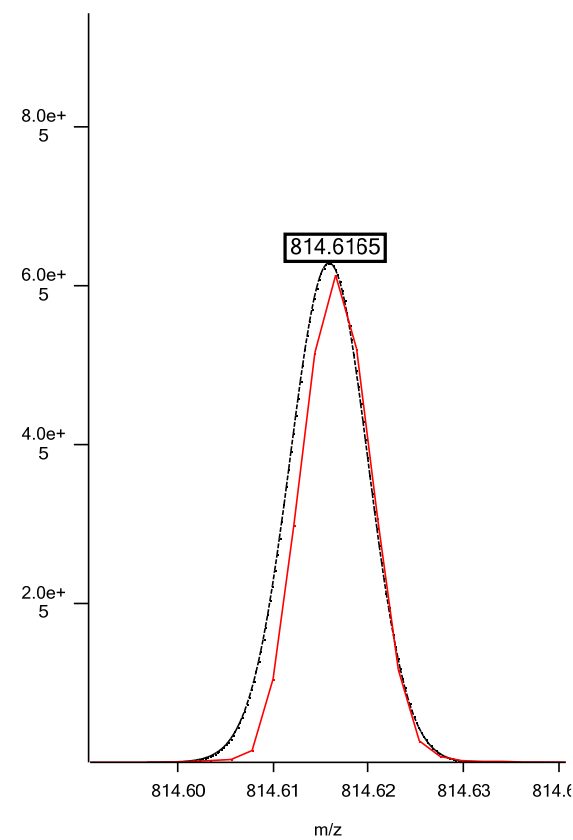
Isotope 1



Isotope 2

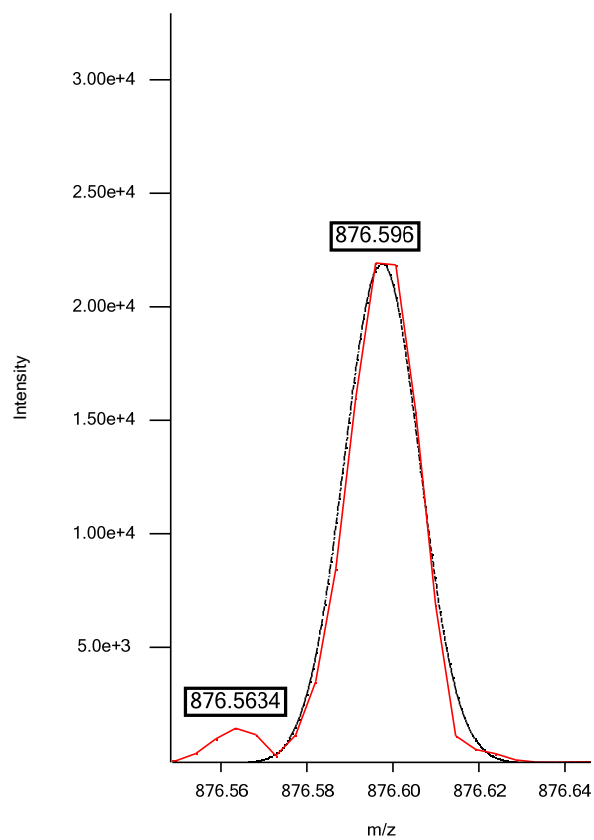


Isotope 3

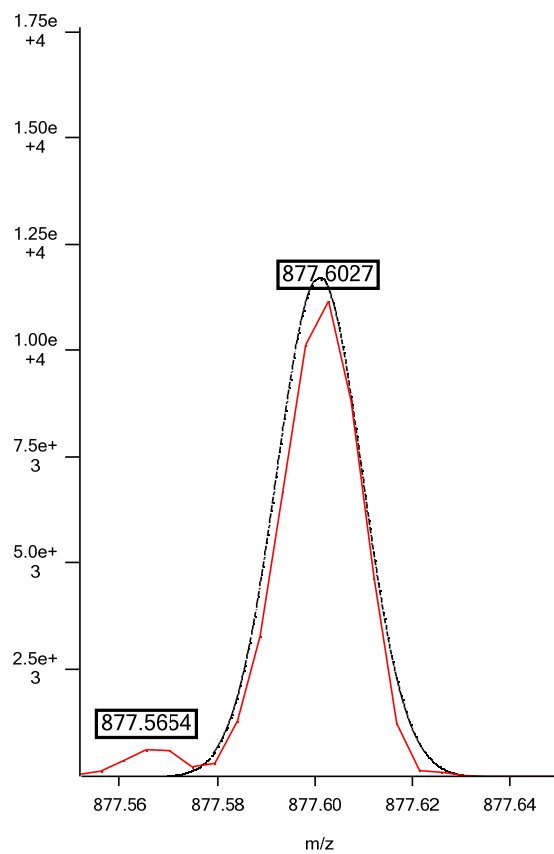


Negative ESI: Oxidized PC 18:0/Hydroperoxy-18:2; $C_{46}H_{87}NO_{12}P$; theoretical m/z 876.5966, (M-H)⁻; isotopic fit 0.0037

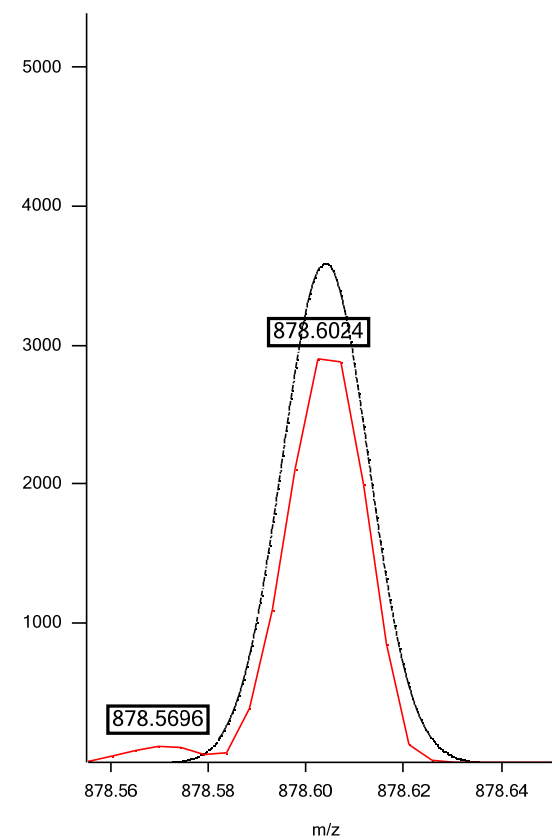
Isotope 1



Isotope 2

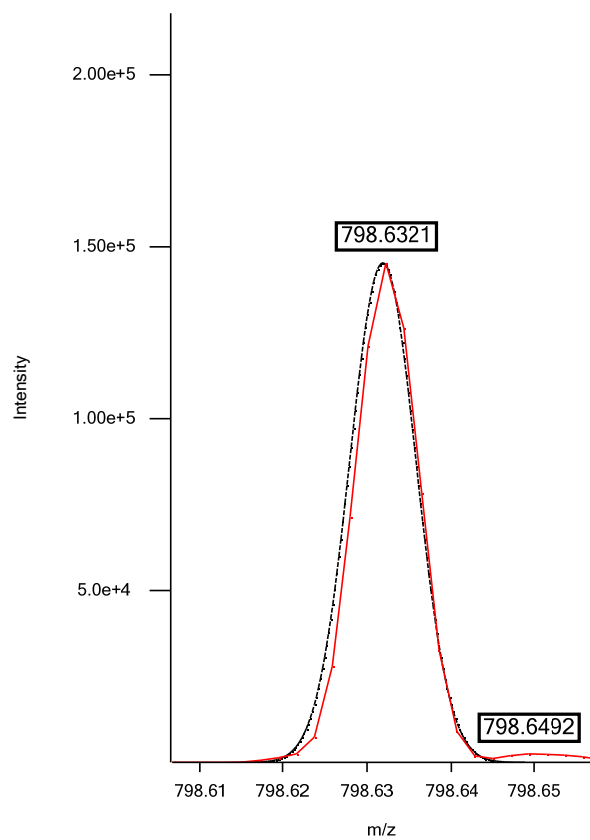


Isotope 3

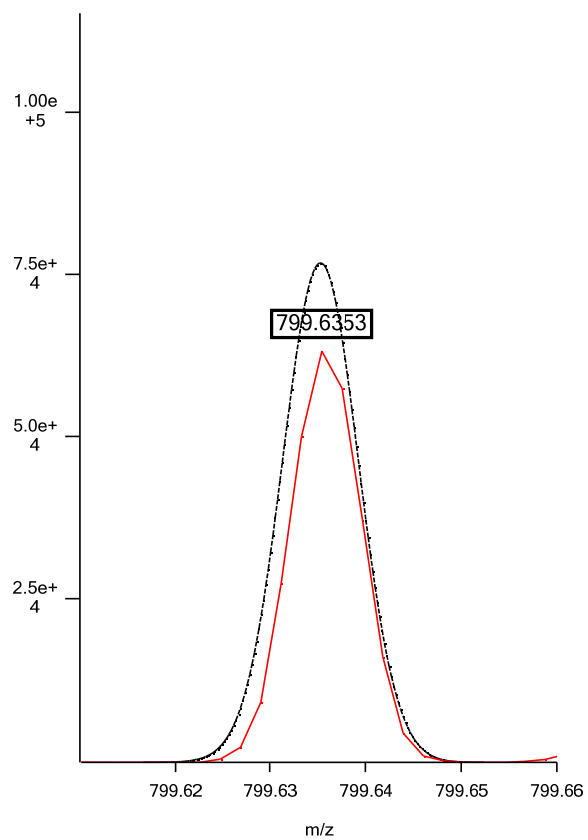


Positive ESI: PC 16:1p/22:2 or 16:0e/22:3; C₄₆H₈₉NO₇P; theoretical m/z 798.6376, (M+H)⁺; isotopic fit 0.0131

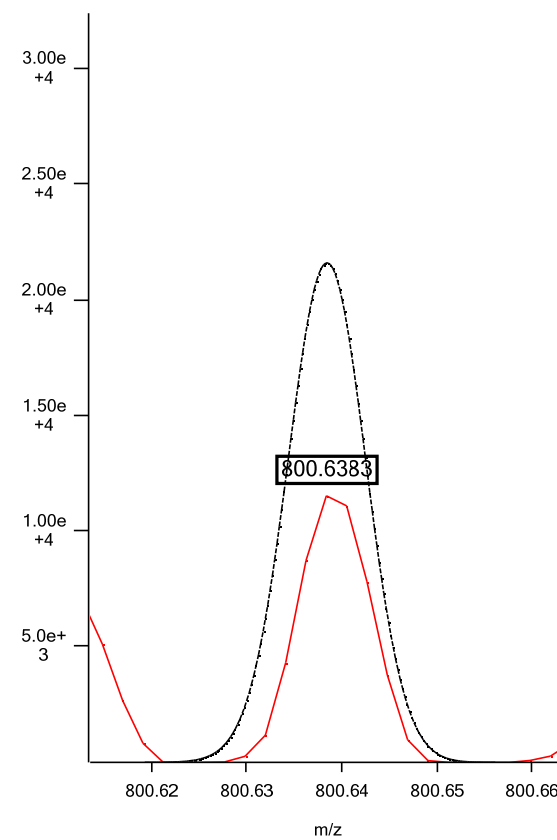
Isotope 1



Isotope 2

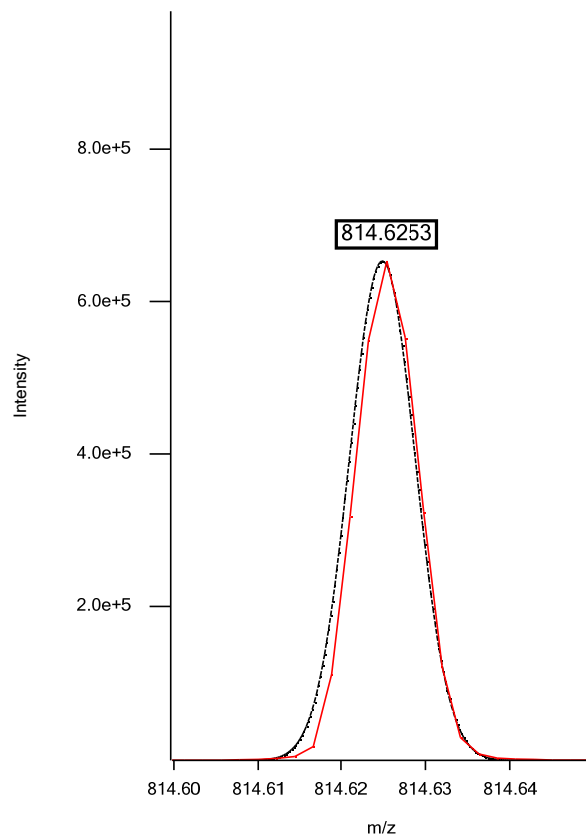


Isotope 3

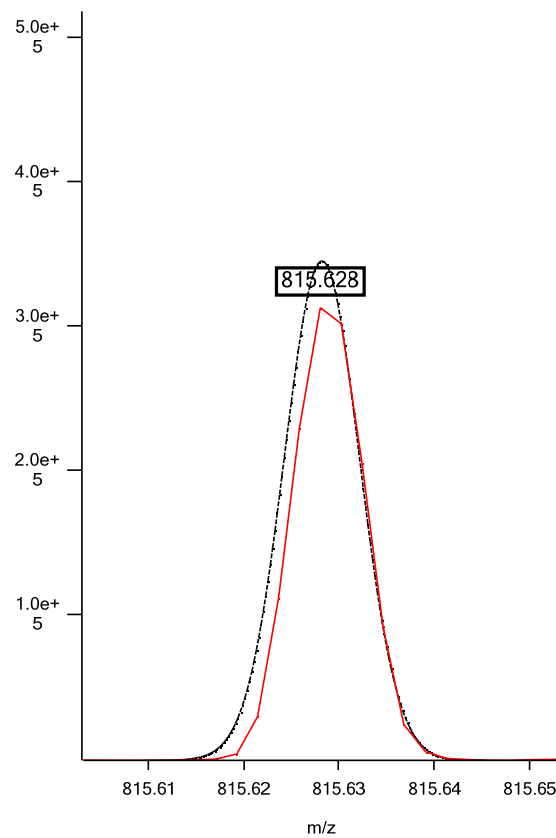


Positive ESI: PC 38:2; C₄₆H₈₉NO₈P; theoretical *m/z* 814.6326, (M+H)⁺; isotopic fit 0.0066

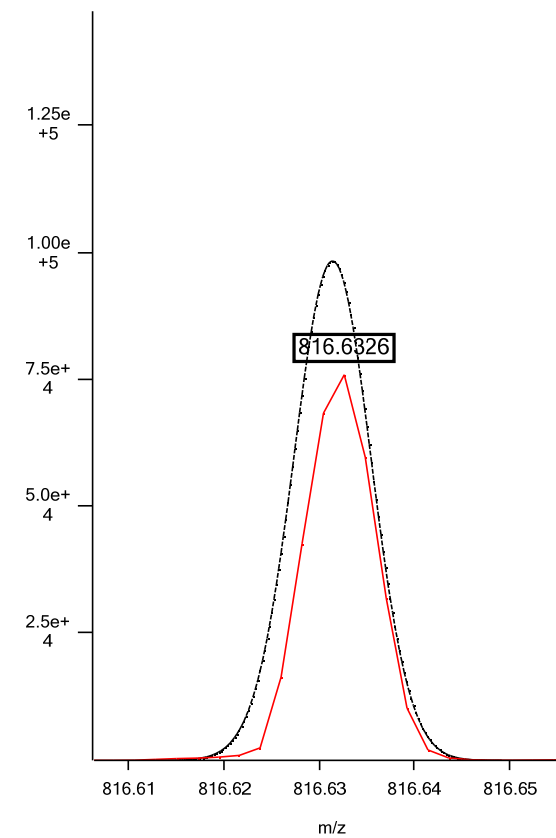
Isotope 1



Isotope 2

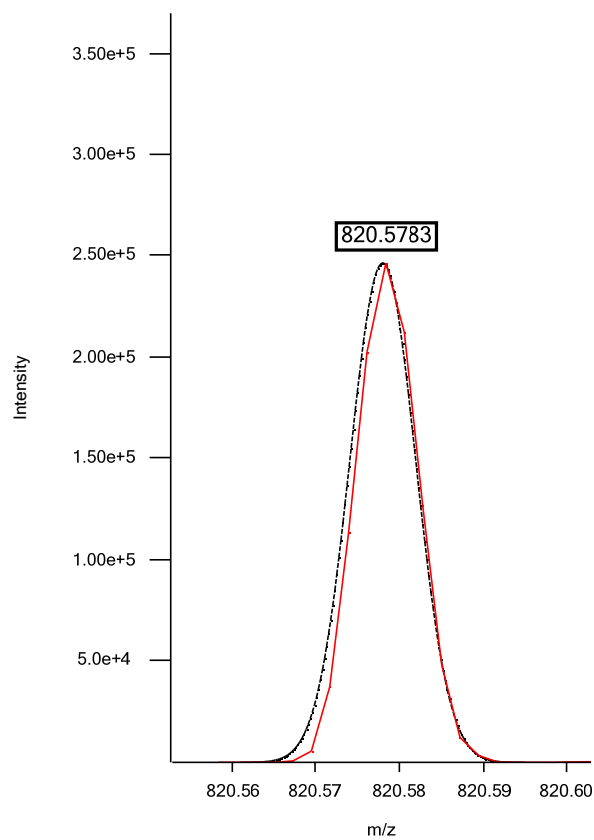


Isotope 3

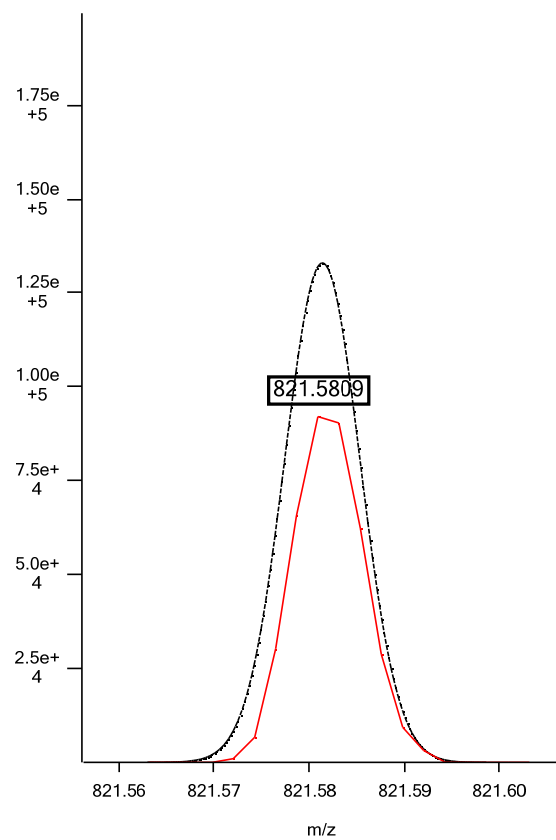


Positive ESI: PC 39:6; C₄₇H₈₃NO₈P; theoretical m/z 820.5856, (M+H)⁺; isotopic fit 0.0236

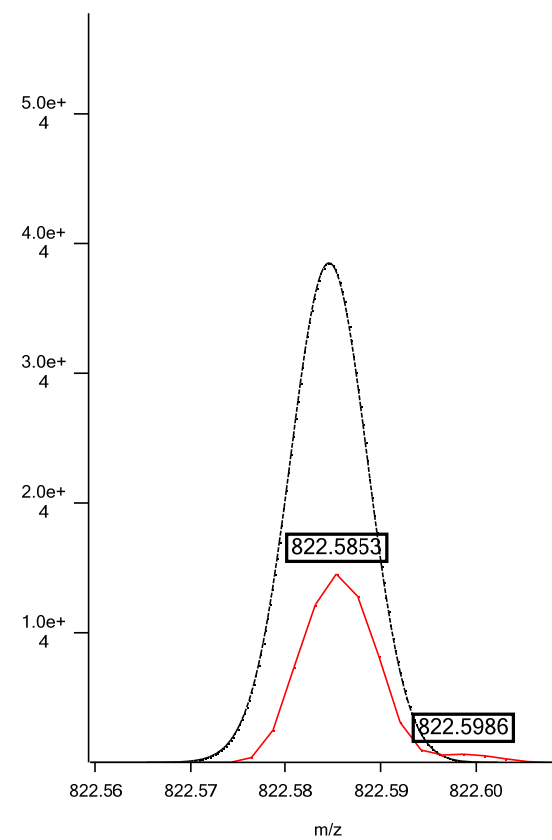
Isotope 1



Isotope 2

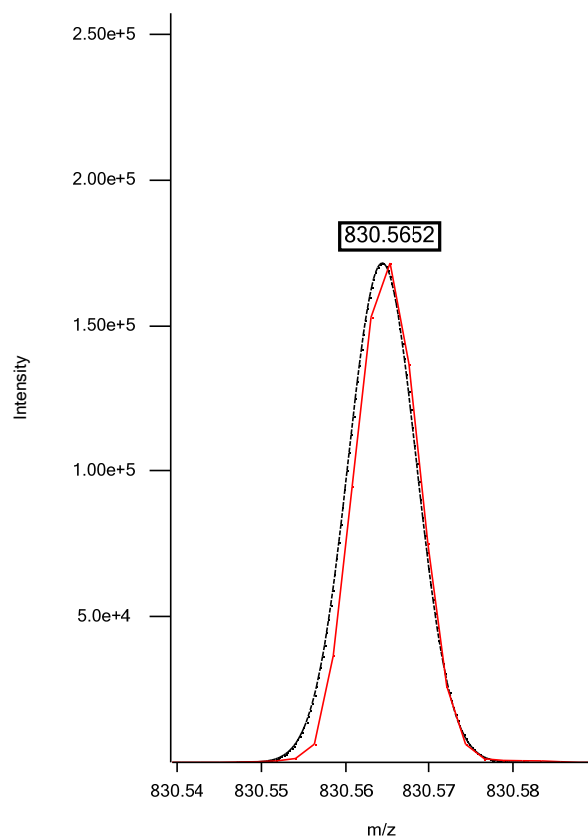


Isotope 3

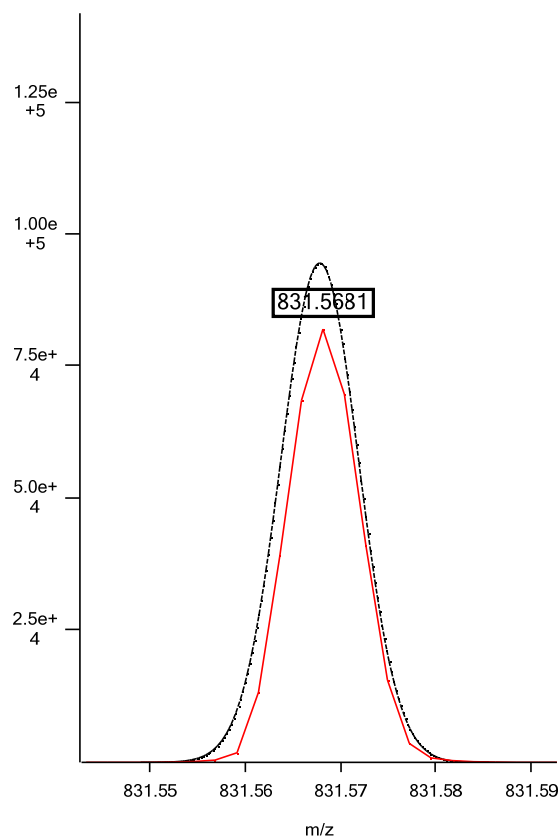


Positive ESI: PC 40:8; C₄₈H₈₁NO₈P; theoretical *m/z* 830.5699, (M+H)⁺; isotopic fit 0.0107

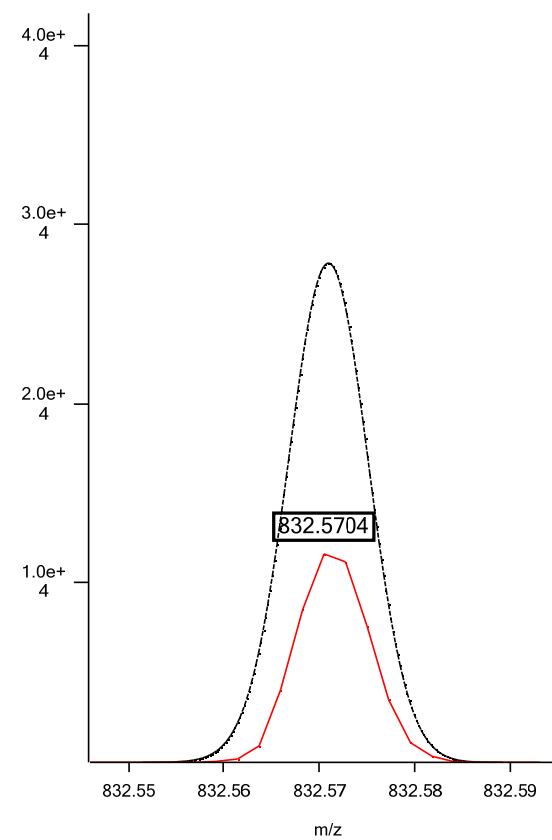
Isotope 1



Isotope 2

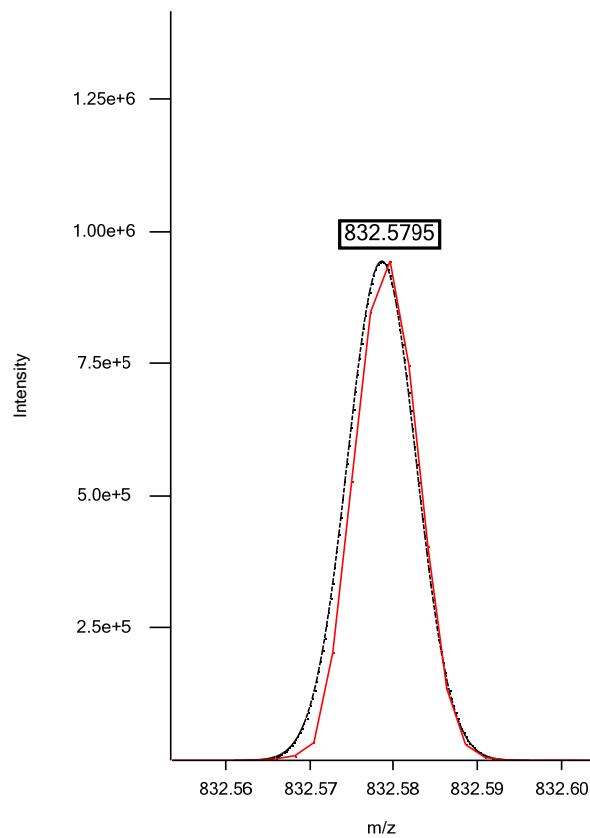


Isotope 3

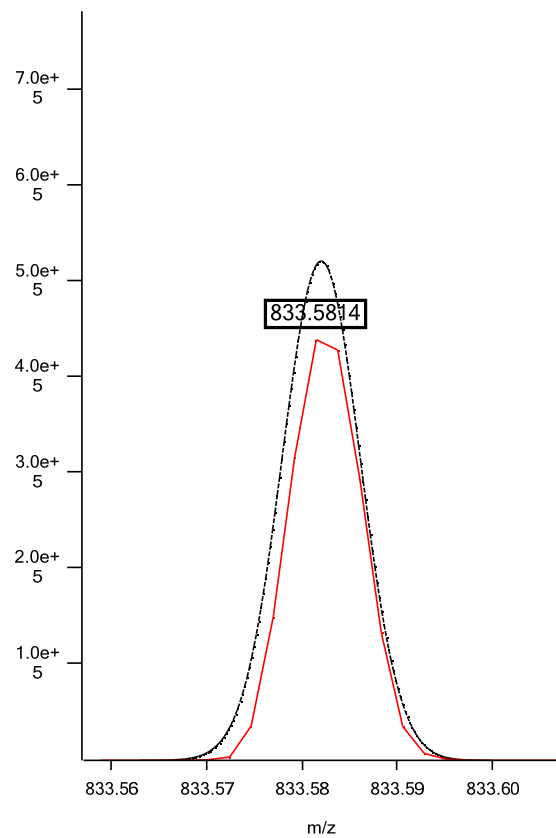


Positive ESI: PC 40:7; C₄₈H₈₃NO₈P; theoretical *m/z* 832.5856, (M+H)⁺; isotopic fit 0.0126

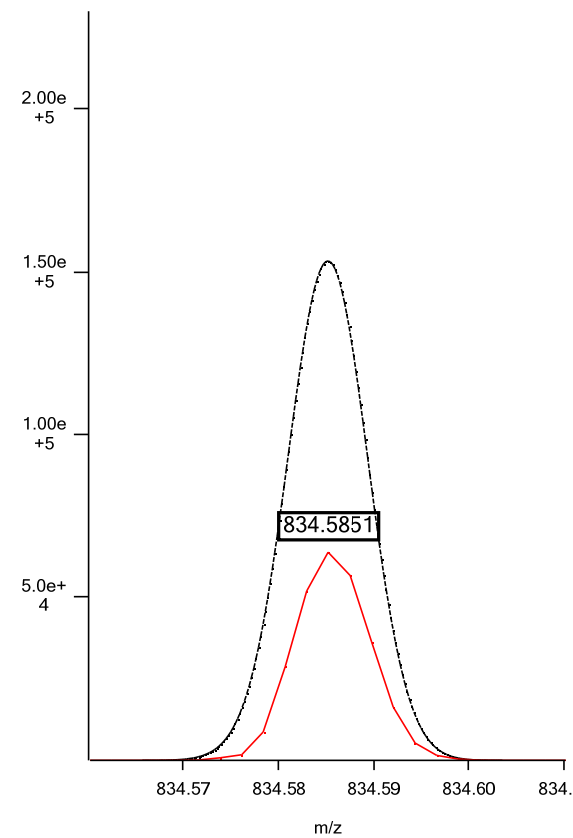
Isotope 1



Isotope 2

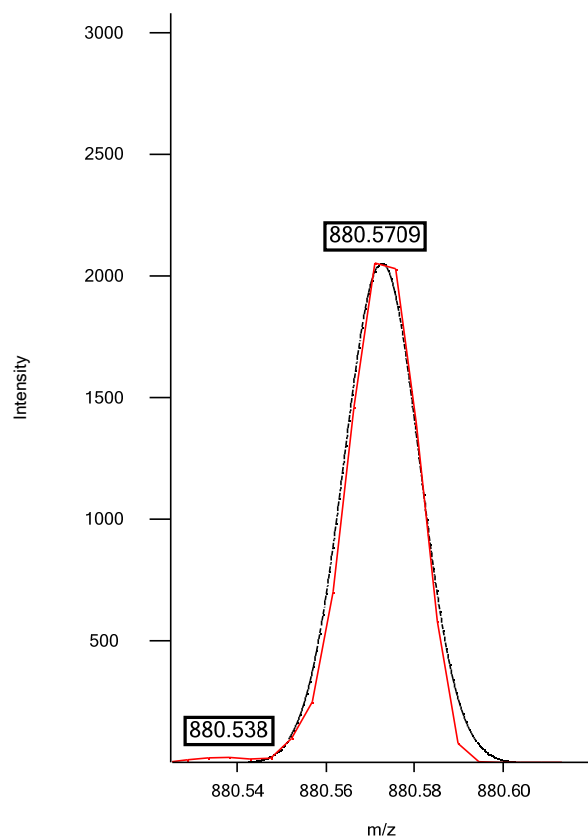


Isotope 3

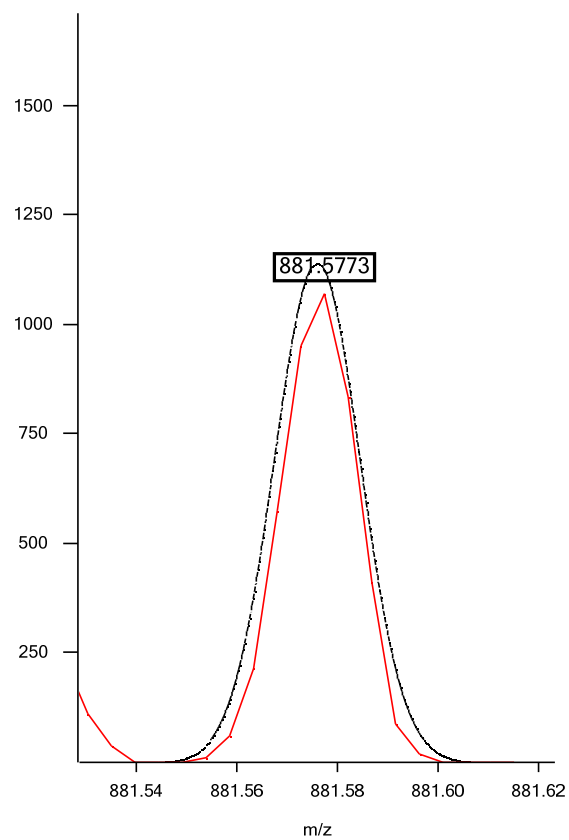


Negative ESI: Oxidized PC 16:0/Hydroxy-22:4; $C_{48}H_{83}NO_{11}P$; theoretical m/z 880.5703, (M-H)⁻; isotopic fit 0.0052

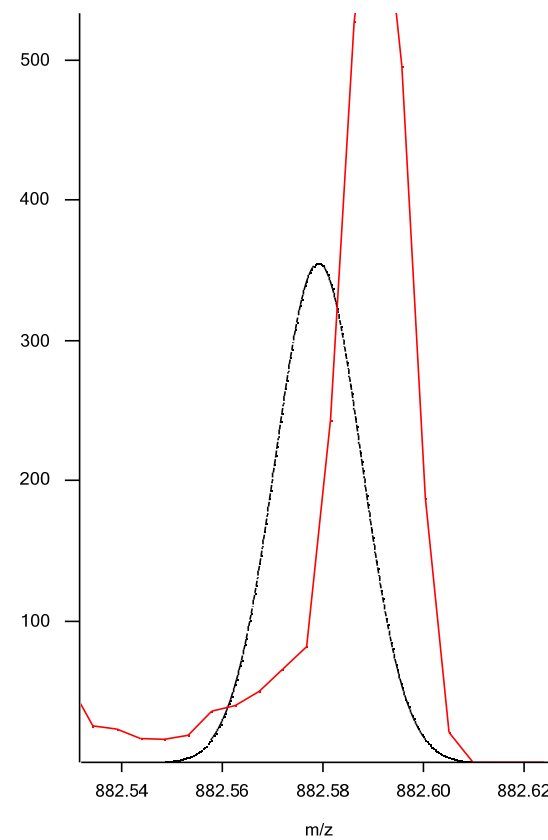
Isotope 1



Isotope 2

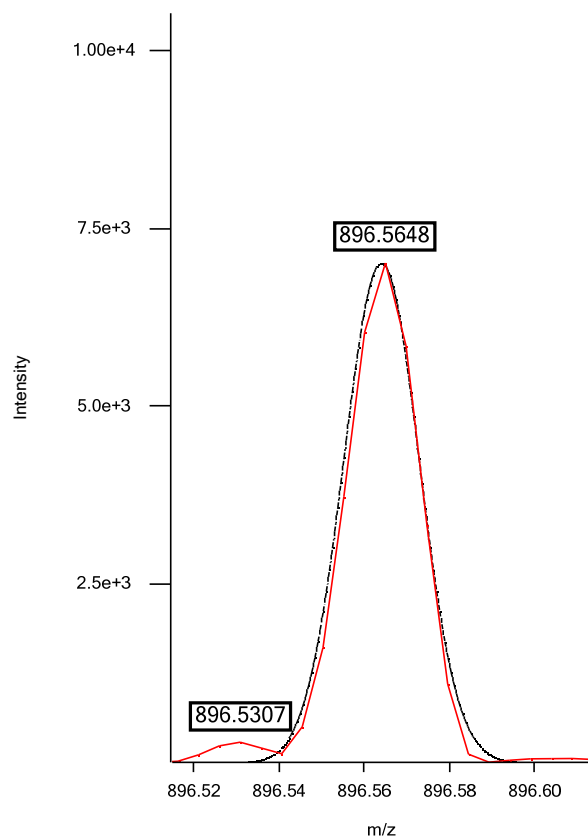


Isotope 3

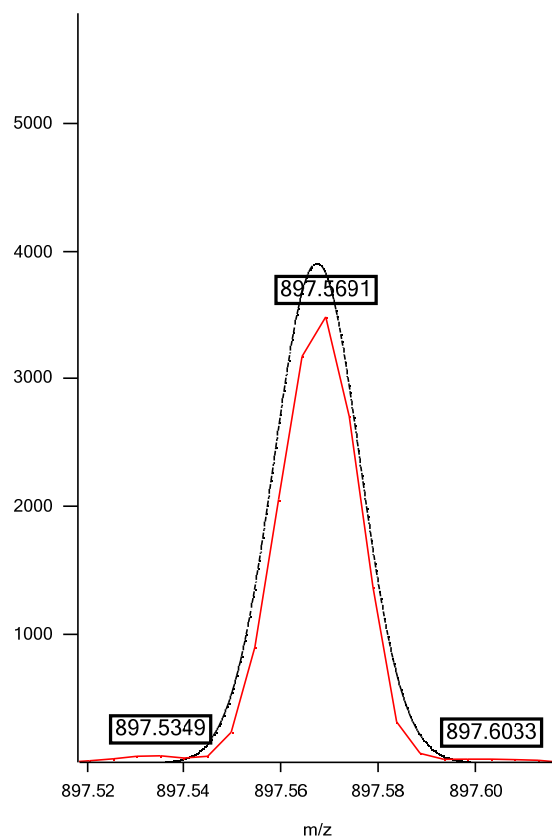


Negative ESI: Oxidized PC 16:0/Hydroperoxy-22:4; $C_{48}H_{83}NO_{12}P$; theoretical m/z 896.5653, (M-H)⁻; isotopic fit 0.0065

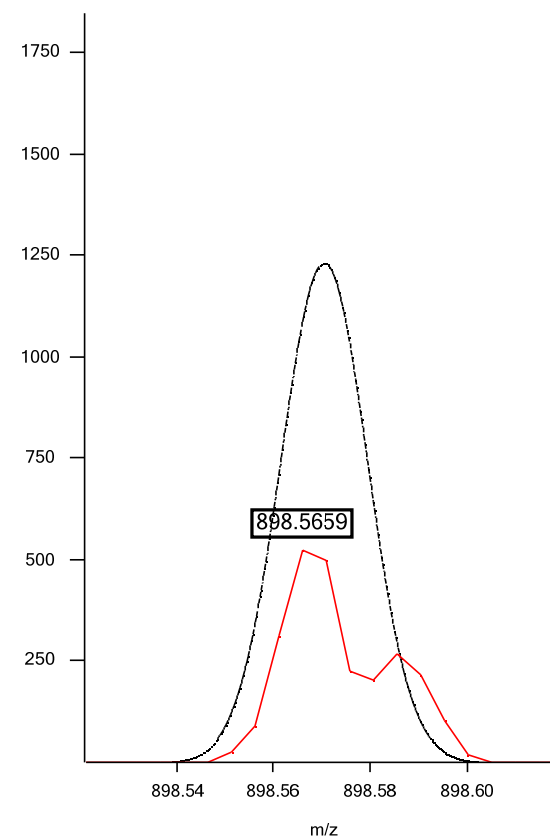
Isotope 1



Isotope 2

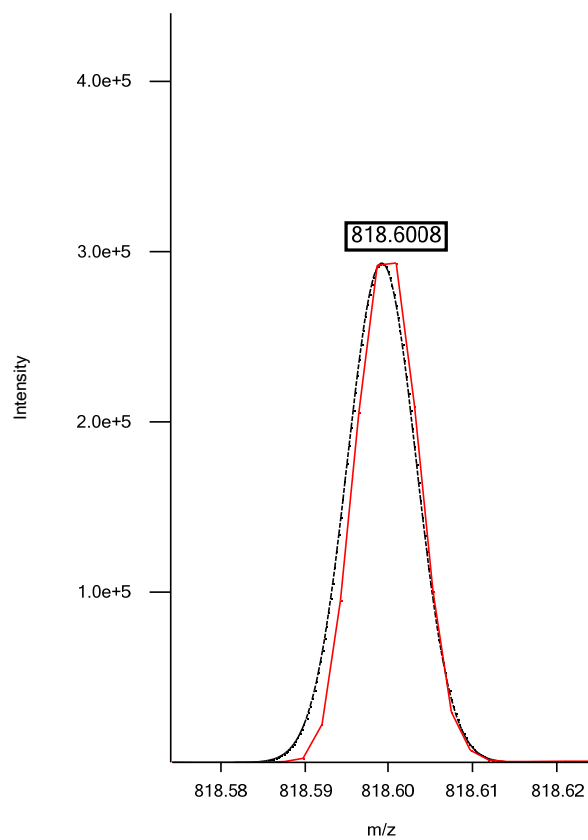


Isotope 3

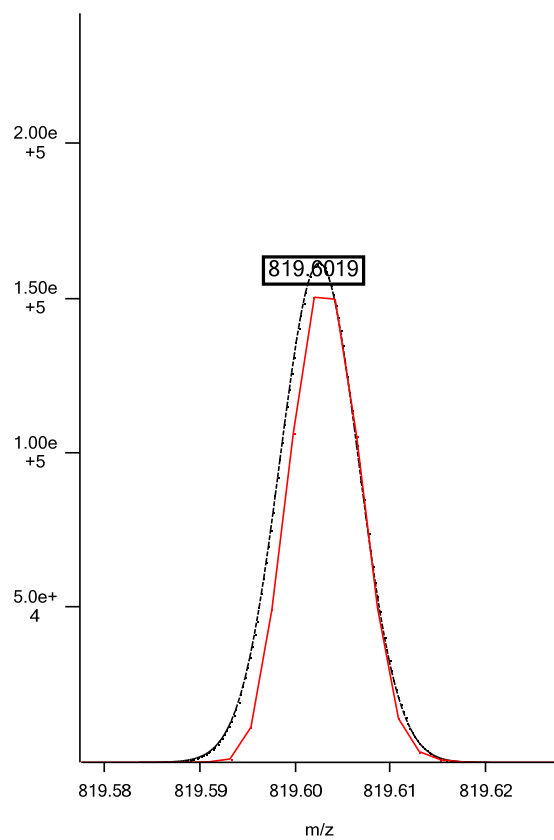


Positive ESI: PC 18:1p/22:6; C₄₈H₈₅NO₇P; theoretical m/z 818.6063, (M+H)⁺; isotopic fit 0.0047

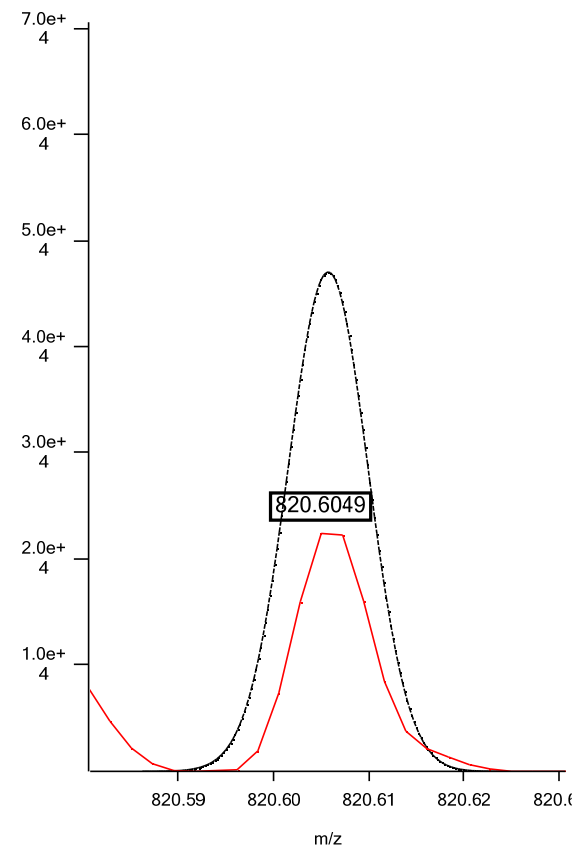
Isotope 1



Isotope 2

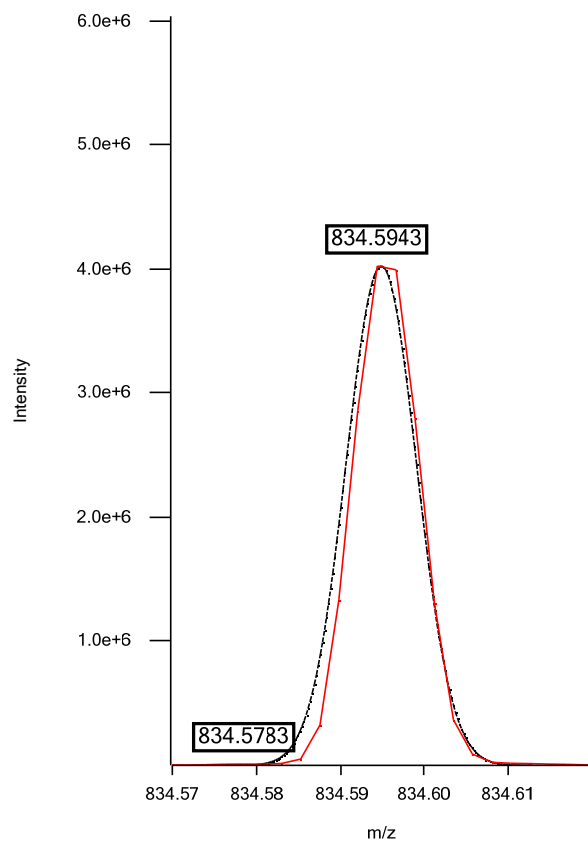


Isotope 3

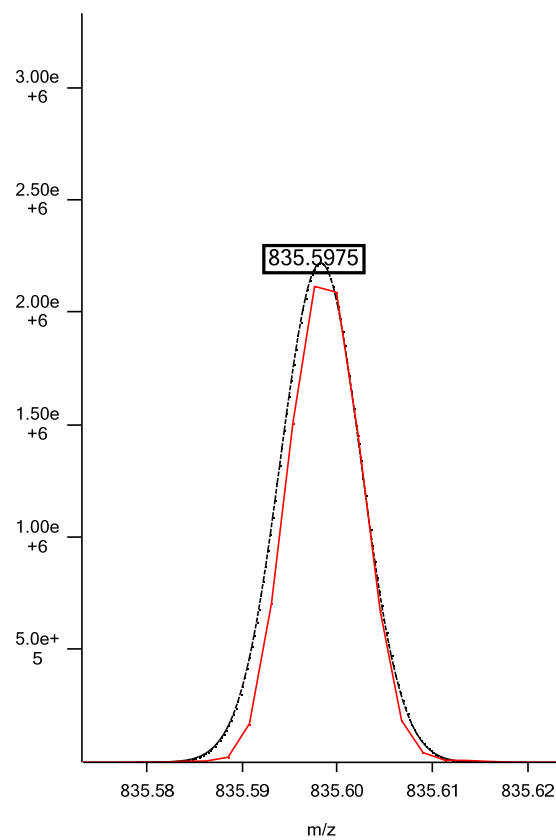


Positive ESI: PC 40:6; C₄₈H₈₅NO₈P; theoretical *m/z* 834.6013, (M+H)⁺; isotopic fit 0.0037

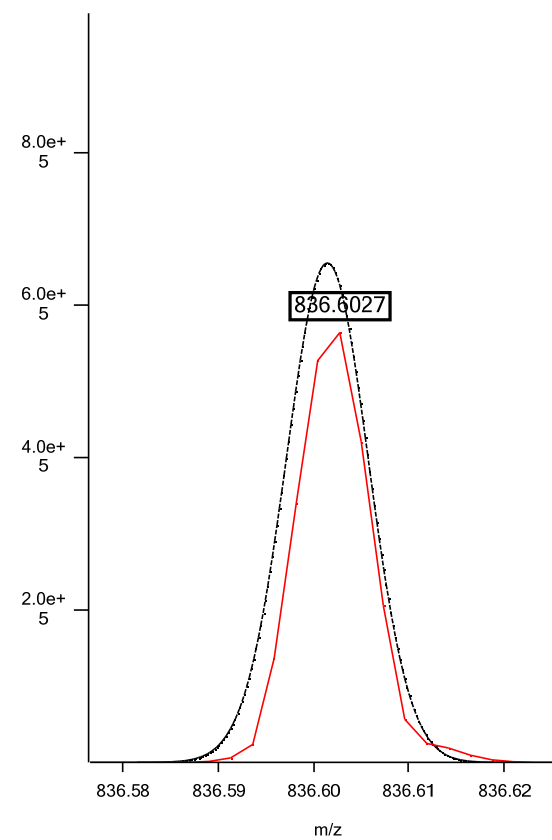
Isotope 1



Isotope 2

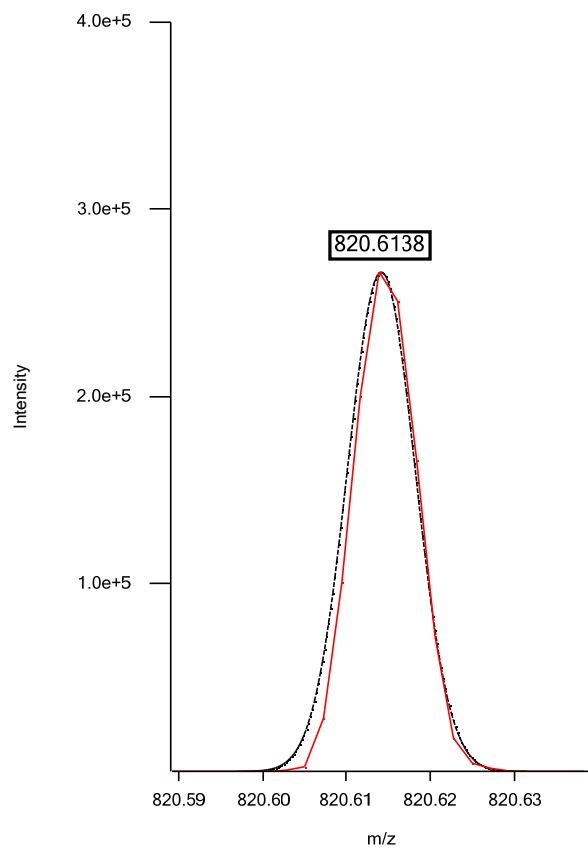


Isotope 3

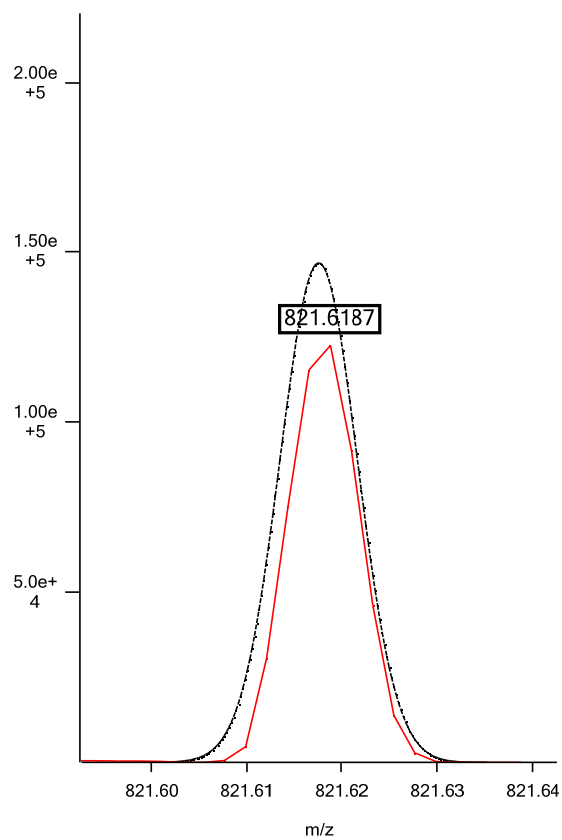


Positive ESI: PC 18:1p/22:5 or 18:0e/22:6; $C_{48}H_{87}NO_7P$; theoretical m/z 820.6220, $(M+H)^+$; isotopic fit 0.0139

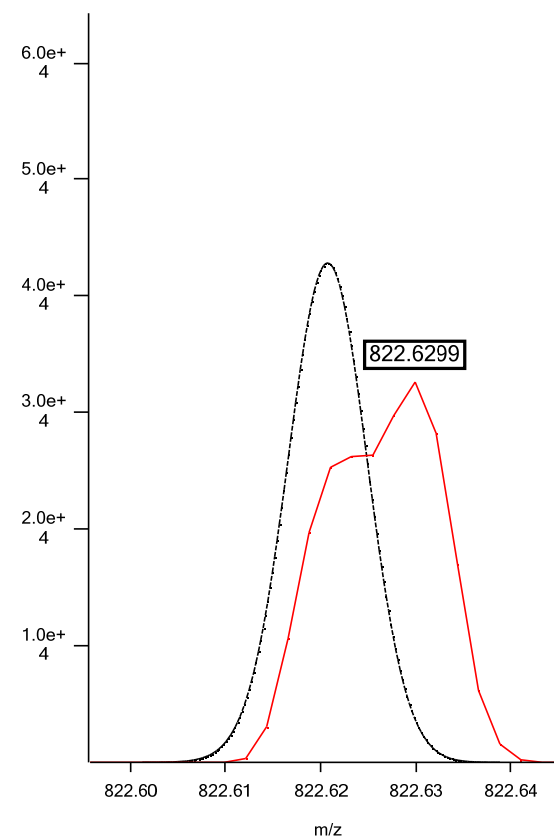
Isotope 1



Isotope 2

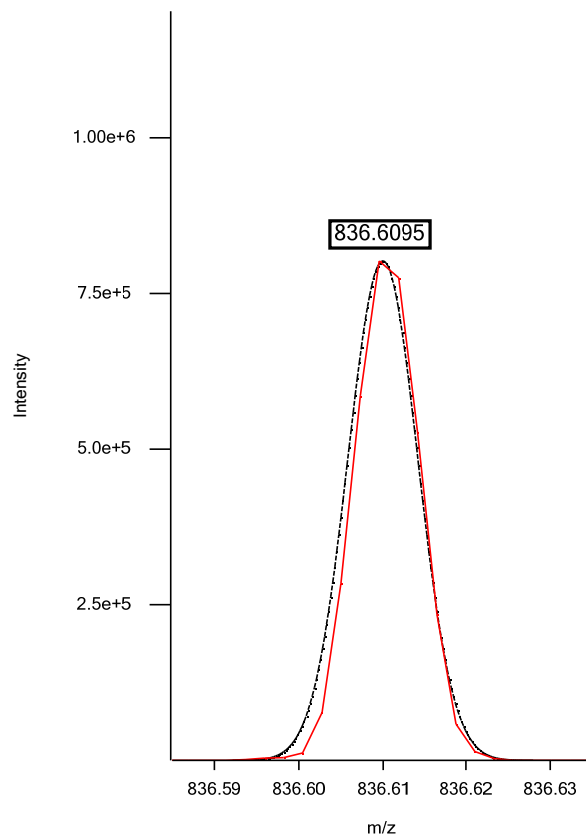


Isotope 3

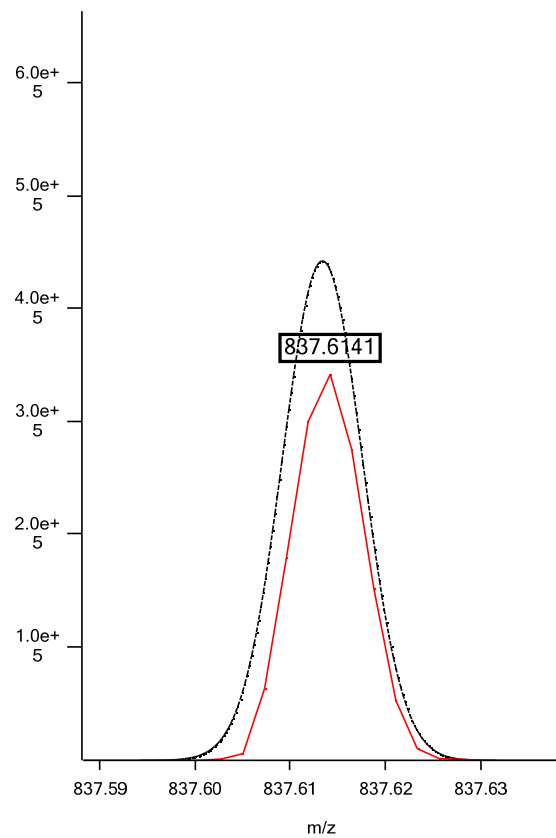


Positive ESI: PC 40:5; C₄₈H₈₇NO₈P; theoretical *m/z* 836.6169, (M+H)⁺; isotopic fit 0.0169

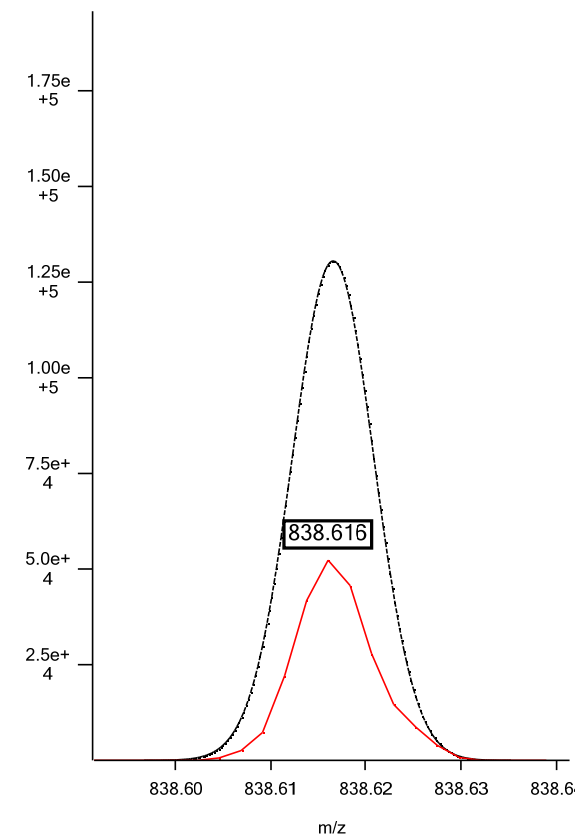
Isotope 1



Isotope 2

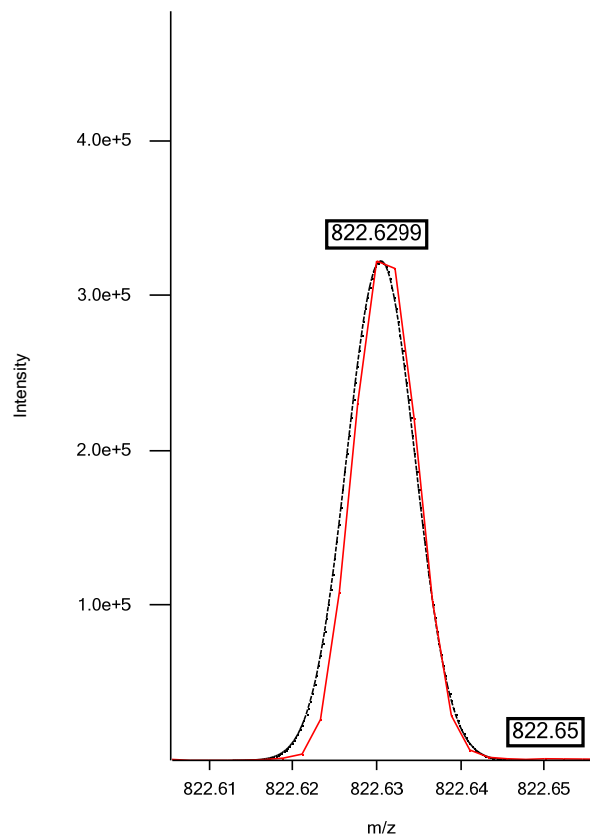


Isotope 3

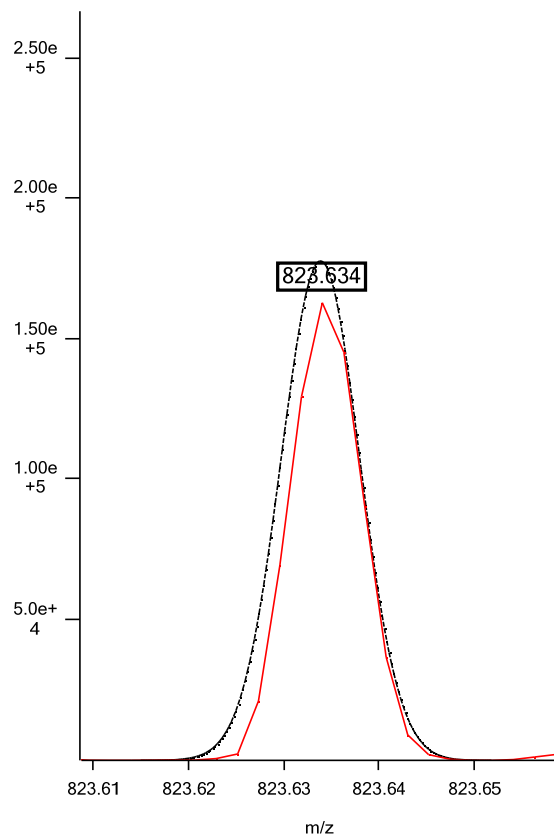


Positive ESI: PC 18:1p/22:4 or 18:0e/22:5; C₄₈H₈₉NO₇P; theoretical *m/z* 822.6376, (M+H)⁺; isotopic fit 0.0062

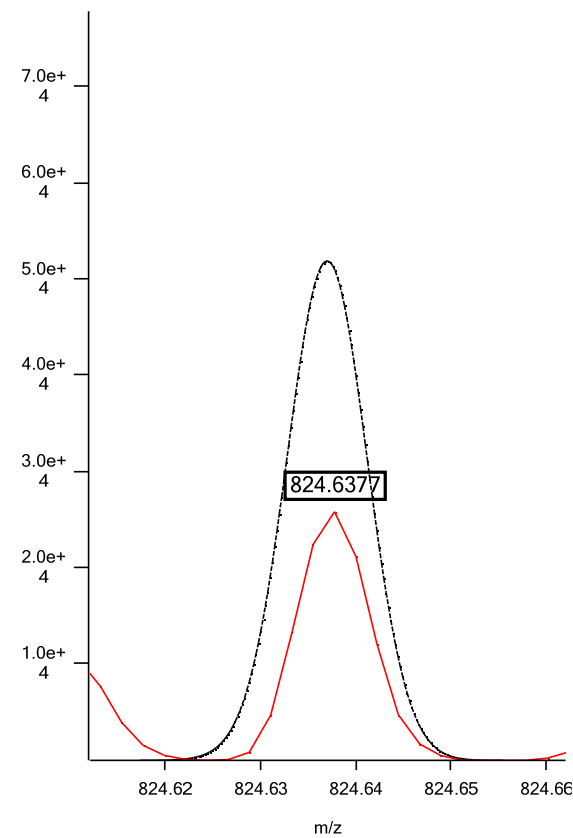
Isotope 1



Isotope 2

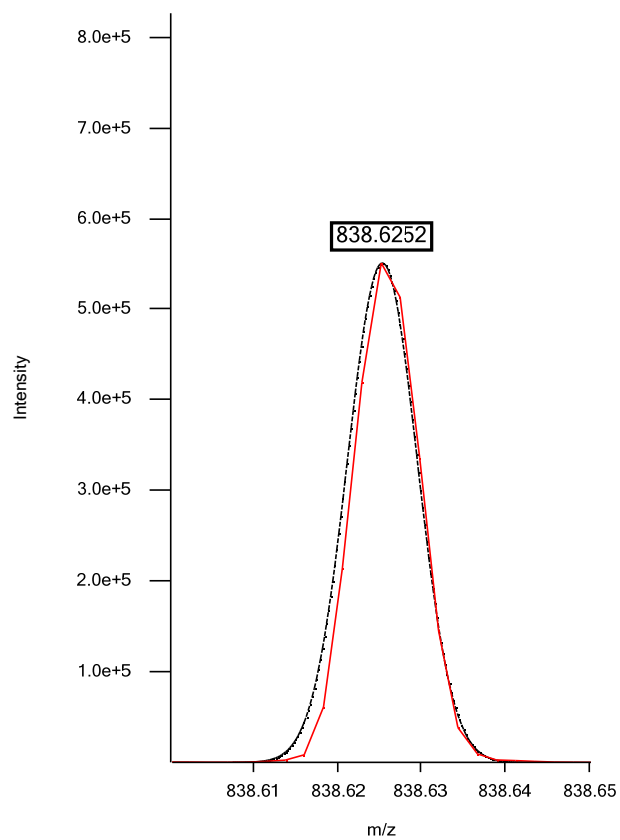


Isotope 3

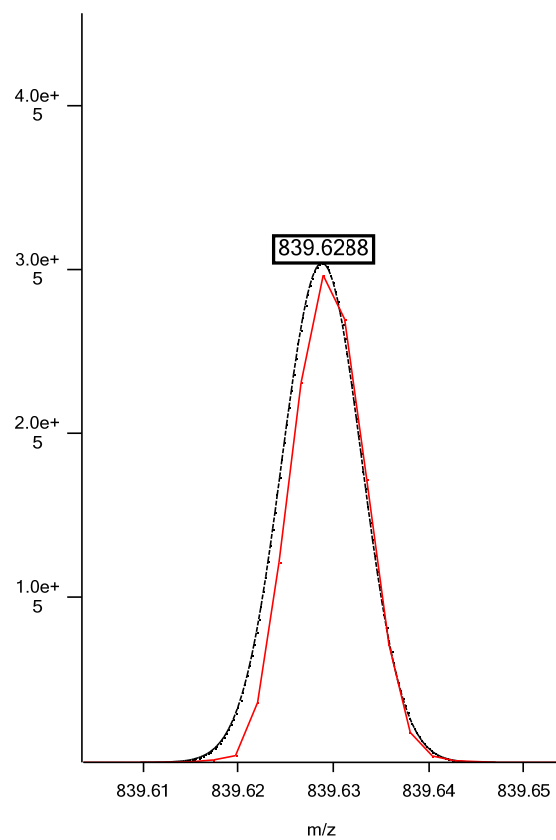


Positive ESI: PC 40:4; C₄₈H₈₉NO₈P; theoretical *m/z* 838.6326, (M+H)⁺; isotopic fit 0.0028

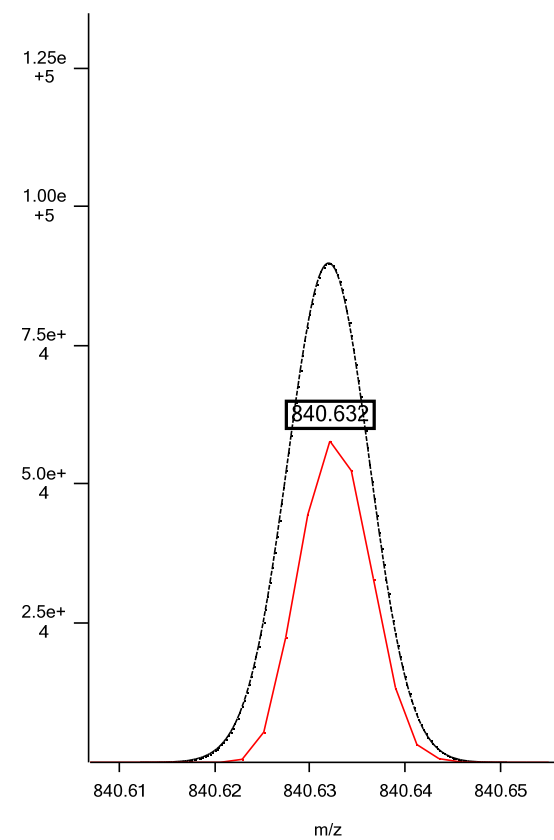
Isotope 1



Isotope 2

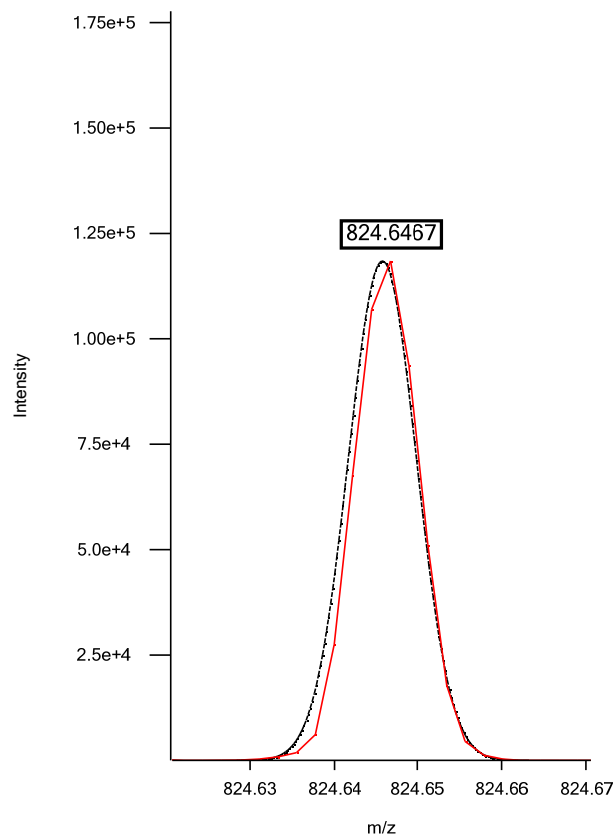


Isotope 3

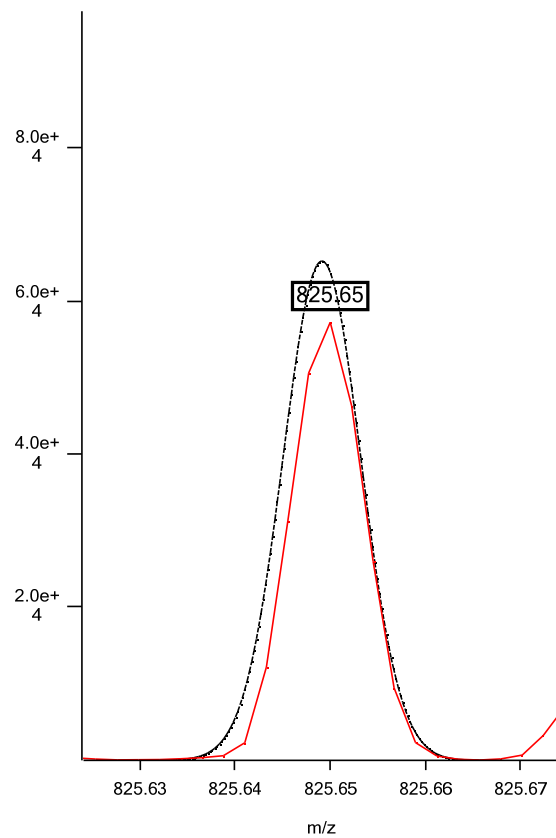


Positive ESI: PC 18:1p/22:3 or 18:0e/22:4; $C_{48}H_{91}NO_7P$; theoretical m/z 824.6533, $(M+H)^+$; isotopic fit 0.0076

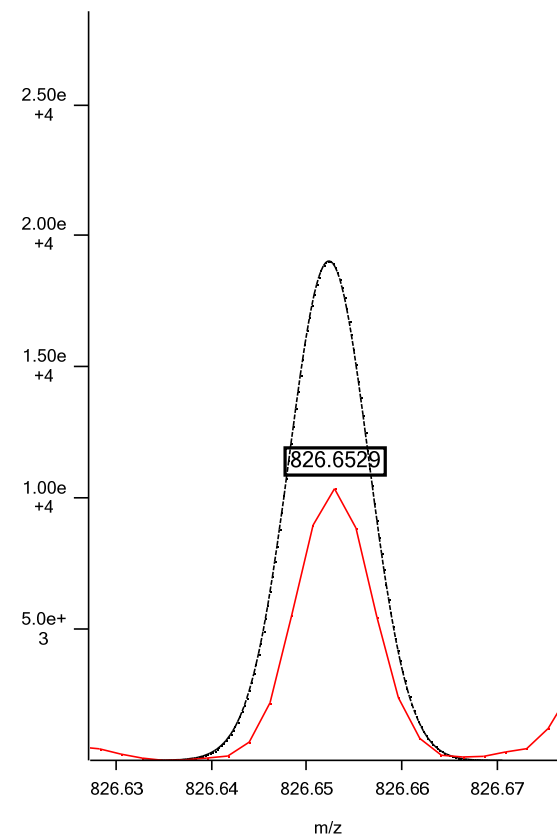
Isotope 1



Isotope 2

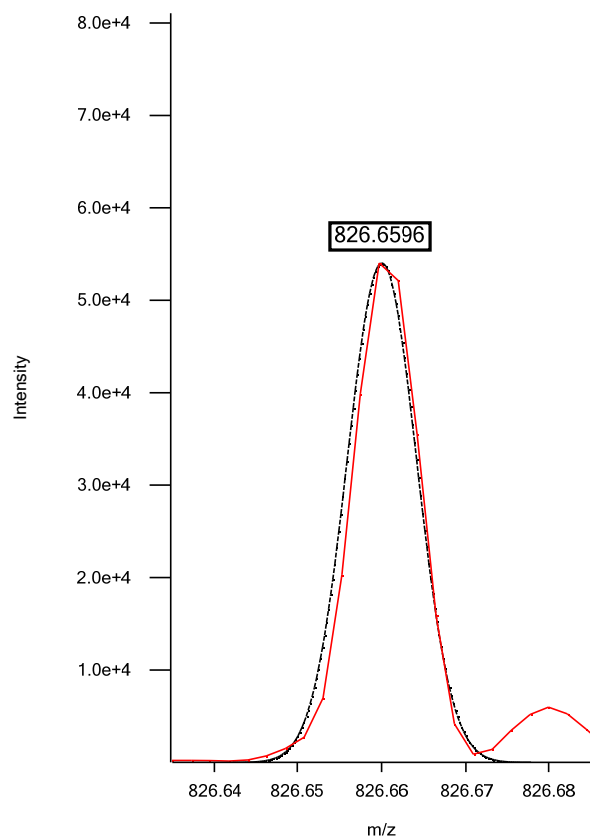


Isotope 3

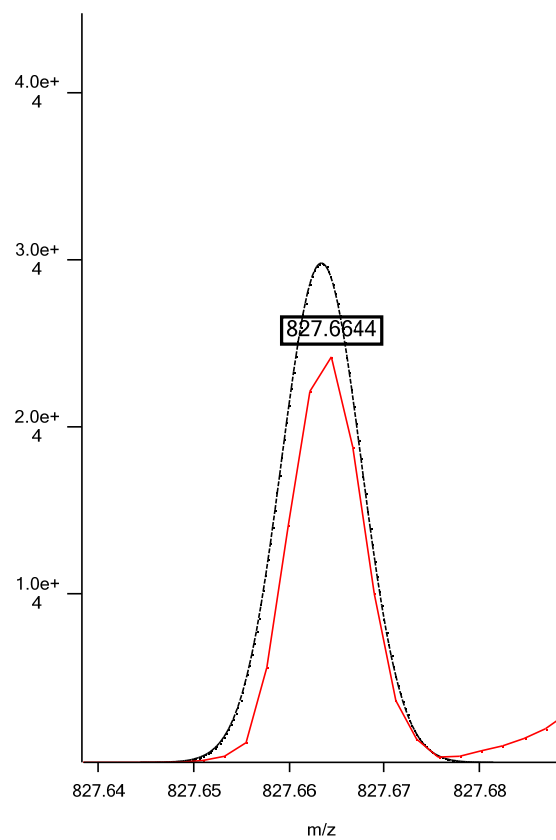


Positive ESI: PC 18:1p/22:2 or 18:0e/22:3; C₄₈H₉₃NO₇P; theoretical *m/z* 826.6689, (M+H)⁺; isotopic fit 0.0119

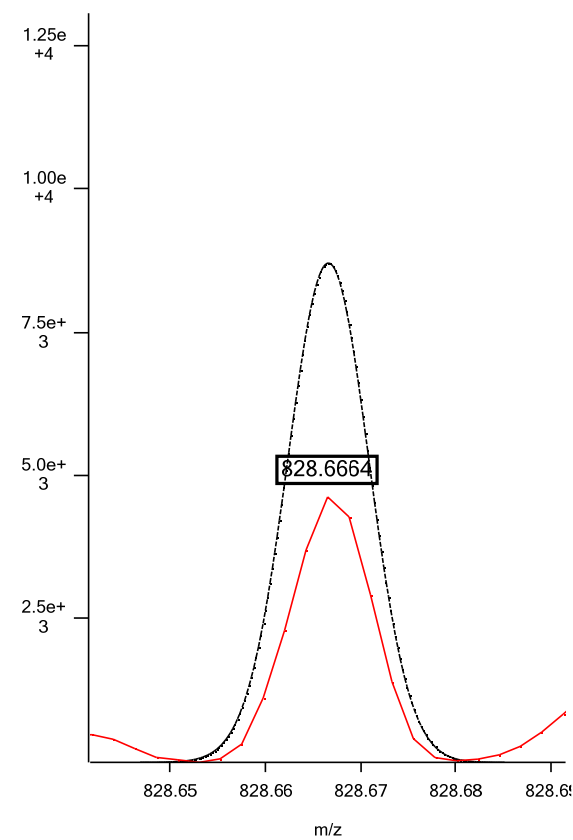
Isotope 1



Isotope 2

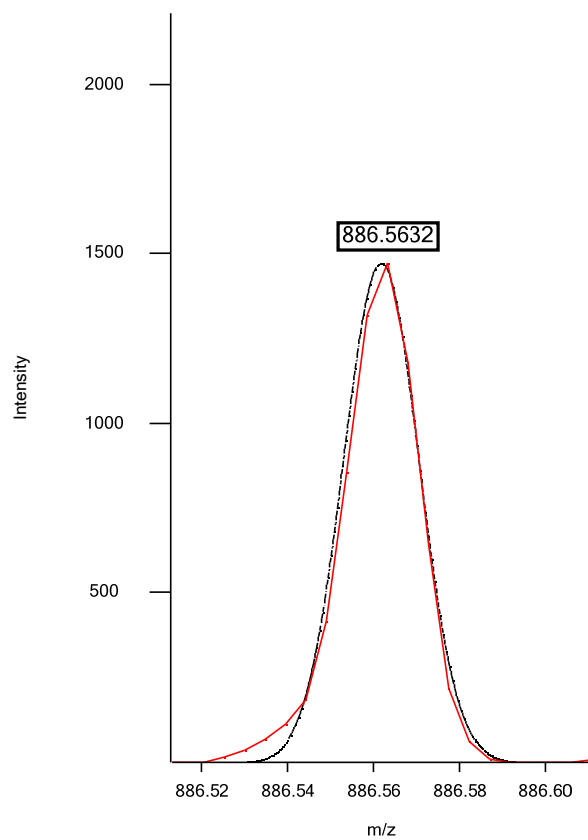


Isotope 3

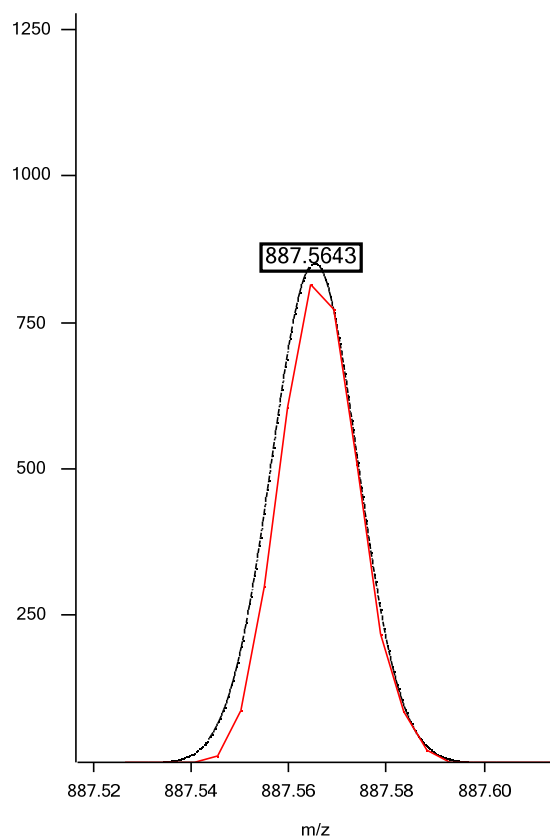


Negative ESI: PC 40:9; C₅₀H₈₁NO₁₀P; theoretical *m/z* 886.5598, (M-H)⁻; isotopic fit 0.0040

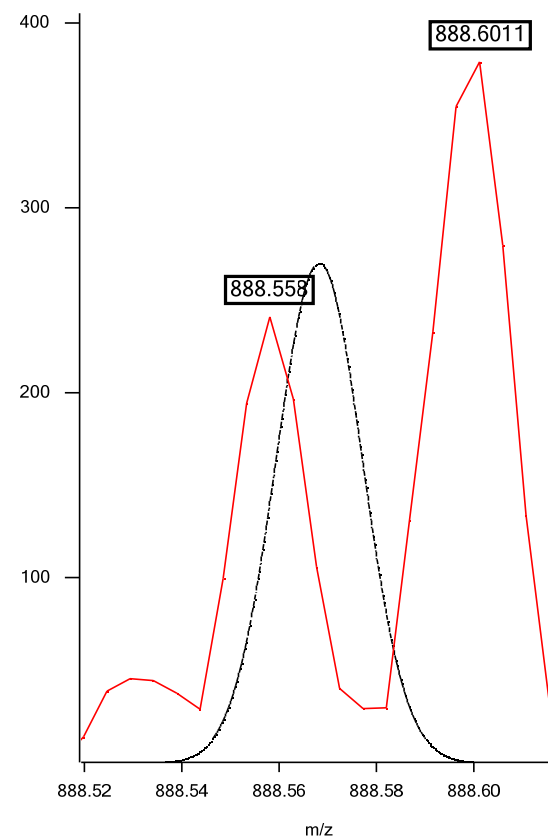
Isotope 1



Isotope 2

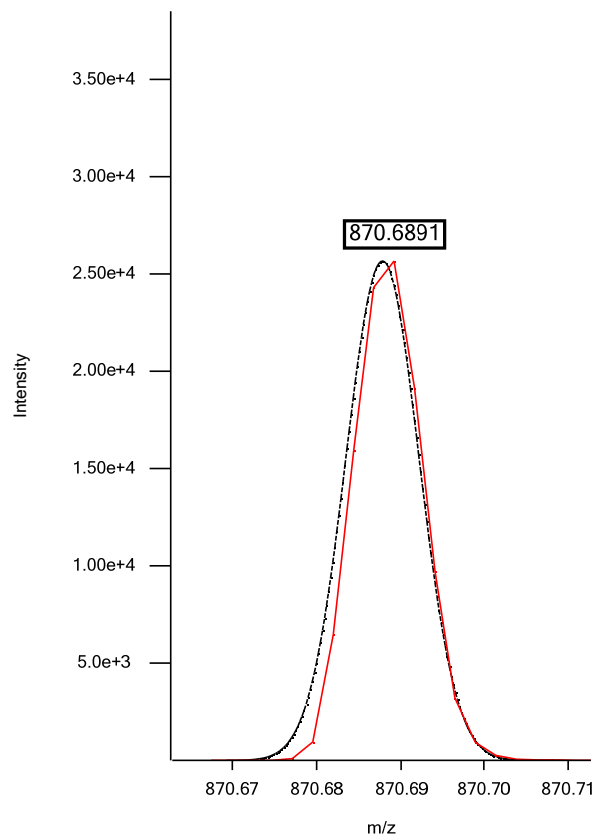


Isotope 3

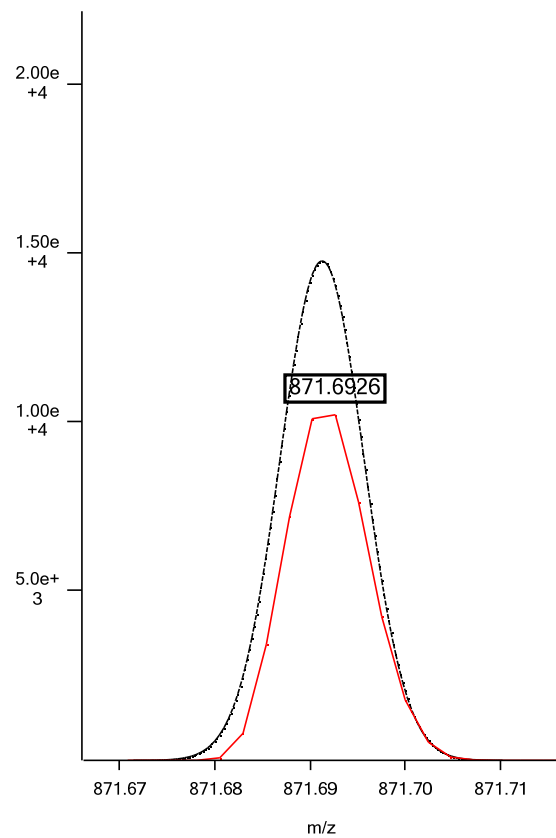


Positive ESI: PC 42:2; C₅₀H₉₇NO₈P; theoretical *m/z* 870.6951, (M+H)⁺; isotopic fit 0.0235

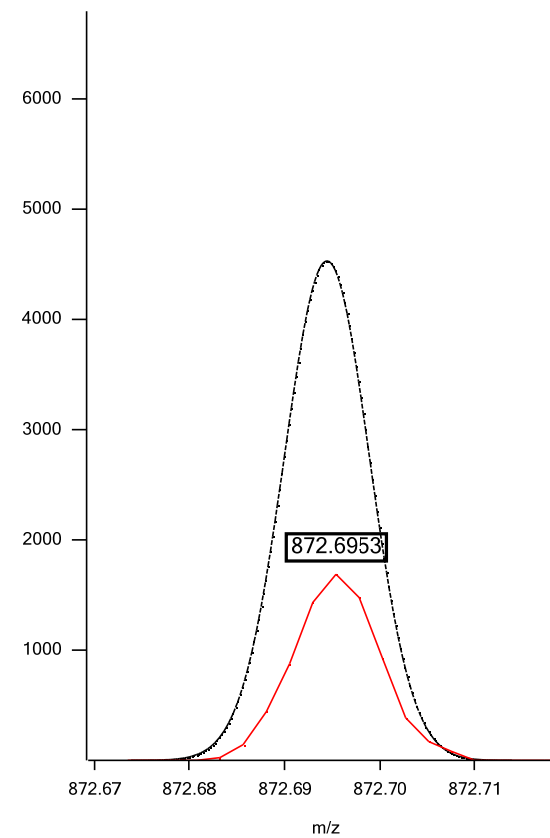
Isotope 1



Isotope 2



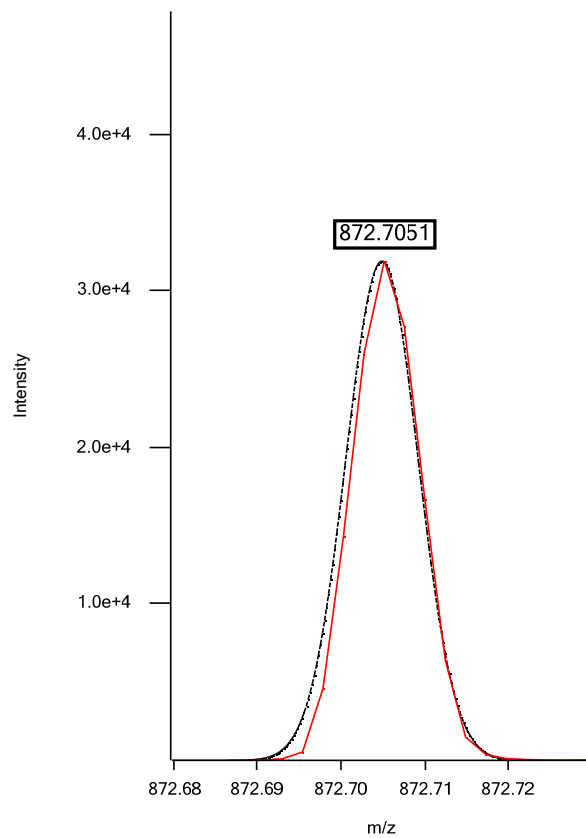
Isotope 3



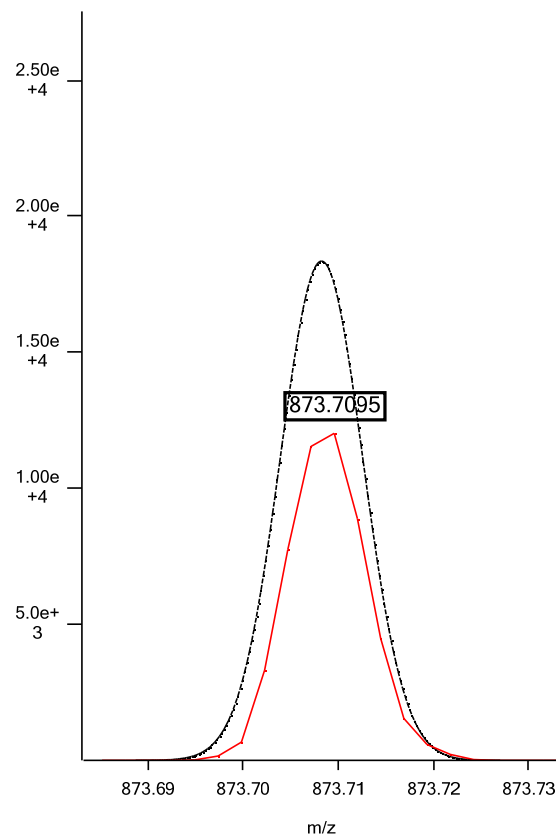
Positive ESI: PC 42:1; C₅₀H₉₉NO₈P; theoretical m/z 872.7108, (M+H)⁺; isotopic fit 0.0318

C50H99NO8P_872.7108_42-1_PC.txt

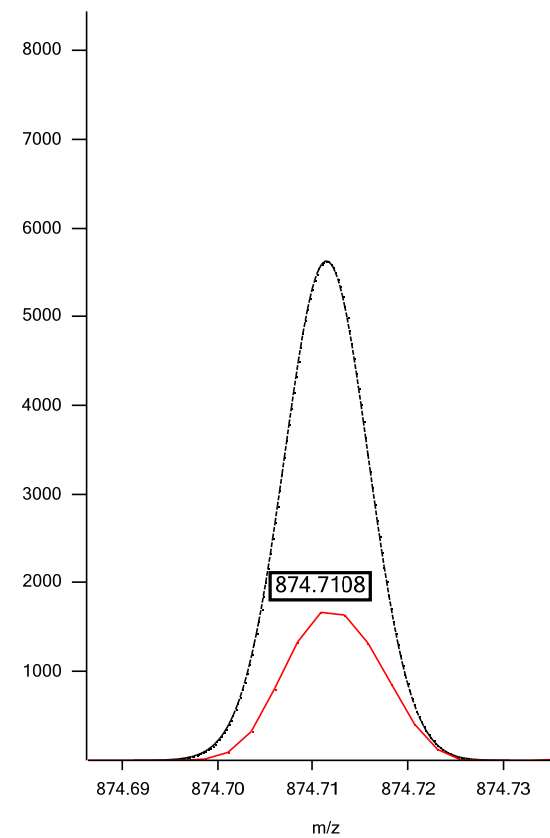
Isotope 1



Isotope 2



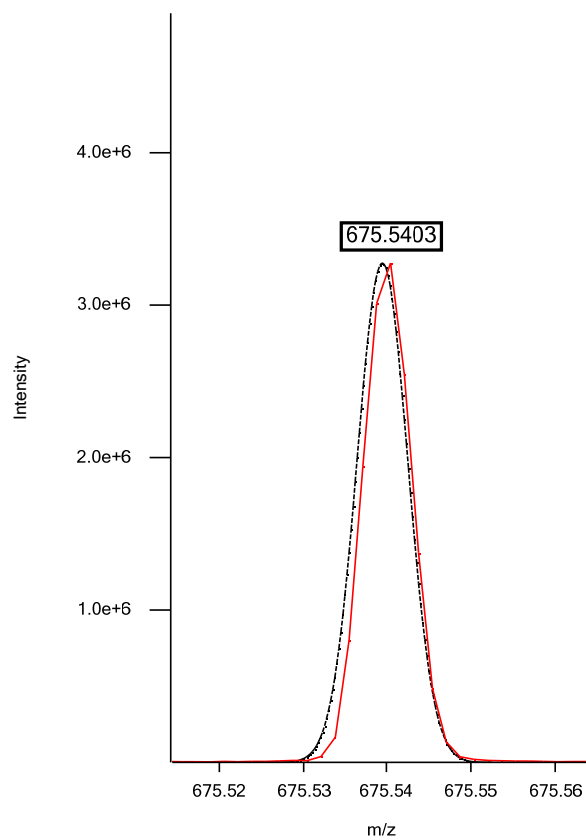
Isotope 3



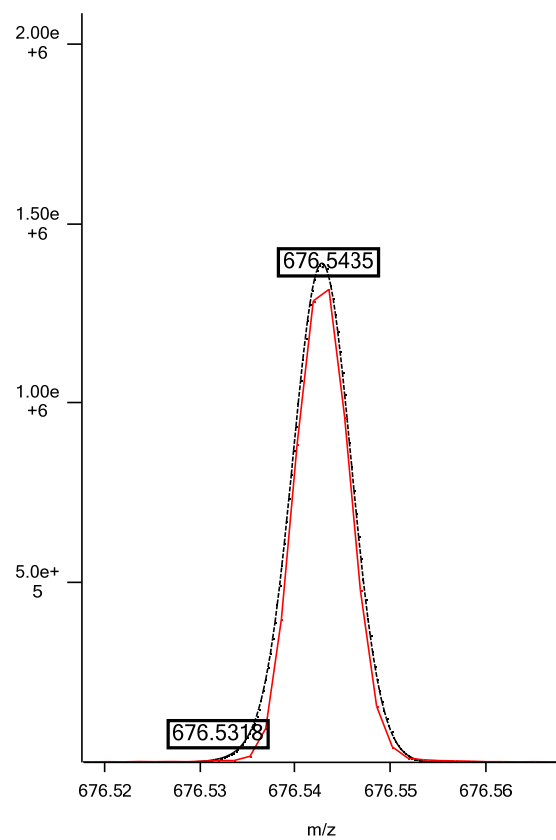
Sphingomyelins

Positive ESI: SM d16:1/16:0; C₃₇H₇₆N₂O₆P; theoretical m/z 675.5441, (M+H)⁺; isotopic fit 0.0065

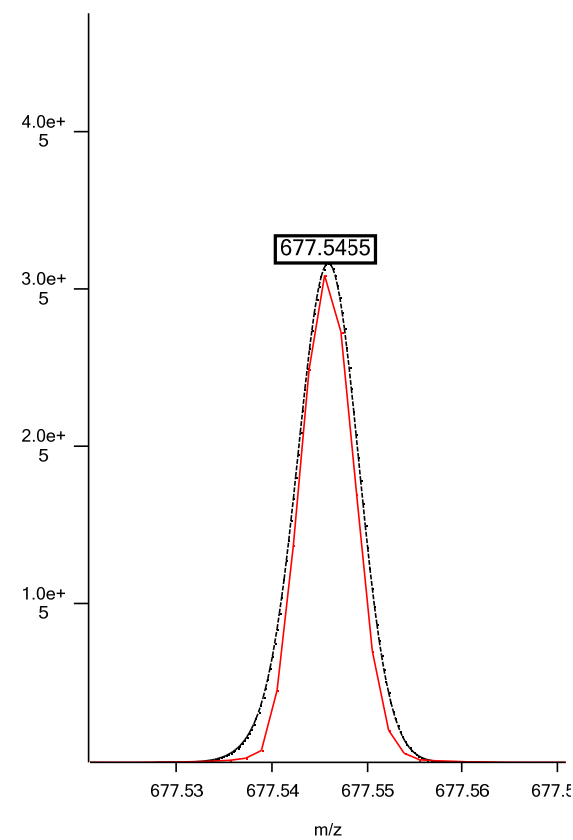
Isotope 1



Isotope 2

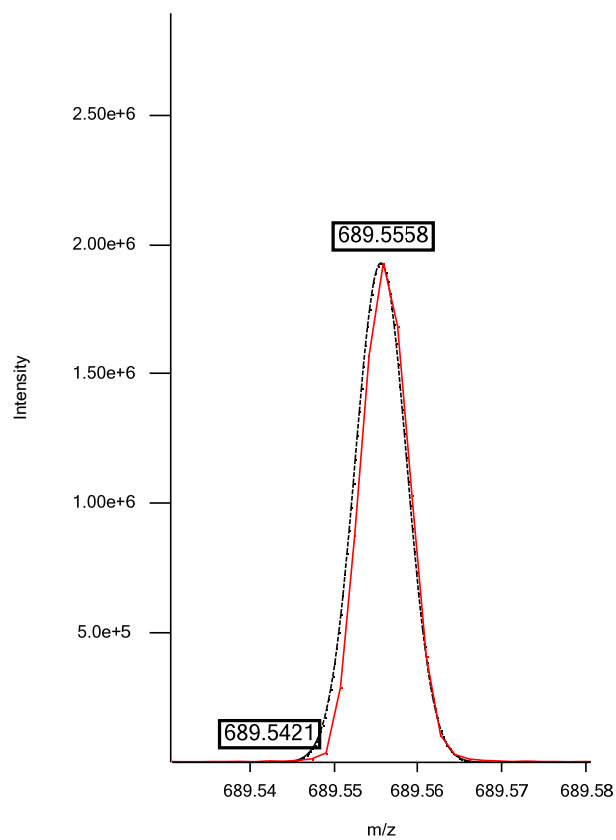


Isotope 3

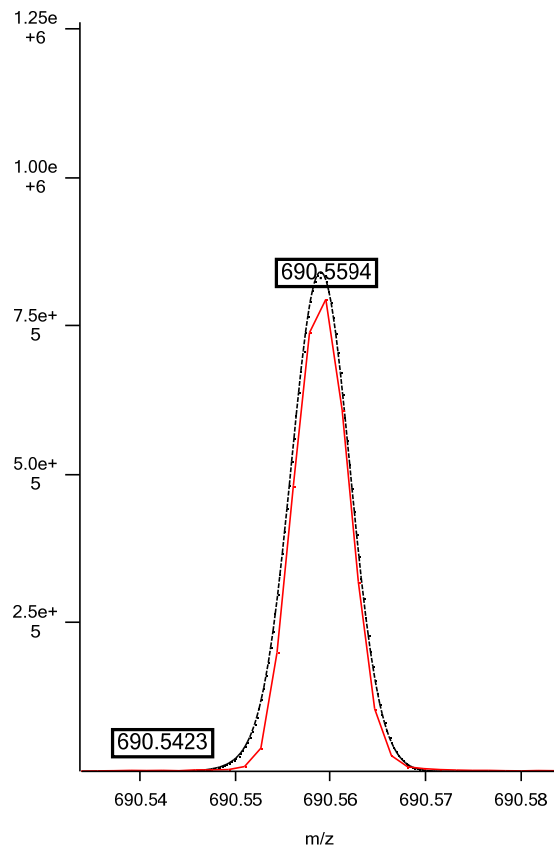


Positive ESI: SM d16:1/17:0; C₃₈H₇₈N₂O₆P; theoretical m/z 689.5597, (M+H)⁺; isotopic fit 0.0098

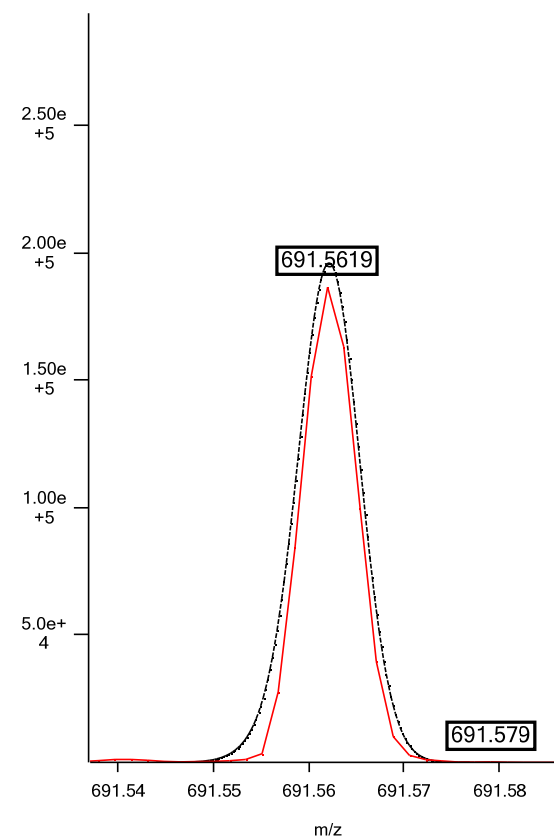
Isotope 1



Isotope 2

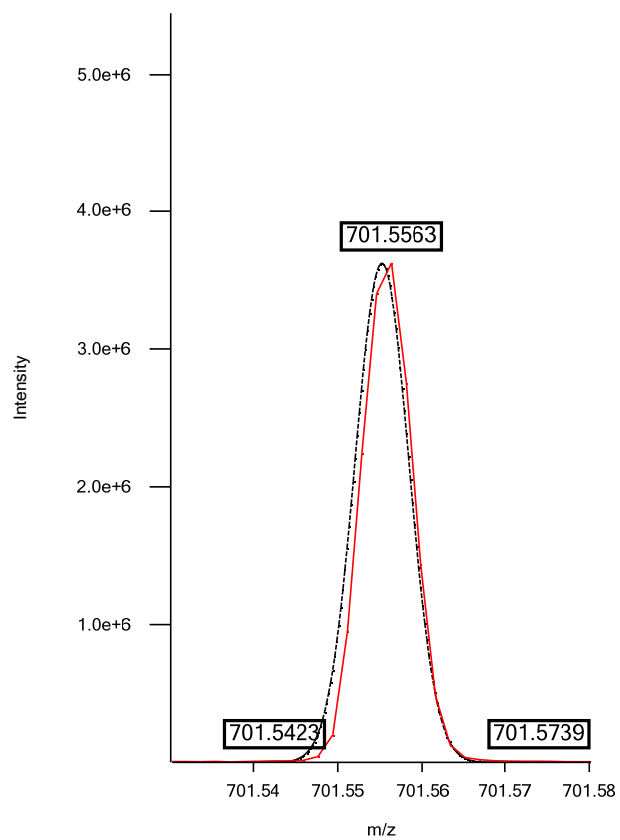


Isotope 3

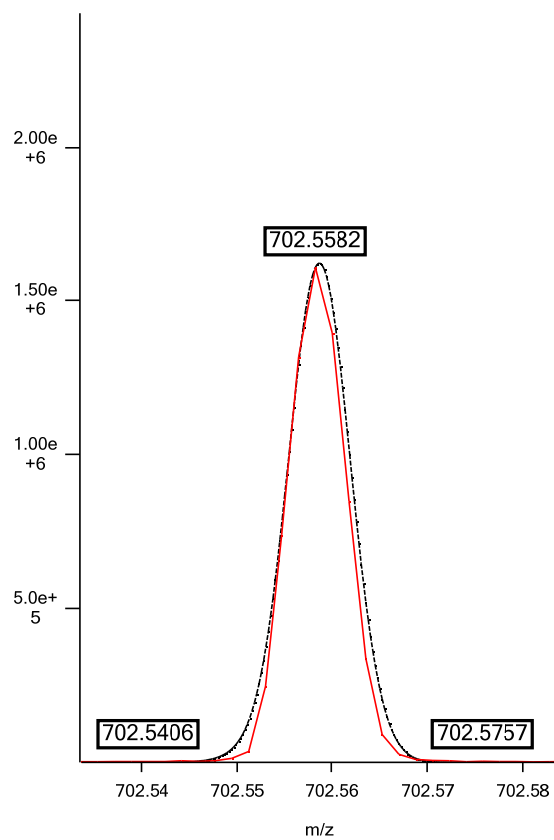


Positive ESI: SM d16:1/18:1; C₃₉H₇₈N₂O₆P; theoretical m/z 701.5597, (M+H)⁺; isotopic fit 0.0058

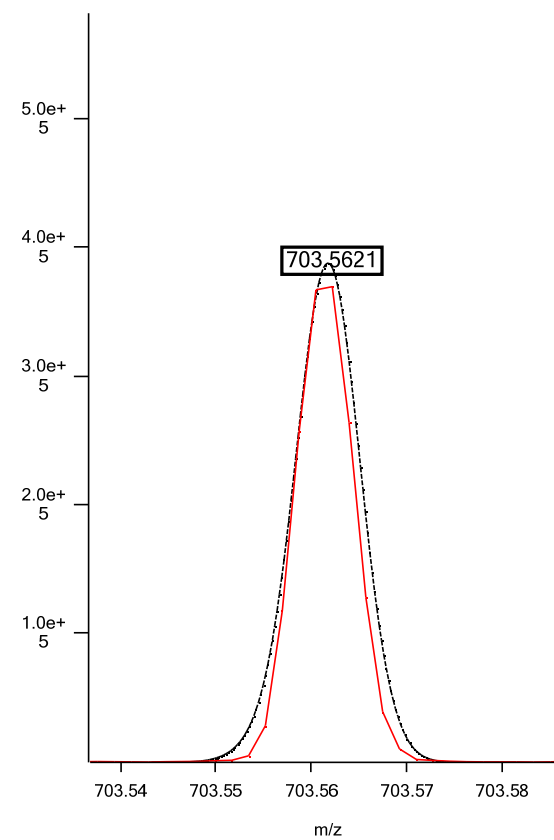
Isotope 1



Isotope 2

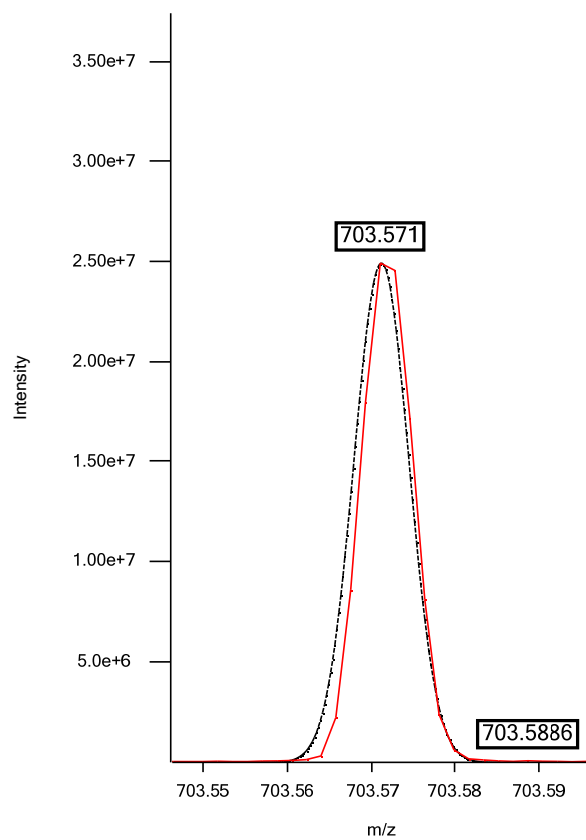


Isotope 3

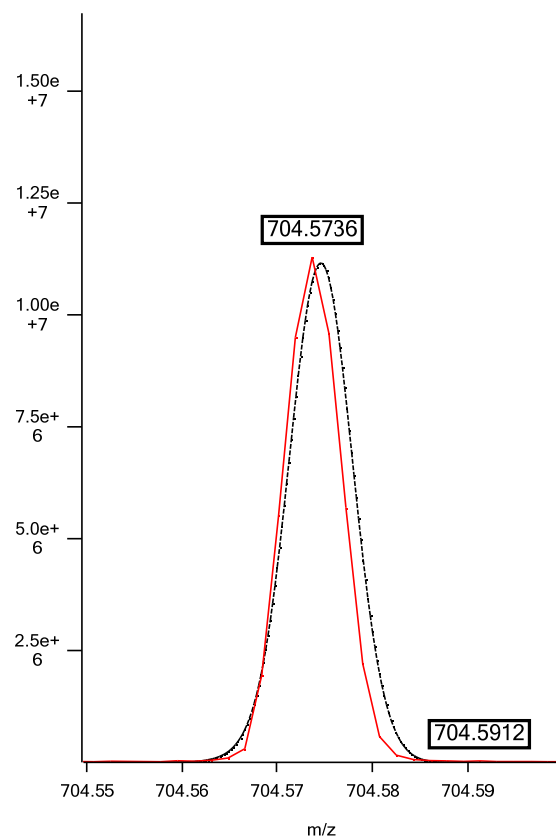


Positive ESI: SM d16:1/18:0; C₃₉H₈₀N₂O₆P; theoretical m/z 703.5754, (M+H)⁺; isotopic fit 0.0168

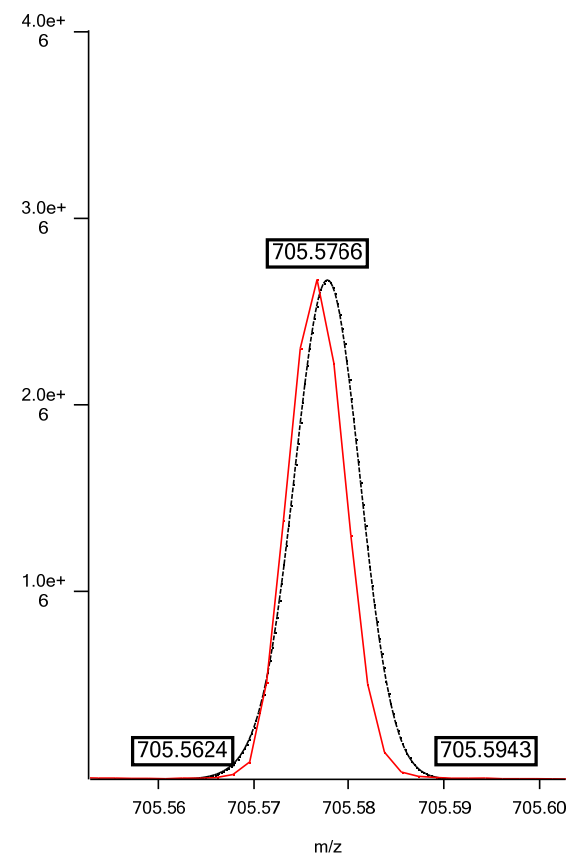
Isotope 1



Isotope 2

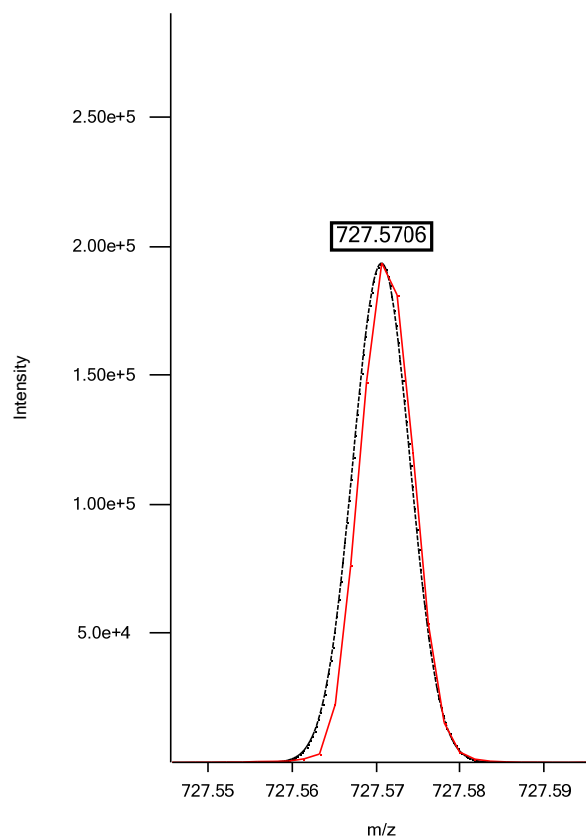


Isotope 3

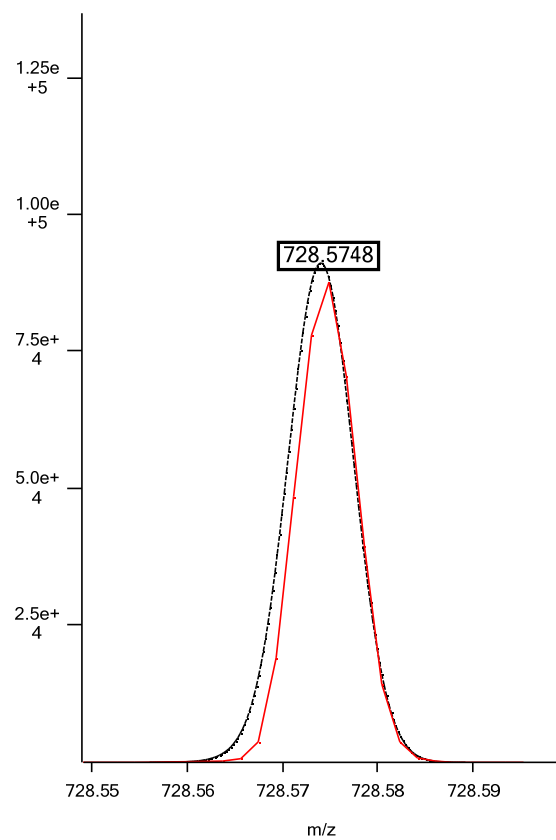


Positive ESI: SM d18:1/18:2; C₄₁H₈₀N₂O₆P; theoretical *m/z* 727.5754, (M+H)⁺; isotopic fit 0.0033

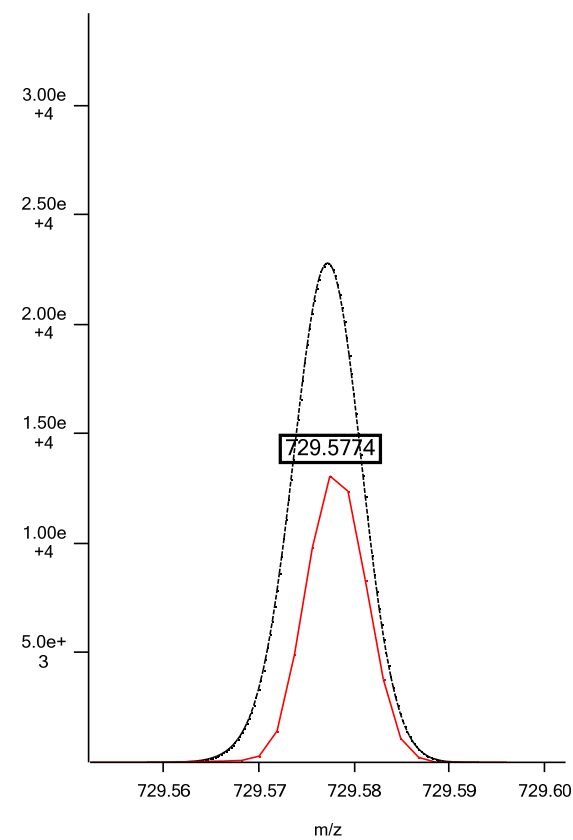
Isotope 1



Isotope 2

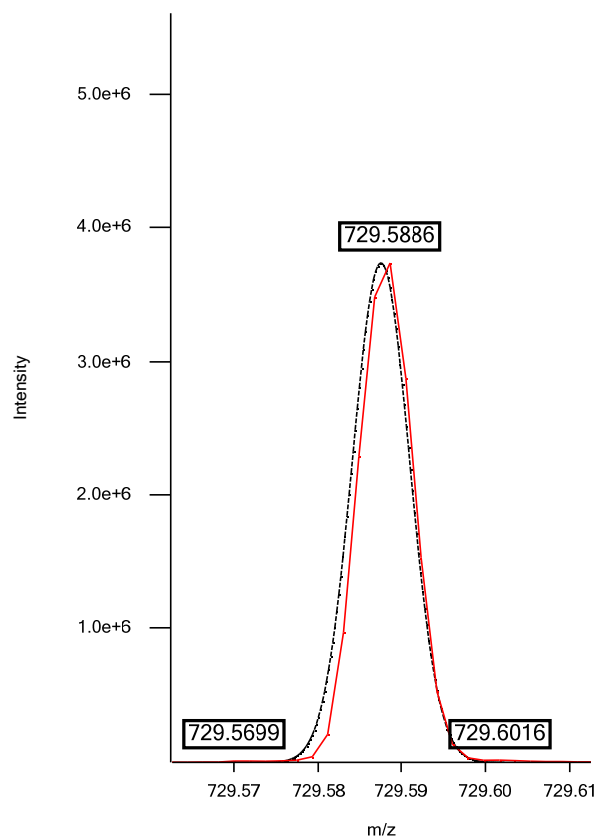


Isotope 3

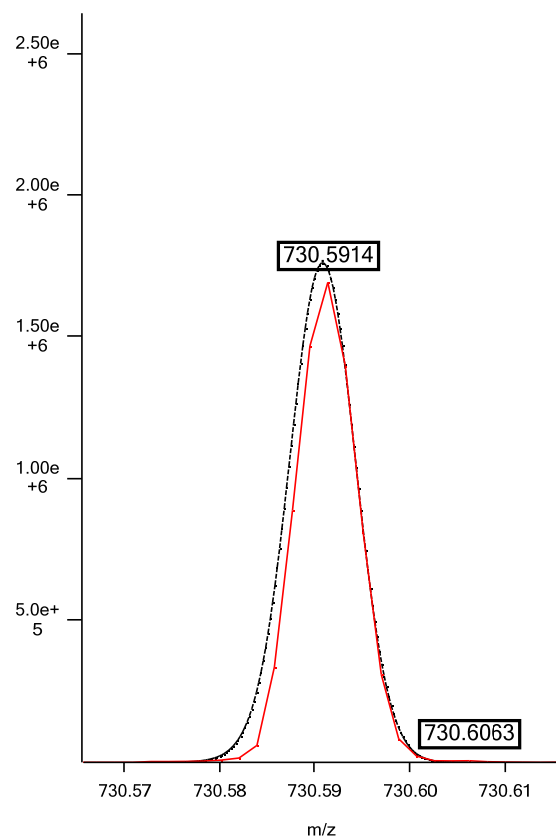


Positive ESI: SM d18:1/18:1; C₄₁H₈₂N₂O₆P; theoretical m/z 729.5910, (M+H)⁺; isotopic fit 0.0028

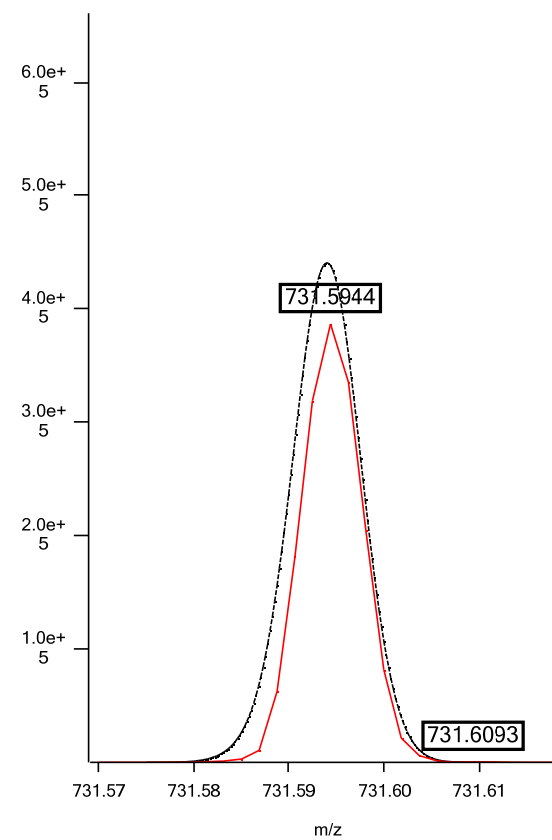
Isotope 1



Isotope 2

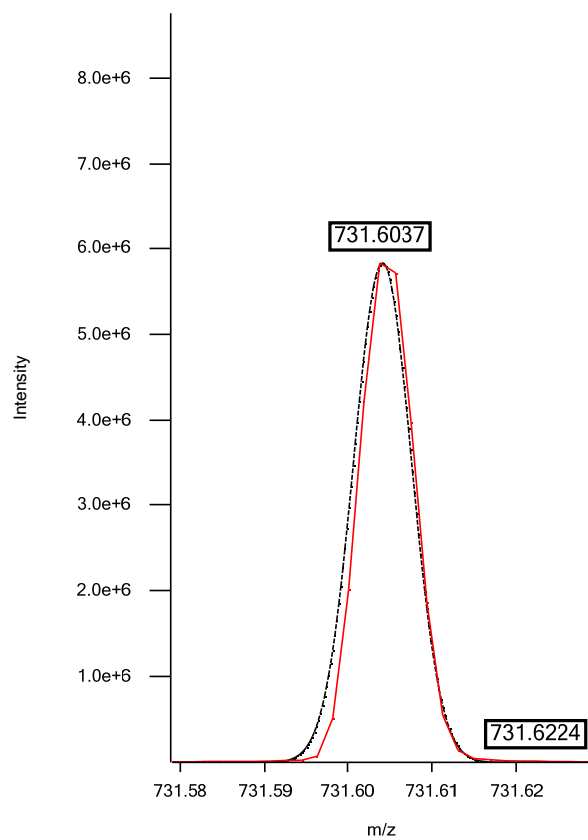


Isotope 3

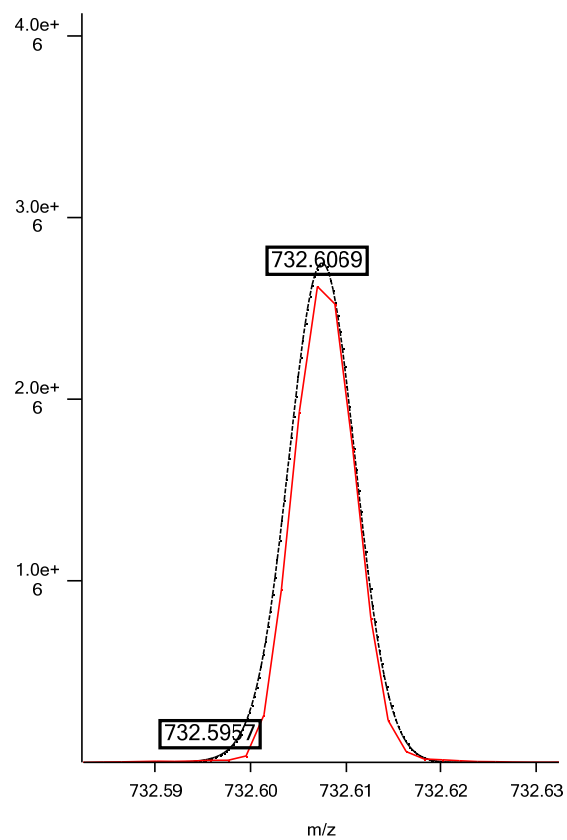


Positive ESI: SM d18:1/18:0; C₄₁H₈₄N₂O₆P; theoretical *m/z* 731.6067, (M+H)⁺; isotopic fit 0.0032

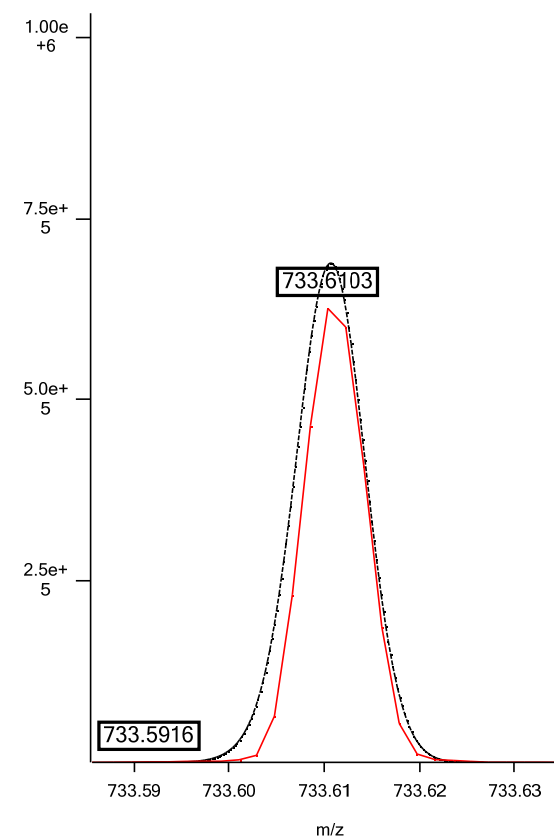
Isotope 1



Isotope 2

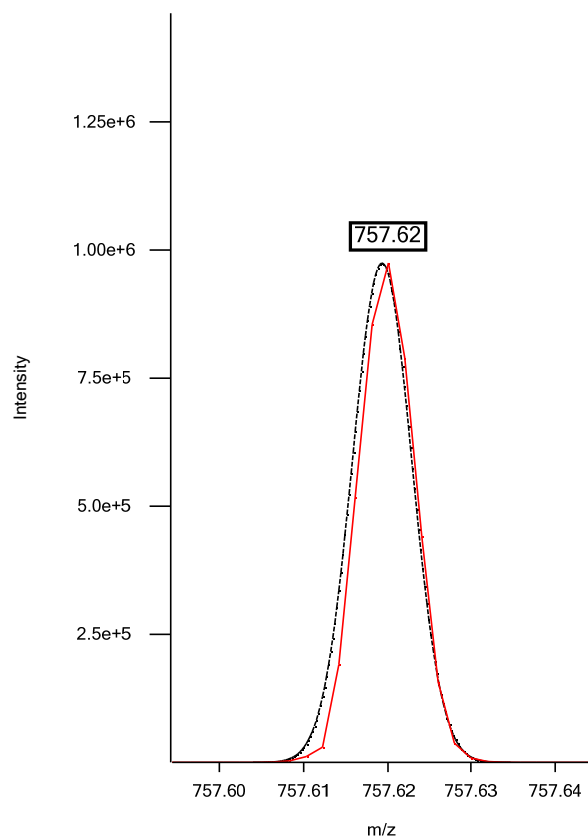


Isotope 3

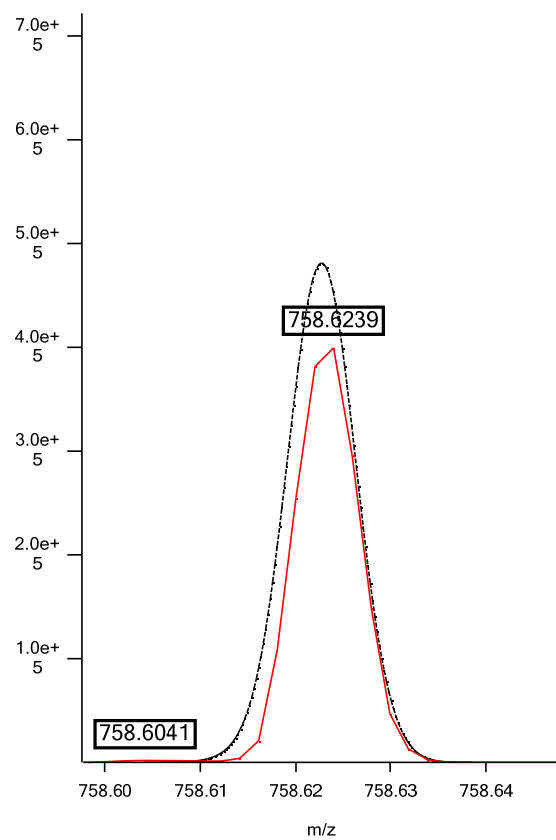


Positive ESI: SM d18:1/20:1; C₄₃H₈₆N₂O₆P; theoretical *m/z* 757.6223, (M+H)⁺; isotopic fit 0.0135

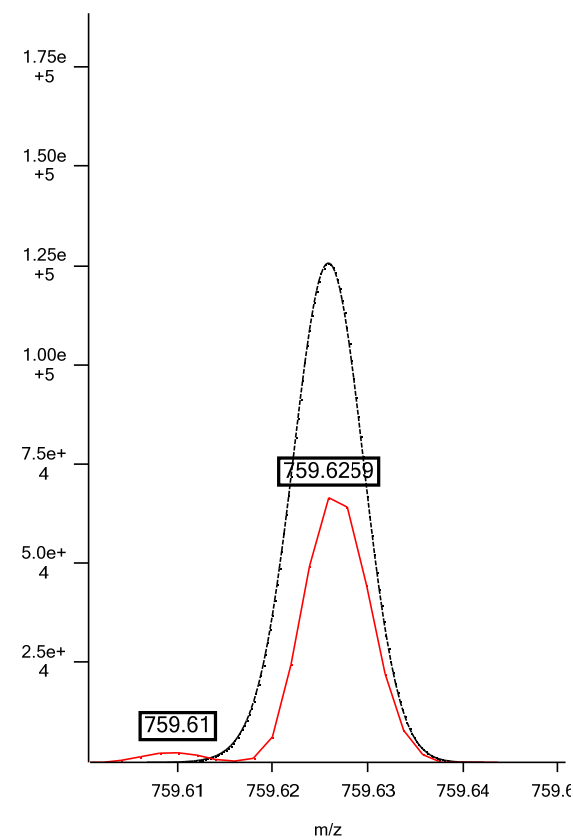
Isotope 1



Isotope 2

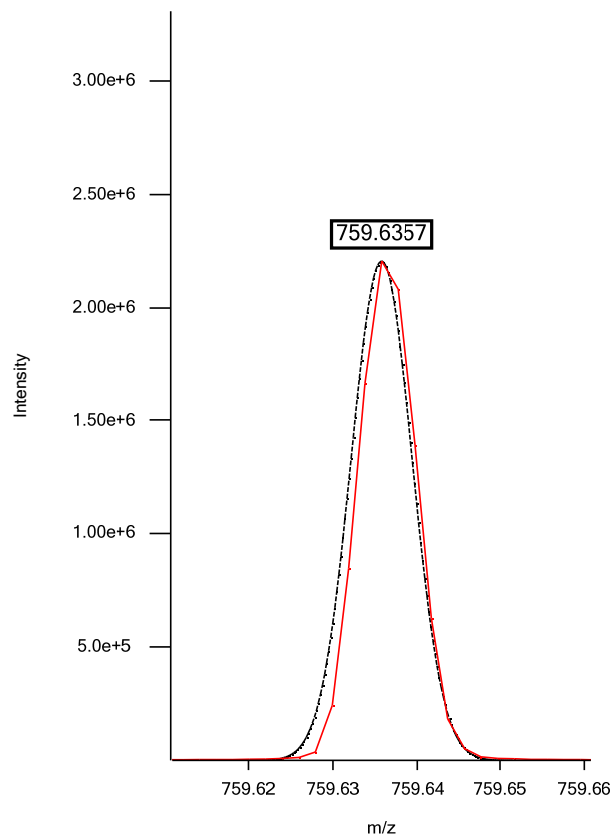


Isotope 3

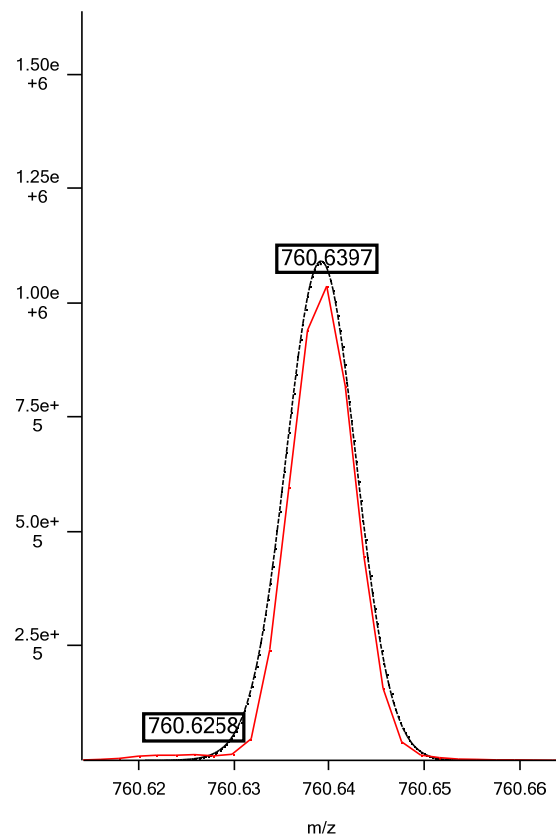


Positive ESI: SM d18:1/20:0; C₄₃H₈₈N₂O₆P; theoretical m/z 759.6380, (M+H)⁺; isotopic fit 0.0052

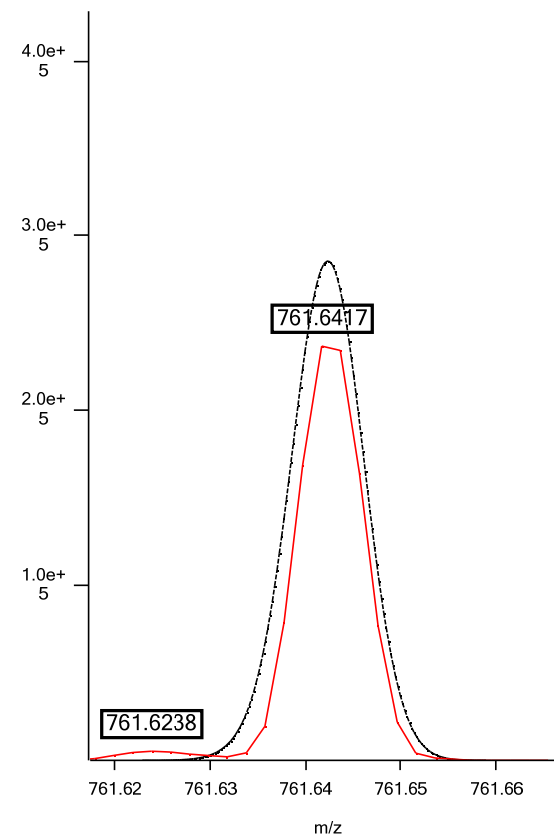
Isotope 1



Isotope 2

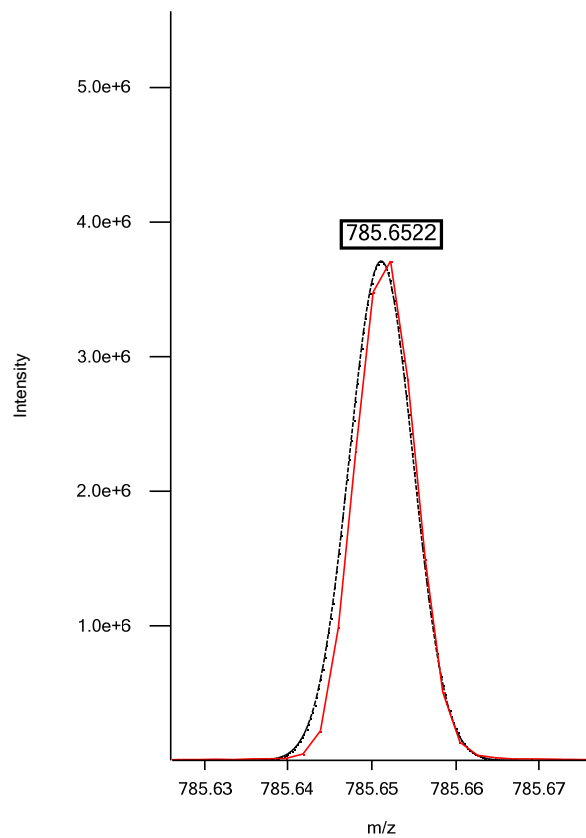


Isotope 3

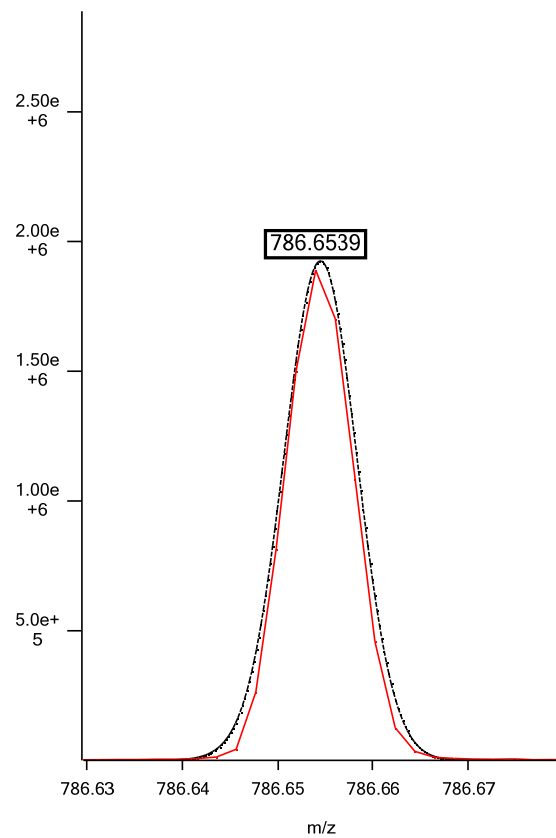


Positive ESI: SM d16:1/24:1; C₄₅H₉₀N₂O₆P; theoretical *m/z* 785.6537, (M+H)⁺; isotopic fit 0.0043

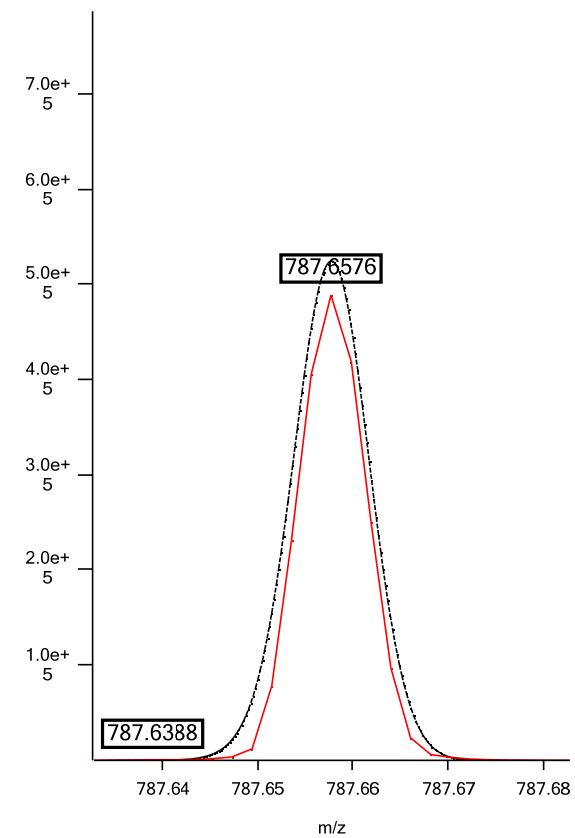
Isotope 1



Isotope 2

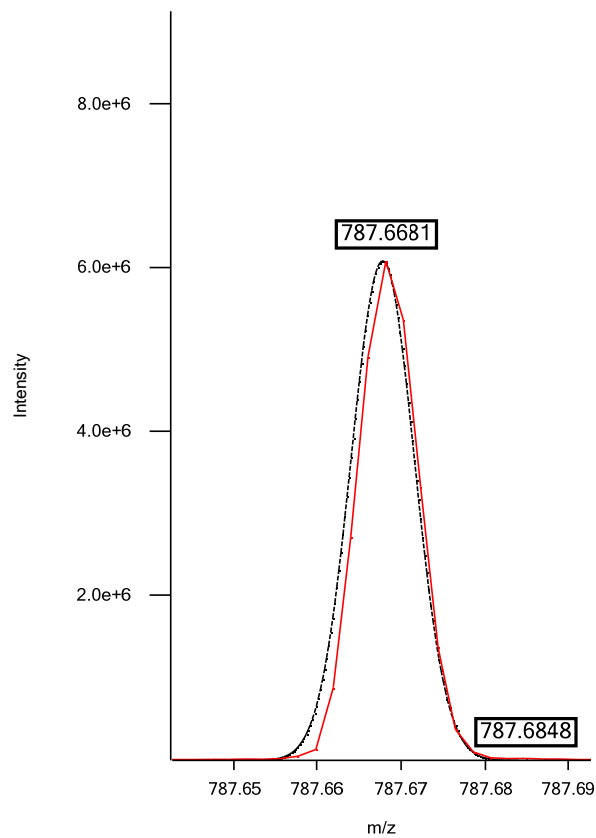


Isotope 3

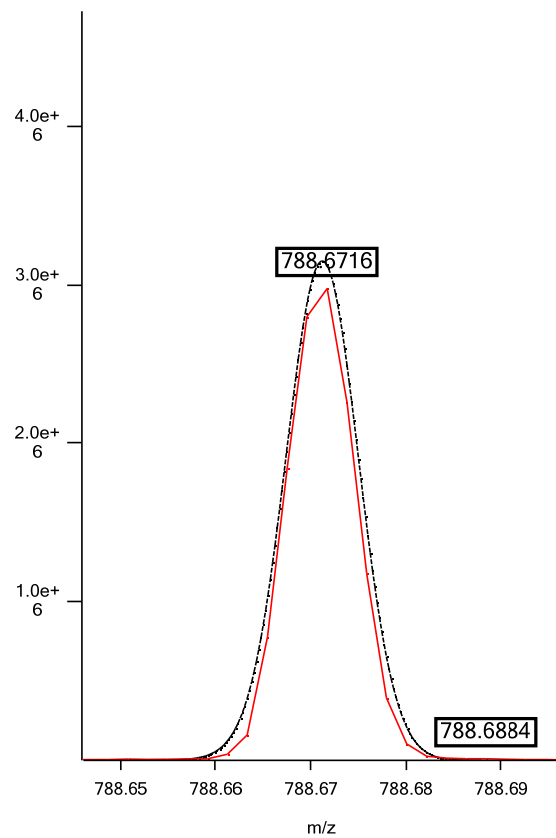


Positive ESI: SM d16:1/24:0; C₄₅H₉₂N₂O₆P; theoretical m/z 787.6693, (M+H)⁺; isotopic fit 0.0090

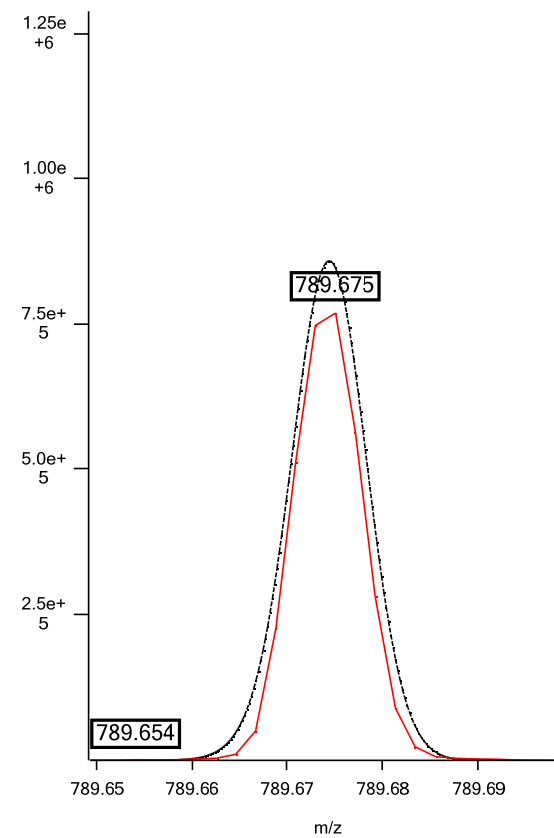
Isotope 1



Isotope 2

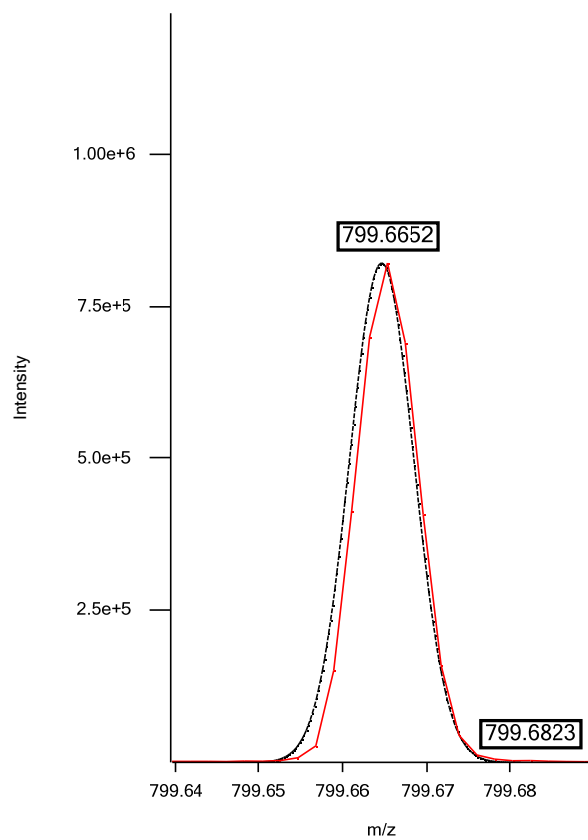


Isotope 3

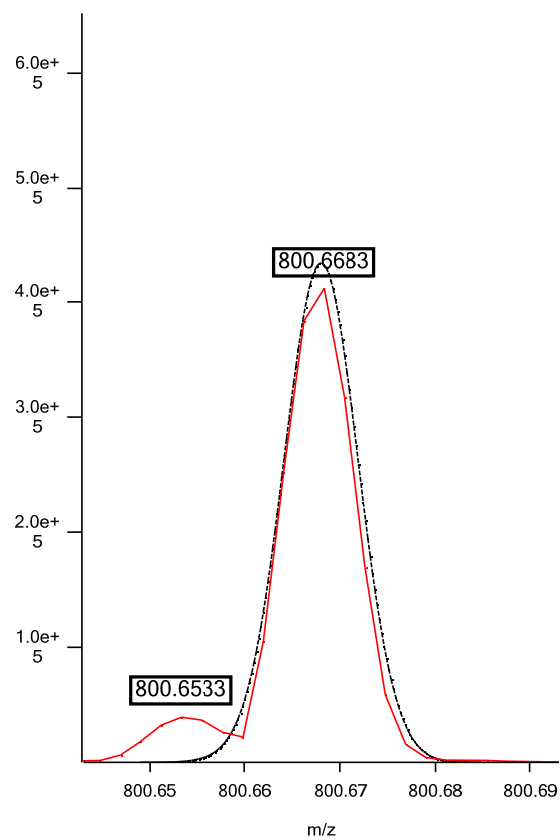


Positive ESI: SM d17:1/24:1; C₄₆H₉₂N₂O₆P; theoretical m/z 799.6693, (M+H)⁺; isotopic fit 0.0074

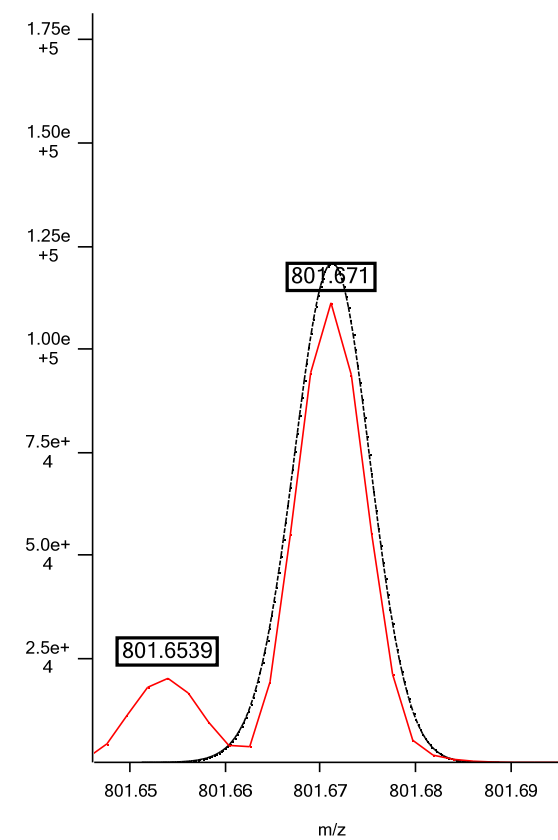
Isotope 1



Isotope 2

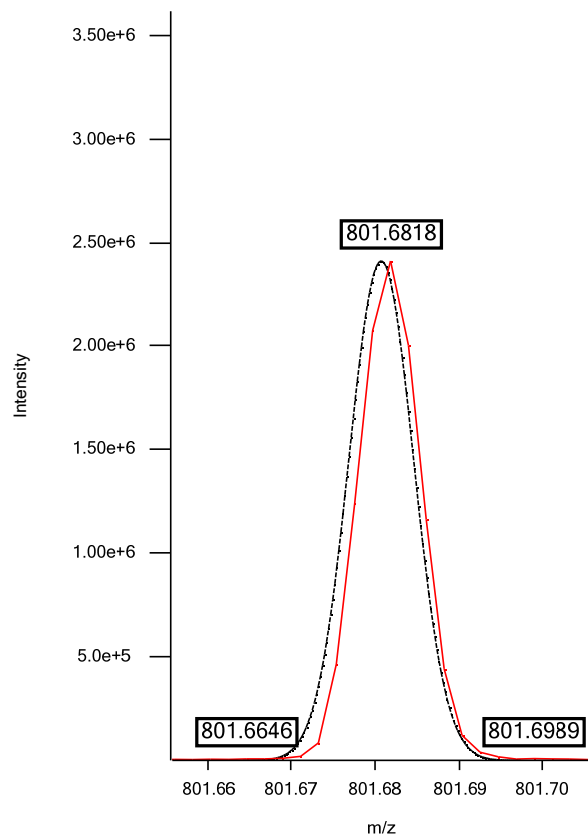


Isotope 3

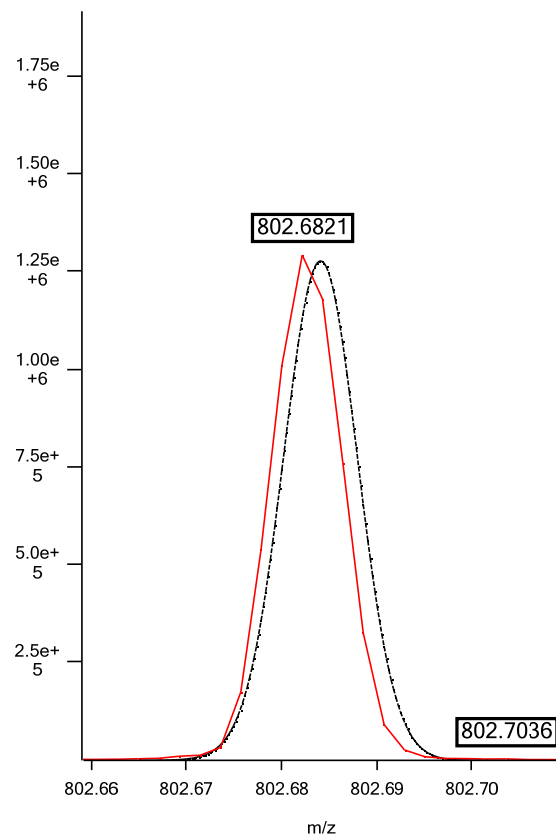


Positive ESI: SM d17:1/24:0; C₄₆H₉₄N₂O₆P; theoretical *m/z* 801.6850, (M+H)⁺; isotopic fit 0.0270

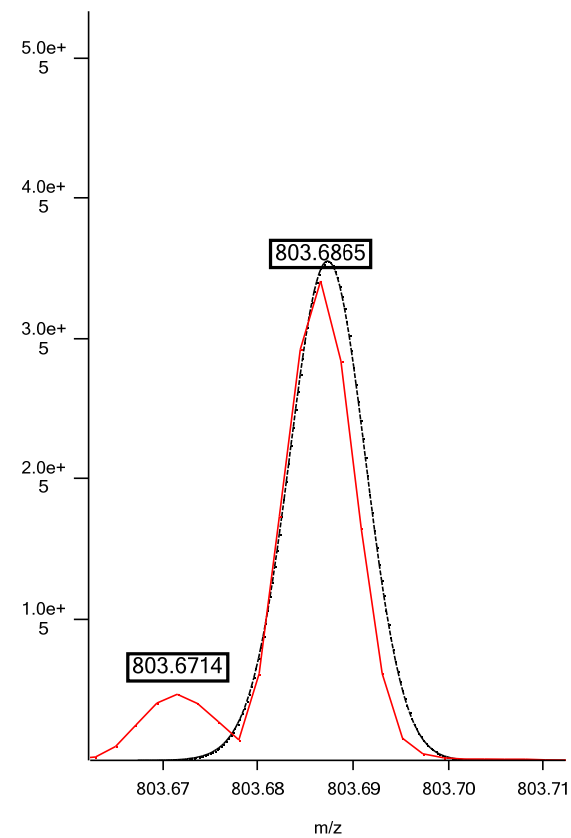
Isotope 1



Isotope 2

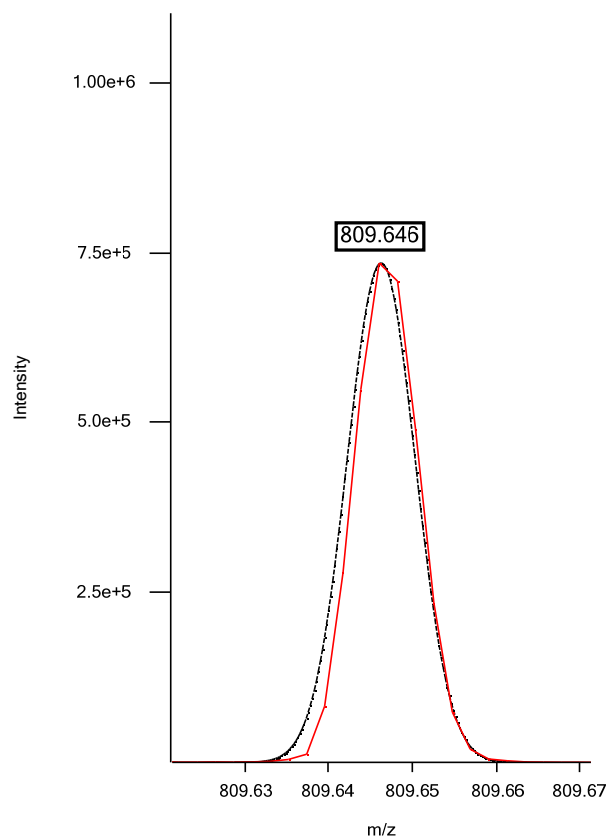


Isotope 3

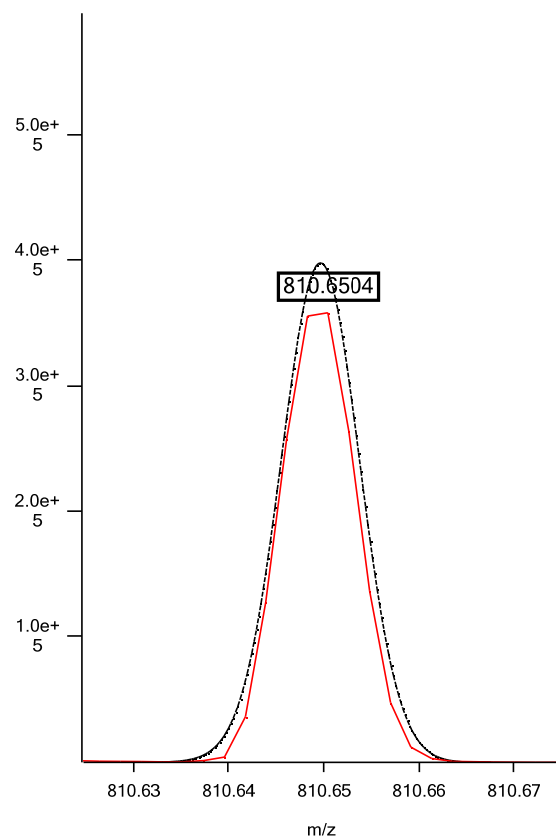


Positive ESI: SM d20:1/22:3; C₄₇H₉₀N₂O₆P; theoretical m/z 809.6536, (M+H)⁺; isotopic fit 0.0082

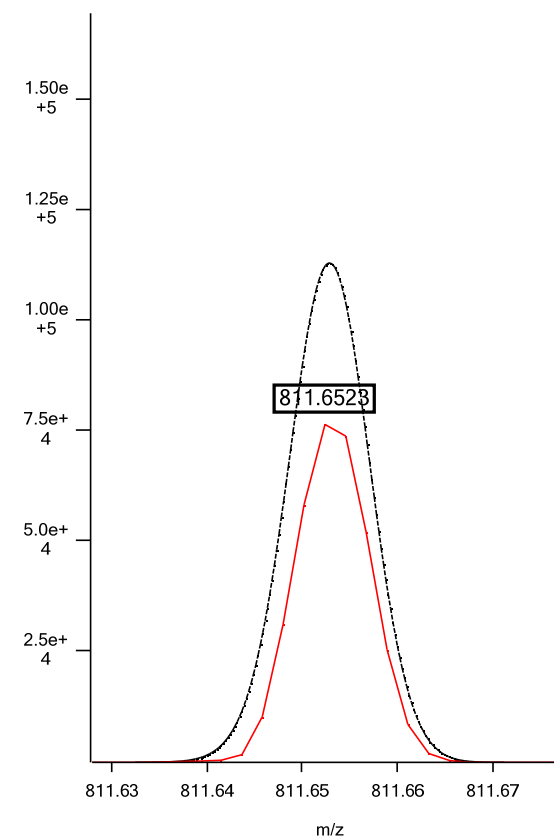
Isotope 1



Isotope 2

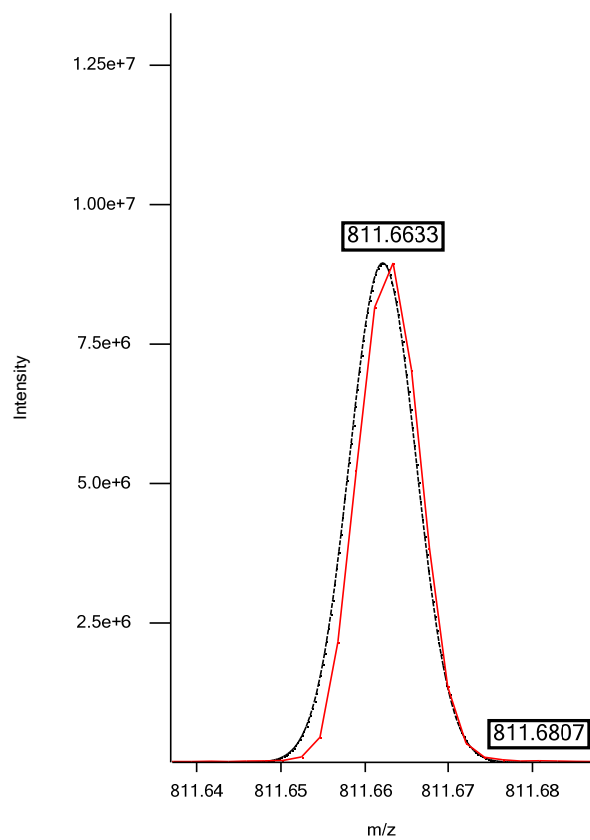


Isotope 3

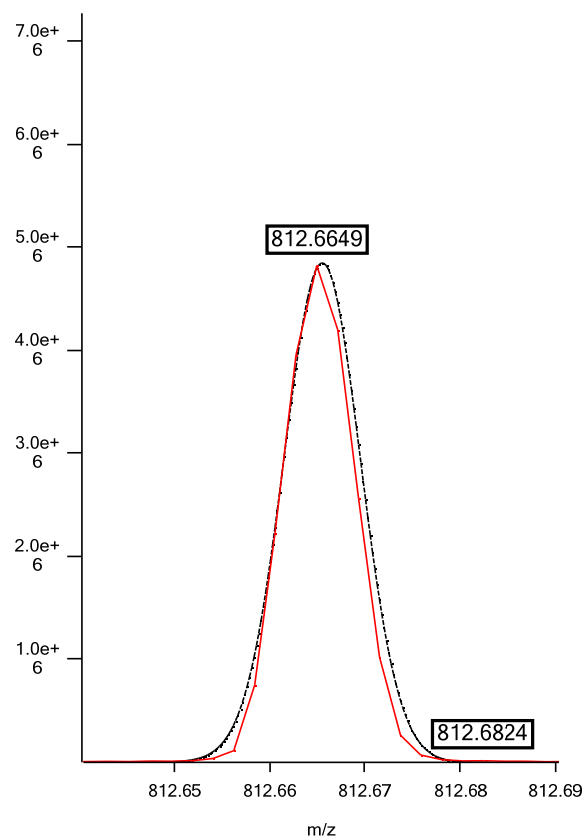


Positive ESI: SM d18:1/24:2; C₄₇H₉₂N₂O₆P; theoretical m/z 811.6693, (M+H)⁺; isotopic fit 0.0088

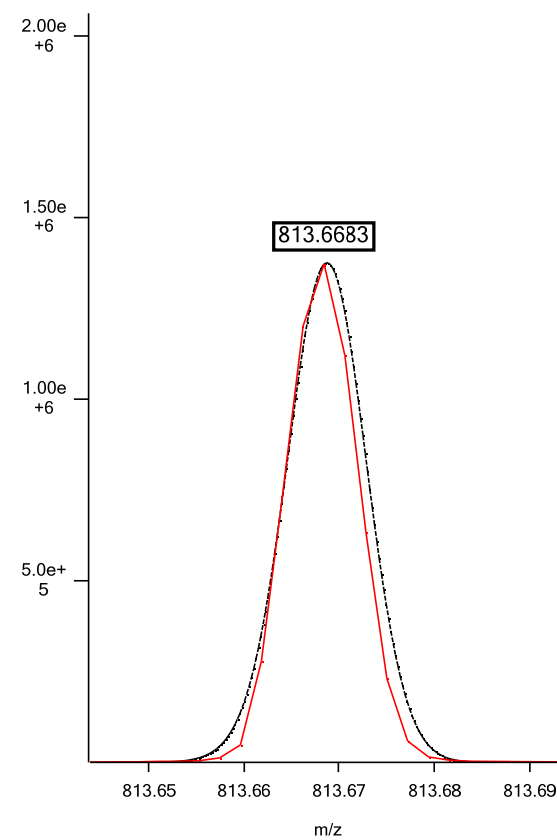
Isotope 1



Isotope 2

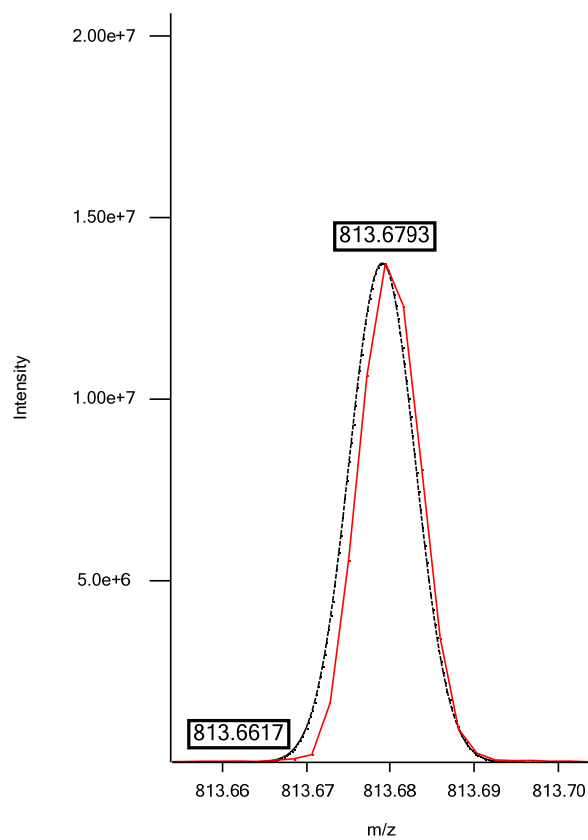


Isotope 3

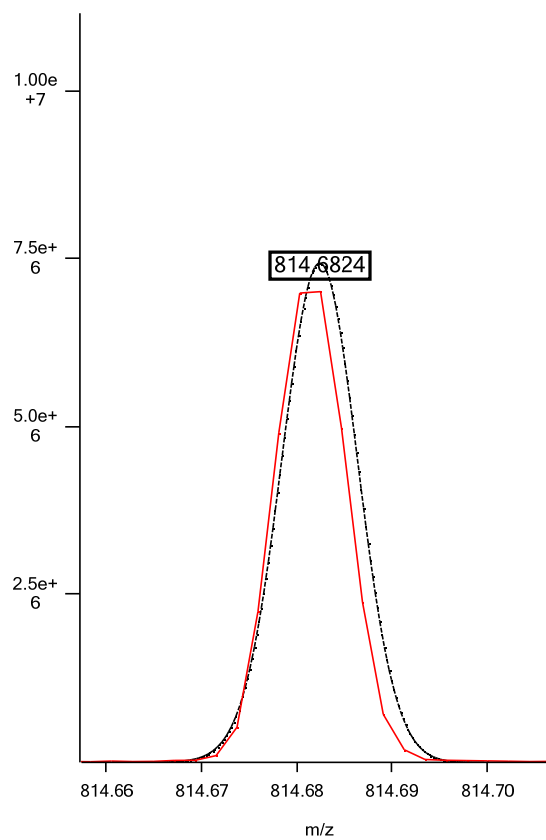


Positive ESI: SM d18:1/24:1; C₄₇H₉₄N₂O₆P; theoretical m/z 813.6849, (M+H)⁺; isotopic fit 0.0177

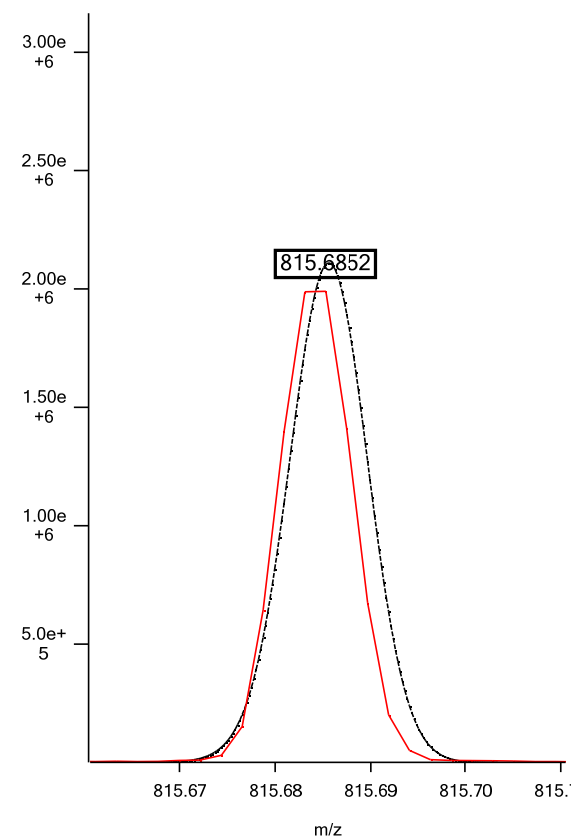
Isotope 1



Isotope 2

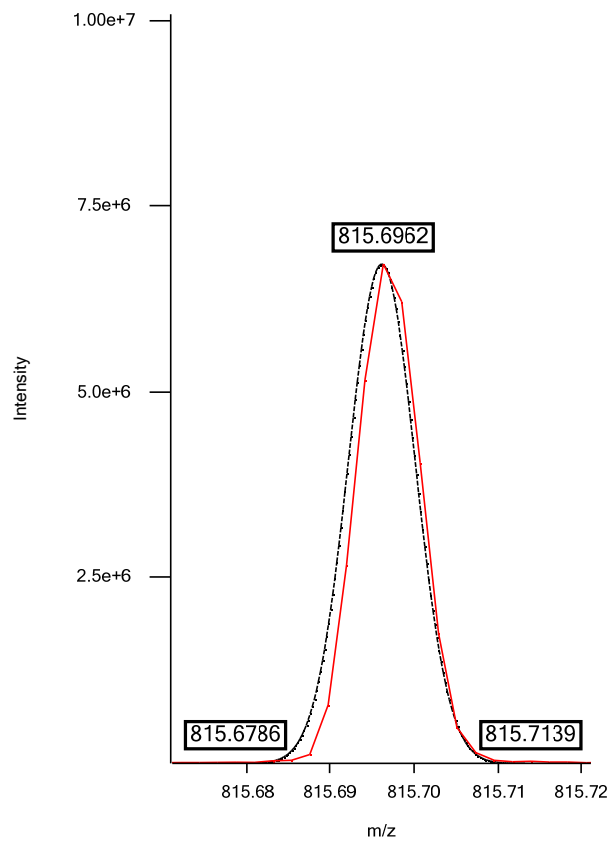


Isotope 3

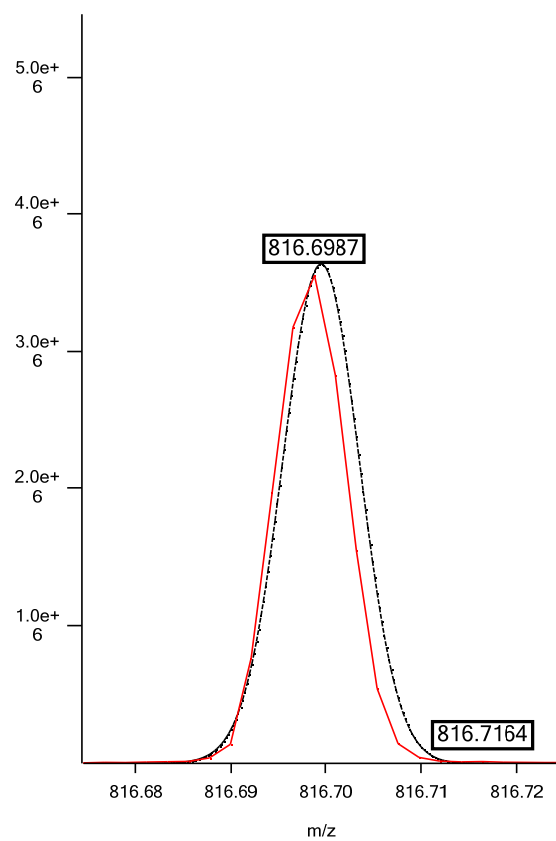


Positive ESI: SM d18:1/24:0; C₄₇H₉₆N₂O₆P; theoretical *m/z* 815.7006, (M+H)⁺; isotopic fit 0.0182

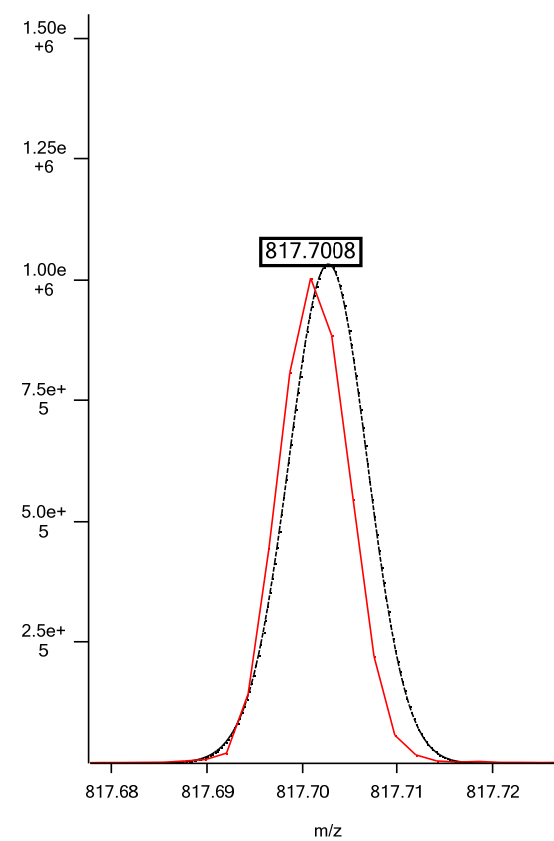
Isotope 1



Isotope 2

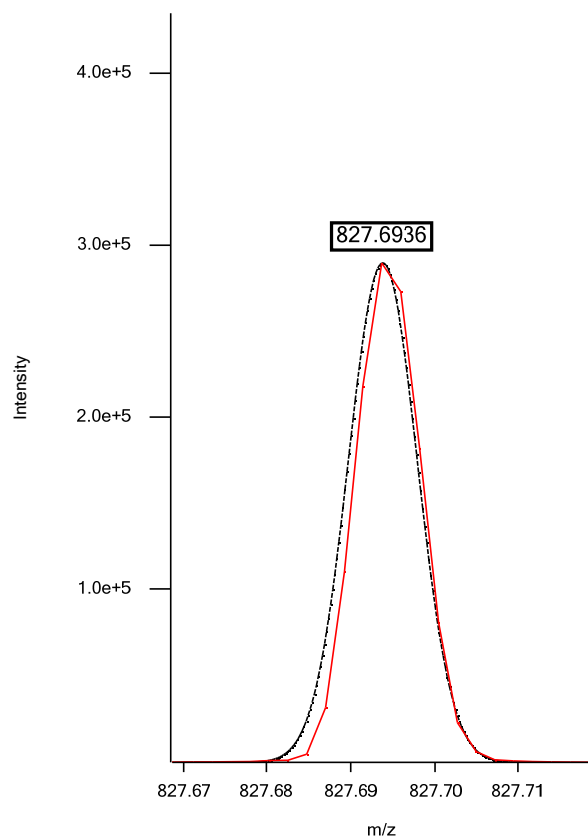


Isotope 3

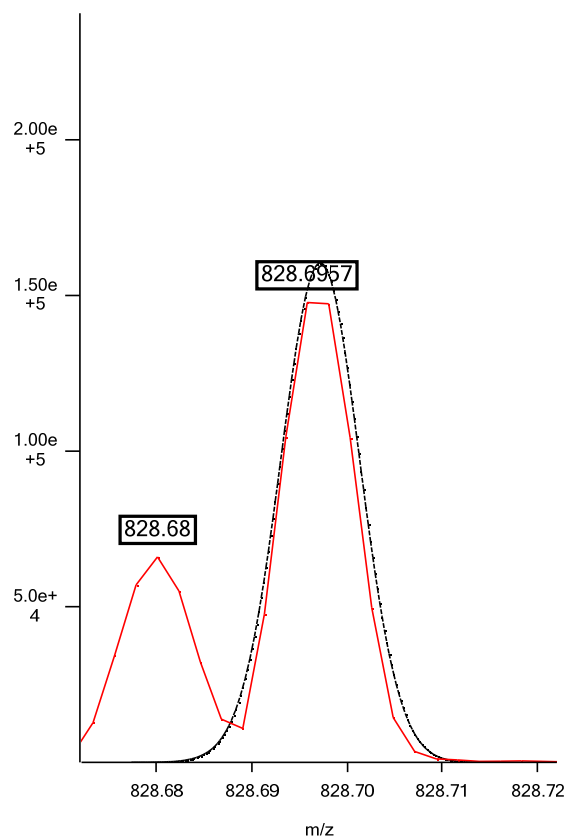


Positive ESI: SM d19:1/24:1; C₄₈H₉₆N₂O₆P; theoretical *m/z* 827.7006, (M+H)⁺; isotopic fit 0.0072

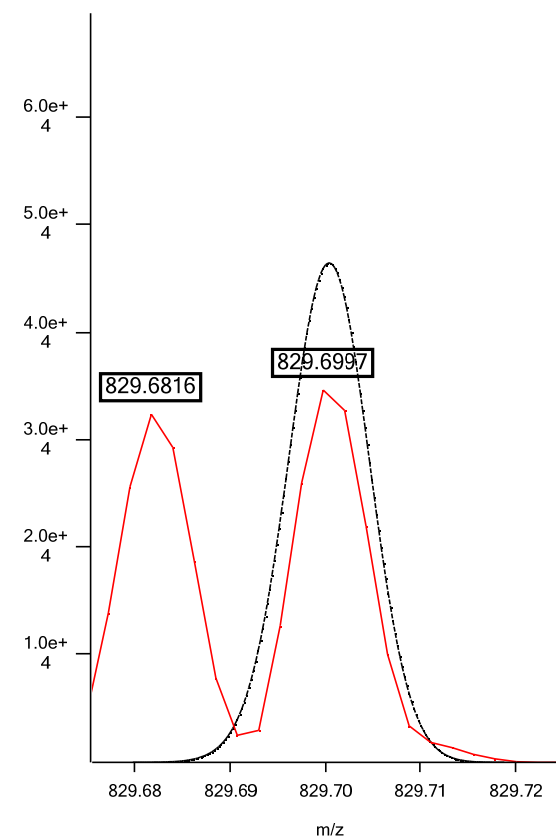
Isotope 1



Isotope 2

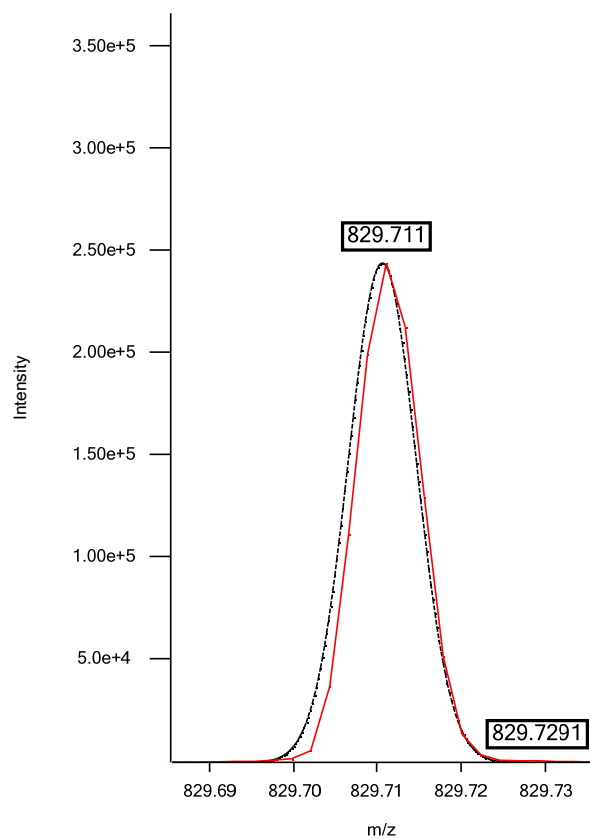


Isotope 3

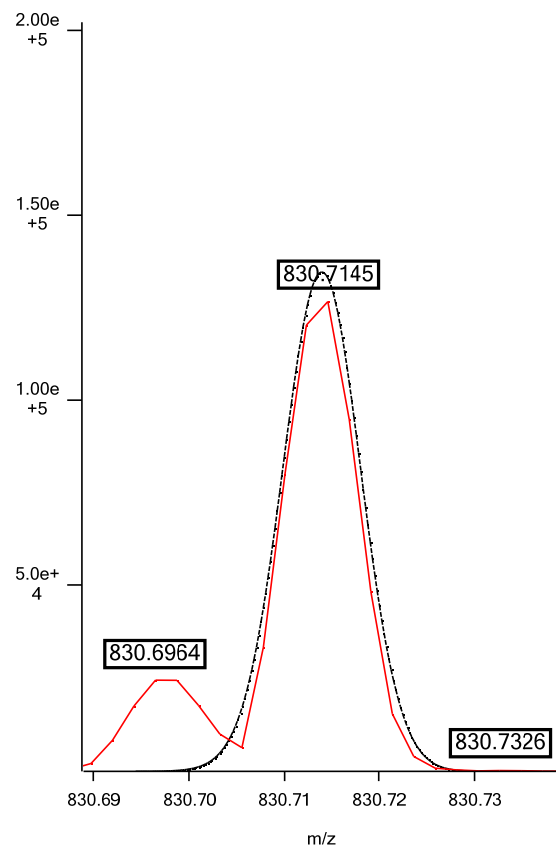


Positive ESI: SM d19:1/24:0; C₄₈H₉₈N₂O₆P; theoretical *m/z* 829.7163, (M+H)⁺; isotopic fit 0.0063

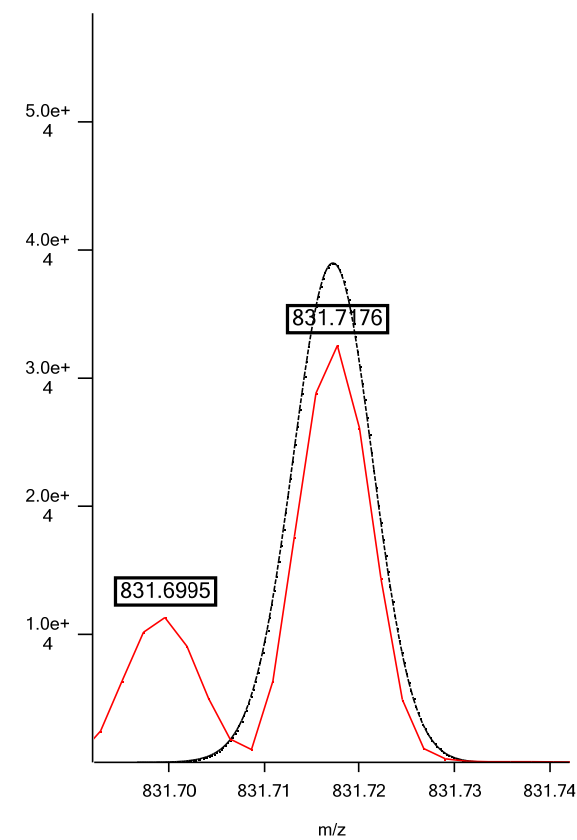
Isotope 1



Isotope 2

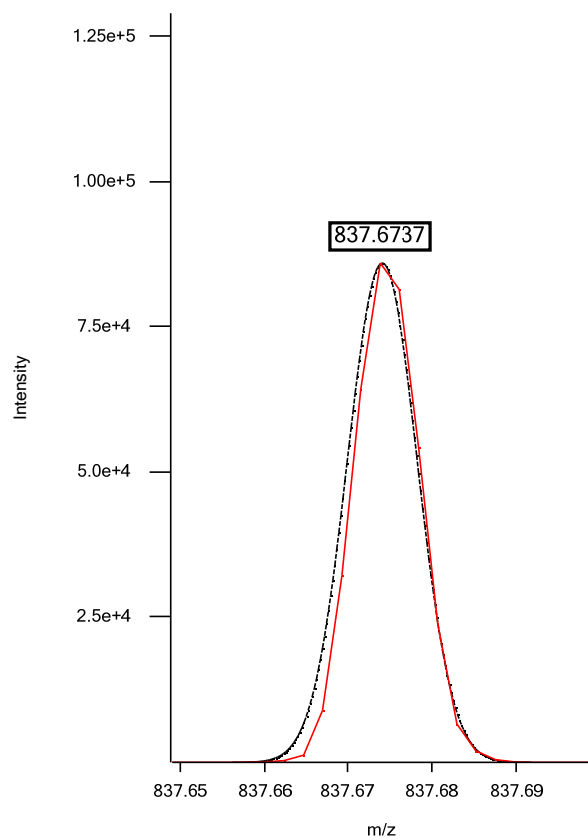


Isotope 3

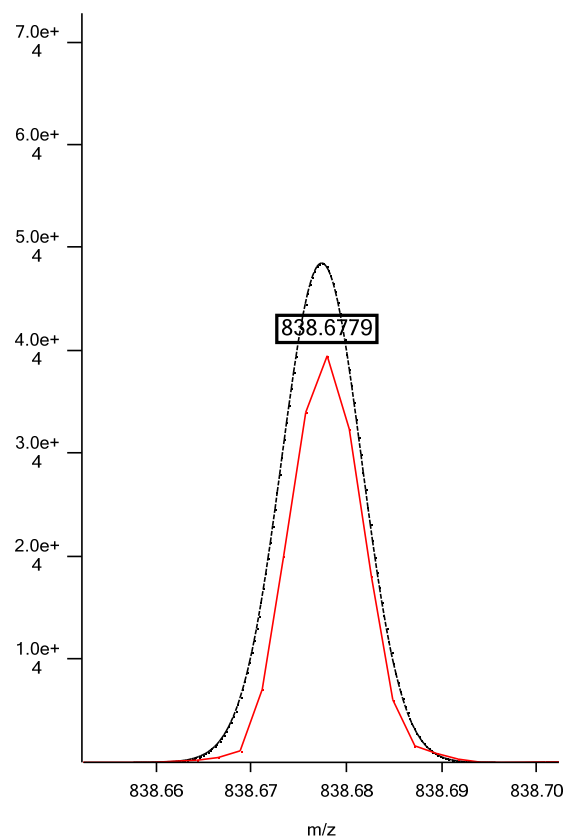


Positive ESI: SM d18:1/26:3; C₄₉H₉₄N₂O₆P; theoretical m/z 837.6849, (M+H)⁺; isotopic fit 0.0168

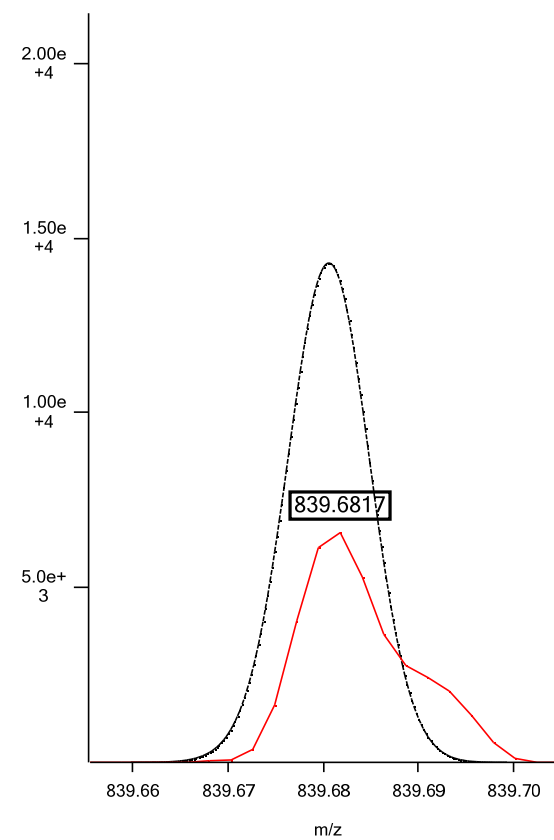
Isotope 1



Isotope 2

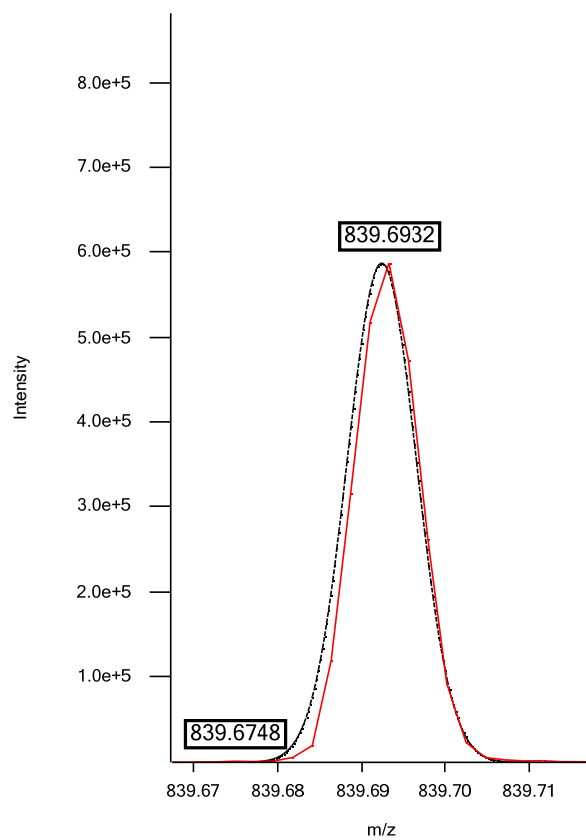


Isotope 3

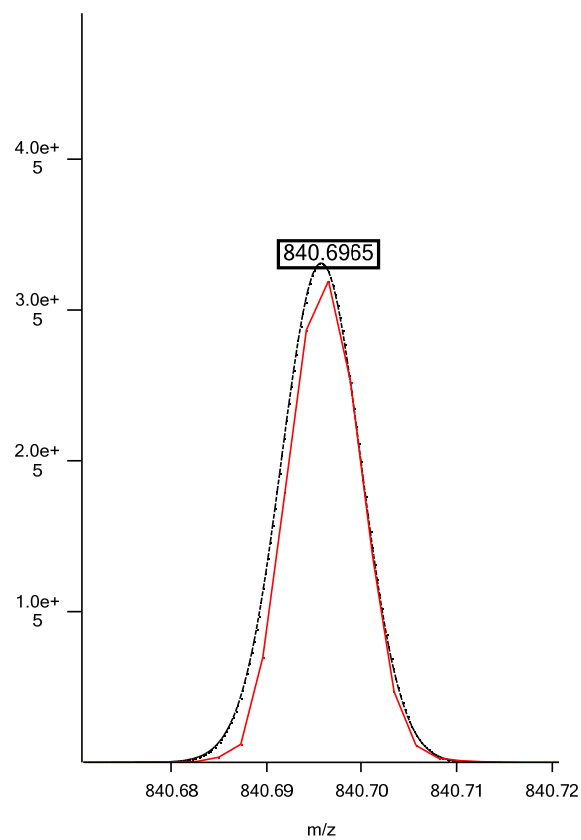


Positive ESI: SM d18:1/26:2; C₄₉H₉₆N₂O₆P; theoretical m/z 839.7006, (M+H)⁺; isotopic fit 0.0076

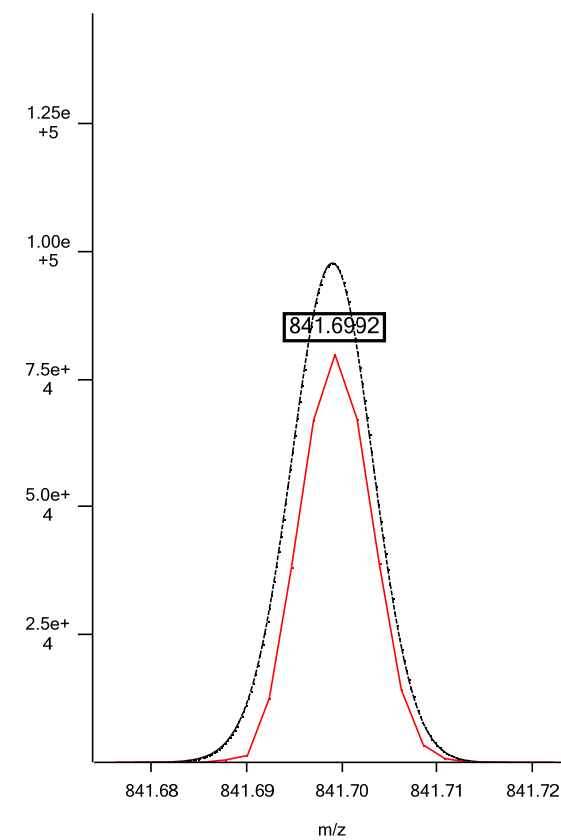
Isotope 1



Isotope 2

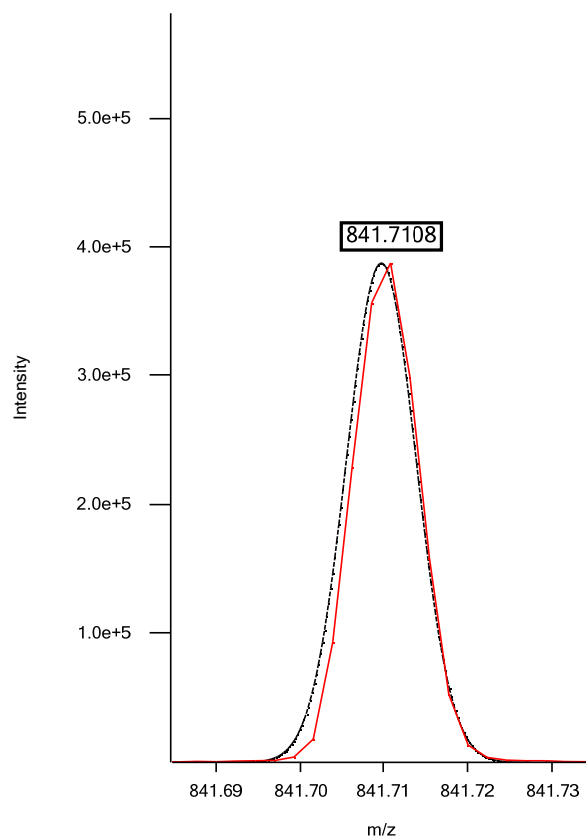


Isotope 3

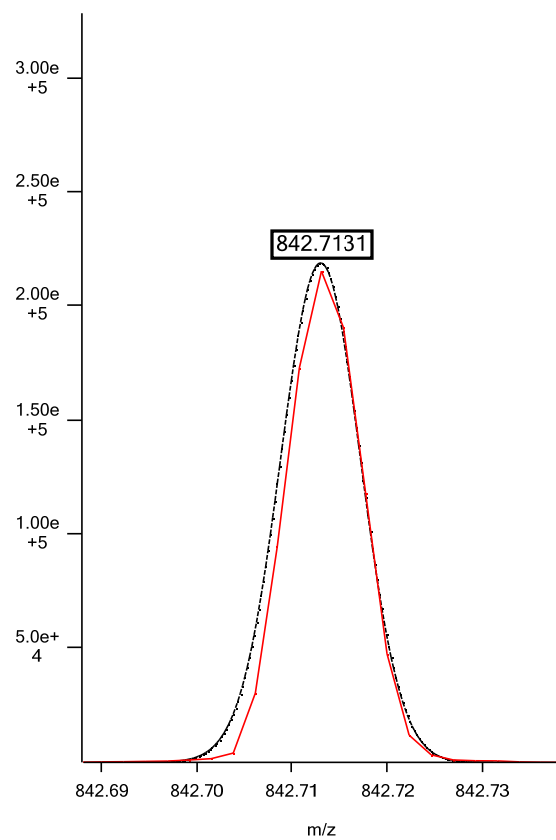


Positive ESI: SM d18:1/26:1; C₄₉H₉₈N₂O₆P; theoretical m/z 841.7163, (M+H)⁺; isotopic fit 0.0043

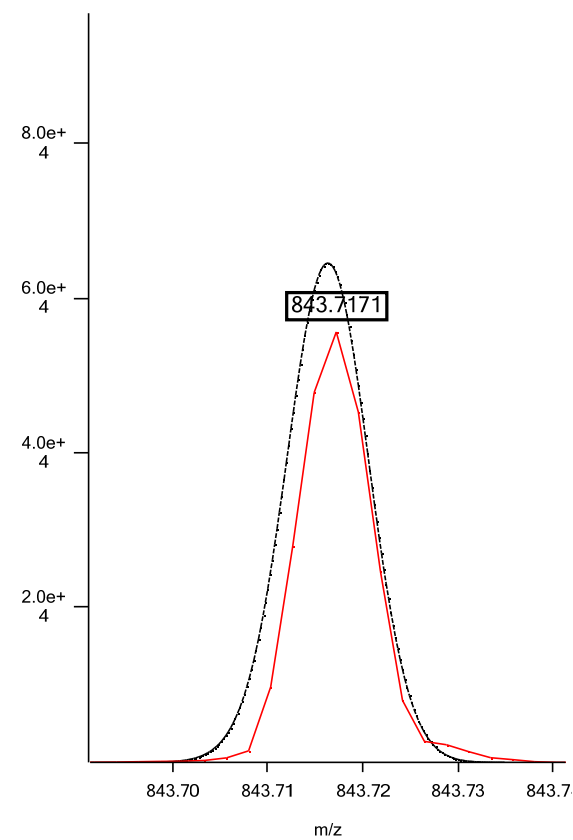
Isotope 1



Isotope 2

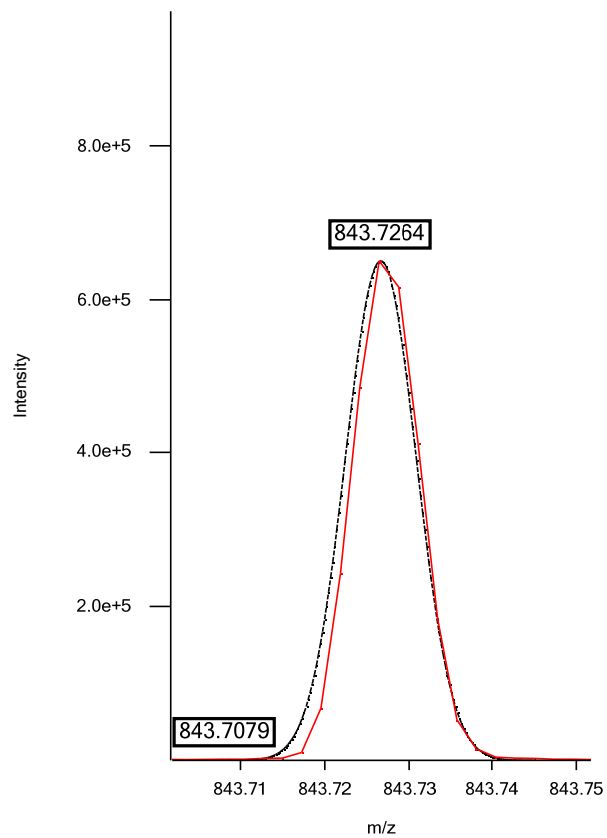


Isotope 3

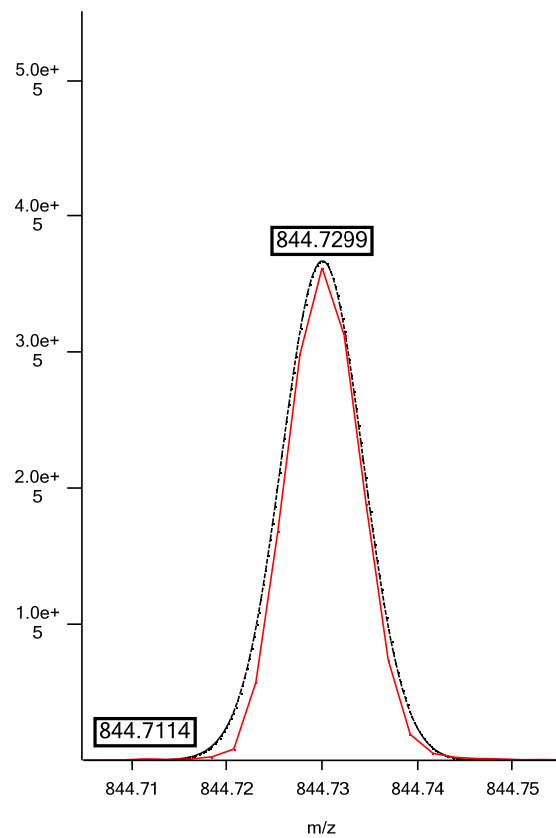


Positive ESI: SM d18:1/26:0; C₄₉H₁₀₀N₂O₆P; theoretical m/z 843.7319, (M+H)⁺; isotopic fit 0.0039

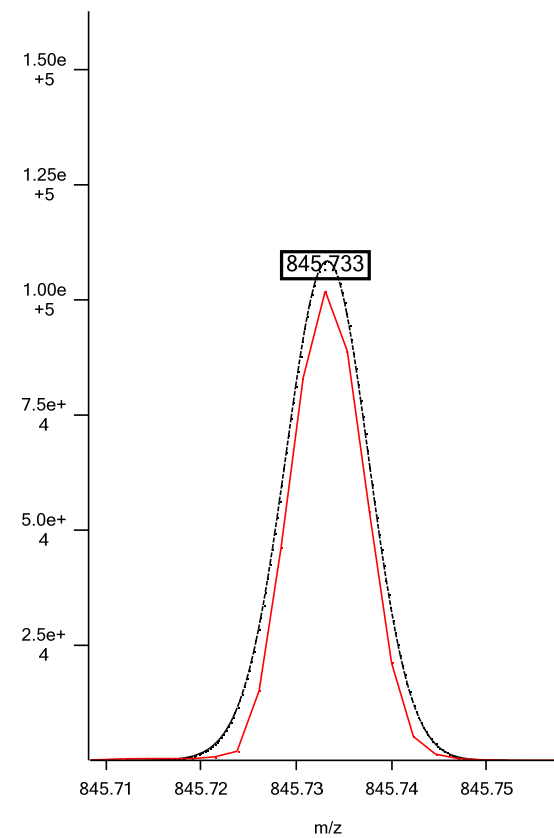
Isotope 1



Isotope 2



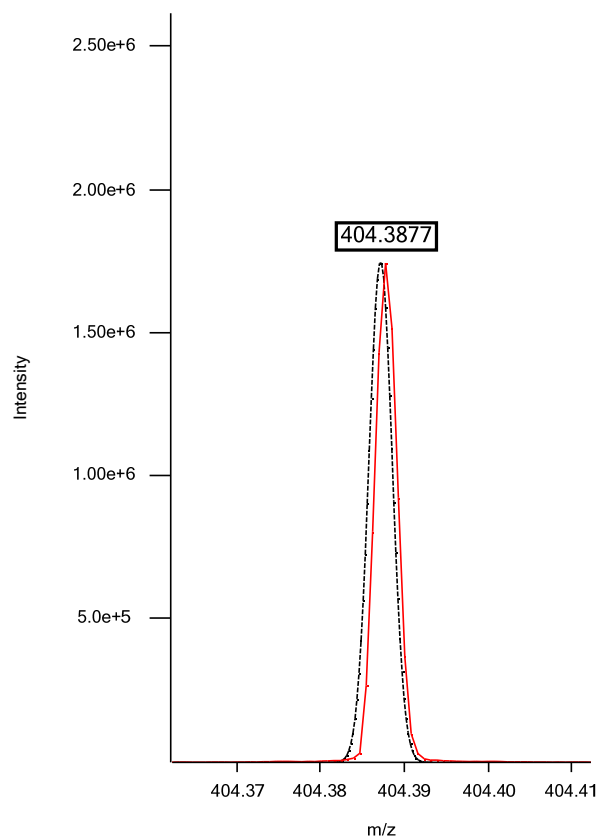
Isotope 3



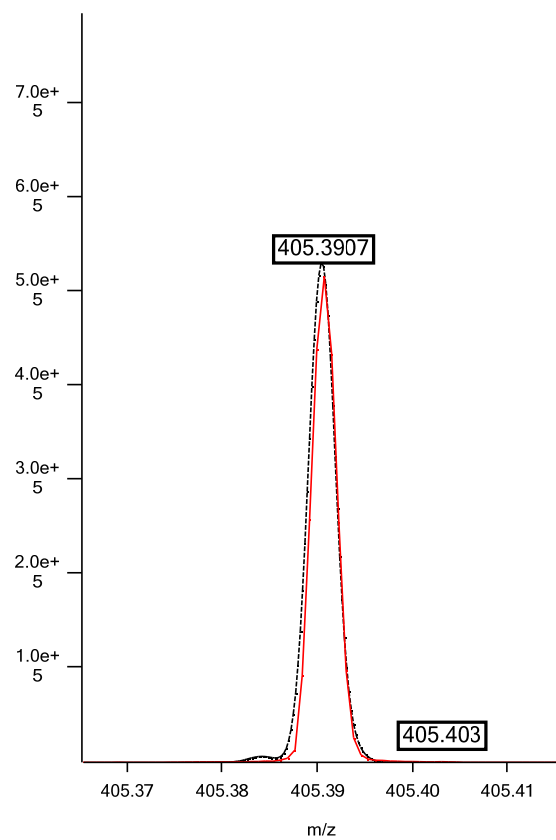
Cholesterol esters

Positive ESI: Cholesterol; C₂₇H₅₀NO; theoretical *m/z* 404.3892, (M+NH₄)⁺; isotopic fit 0.0406

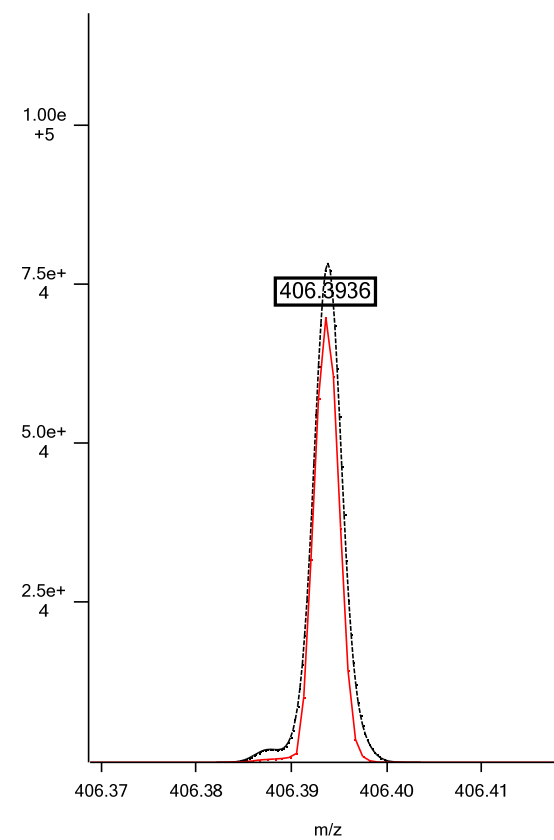
Isotope 1



Isotope 2

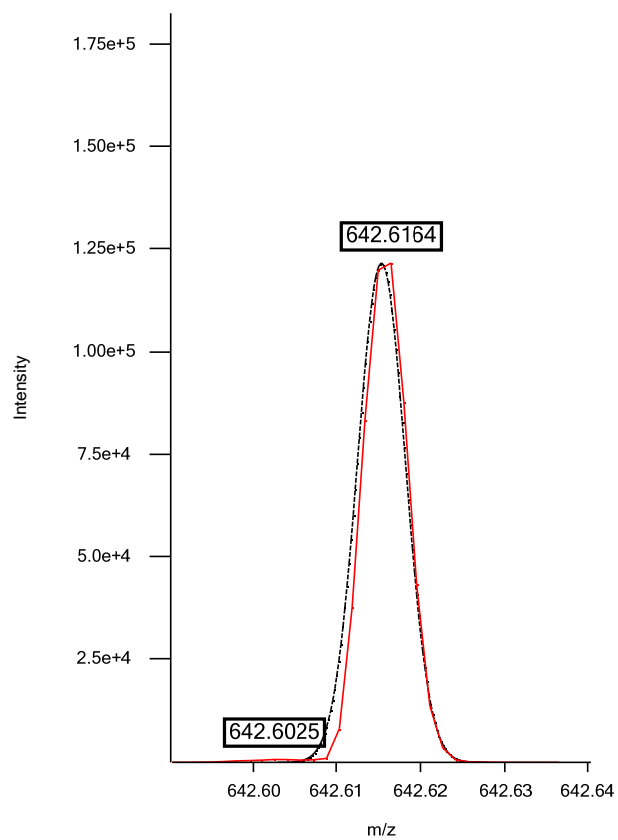


Isotope 3

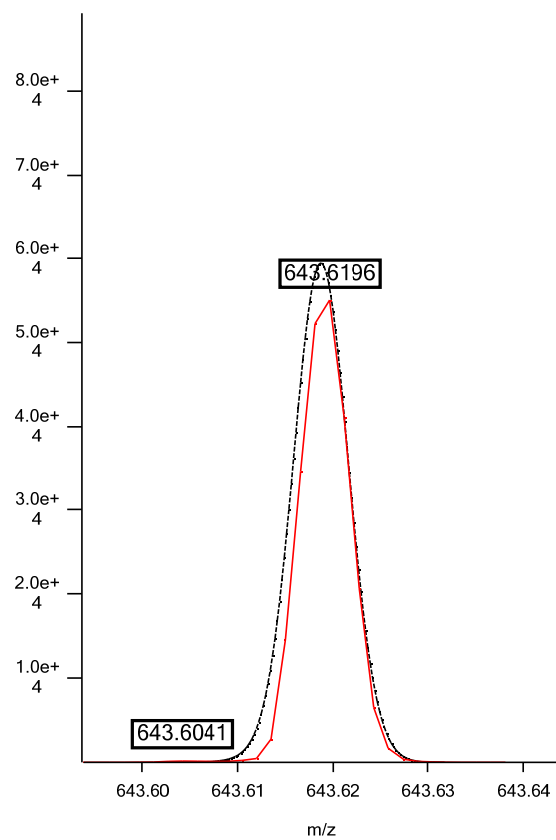


Positive ESI: CE 16:0; C₄₃H₈₀NO₂; theoretical m/z 642.6189, (M+NH₄)⁺; isotopic fit 0.0046

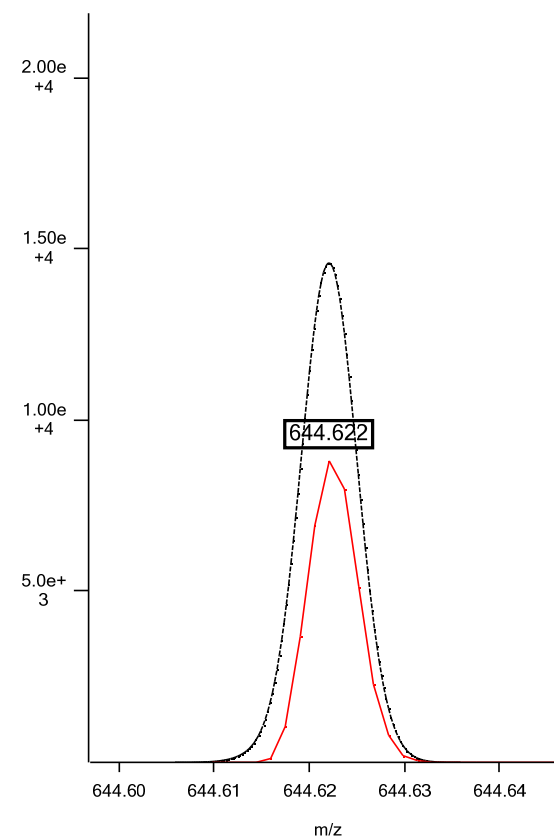
Isotope 1



Isotope 2

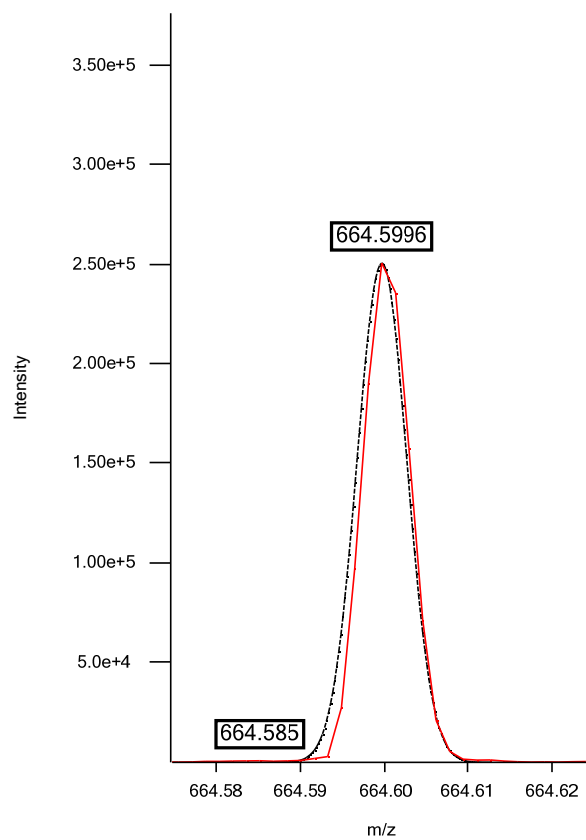


Isotope 3

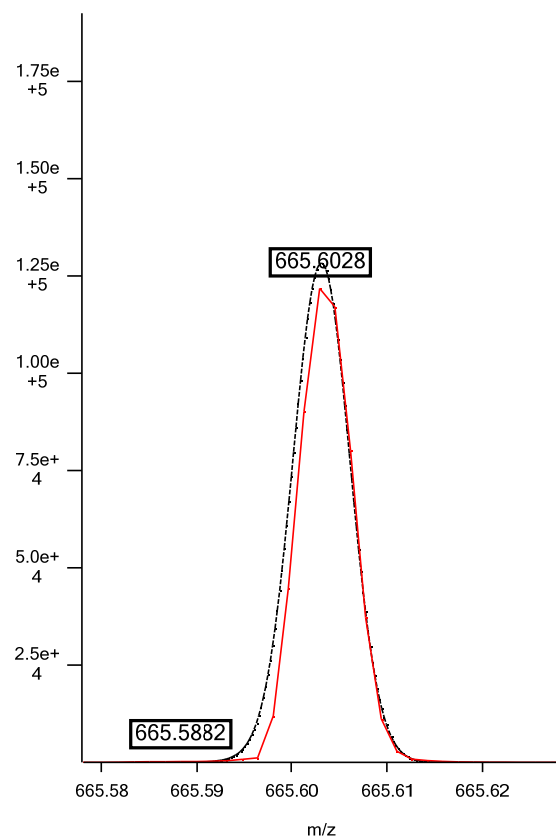


Positive ESI: CE 18:3; C₄₅H₇₈NO₂; theoretical m/z 664.6032, (M+NH₄)⁺; isotopic fit 0.0058

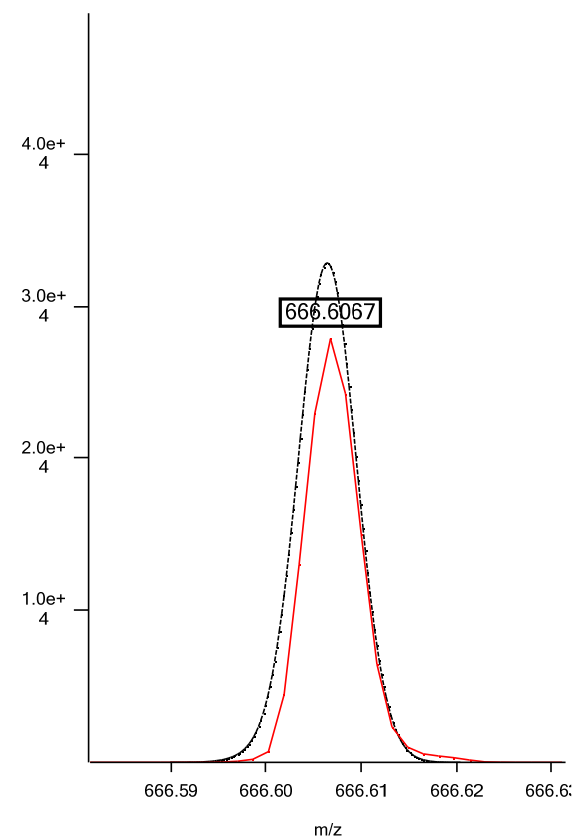
Isotope 1



Isotope 2

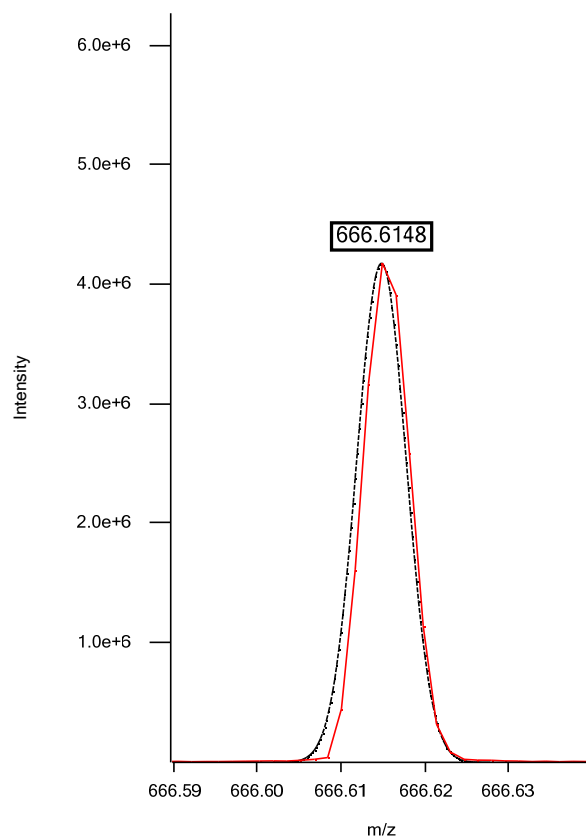


Isotope 3

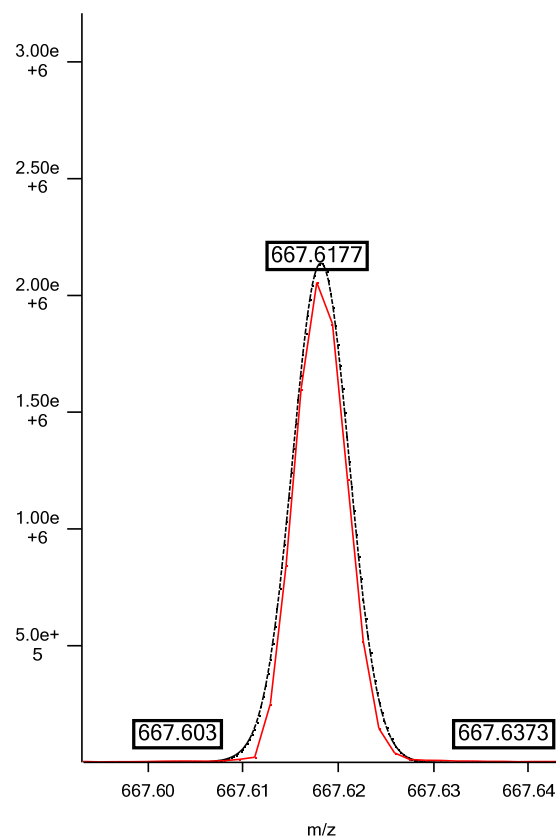


Positive ESI: CE 18:2; C₄₅H₈₀NO₂; theoretical *m/z* 666.6189, (M+NH₄)⁺; isotopic fit 0.0139

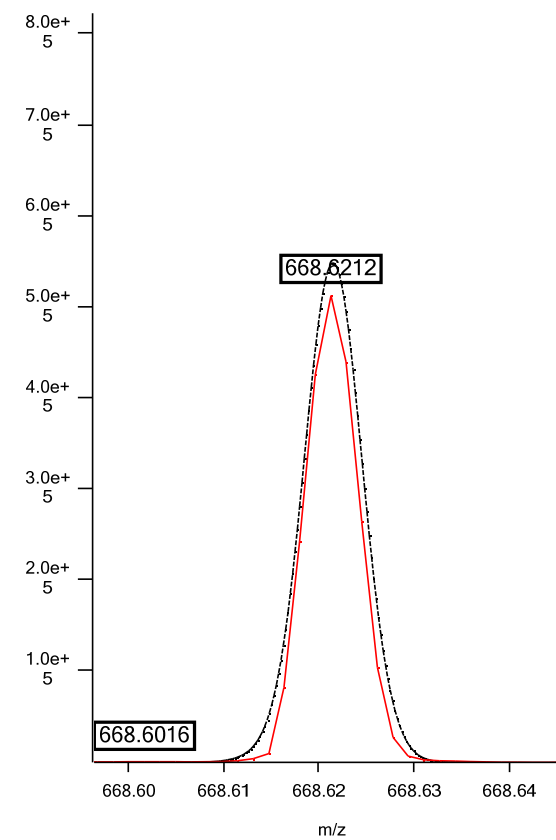
Isotope 1



Isotope 2

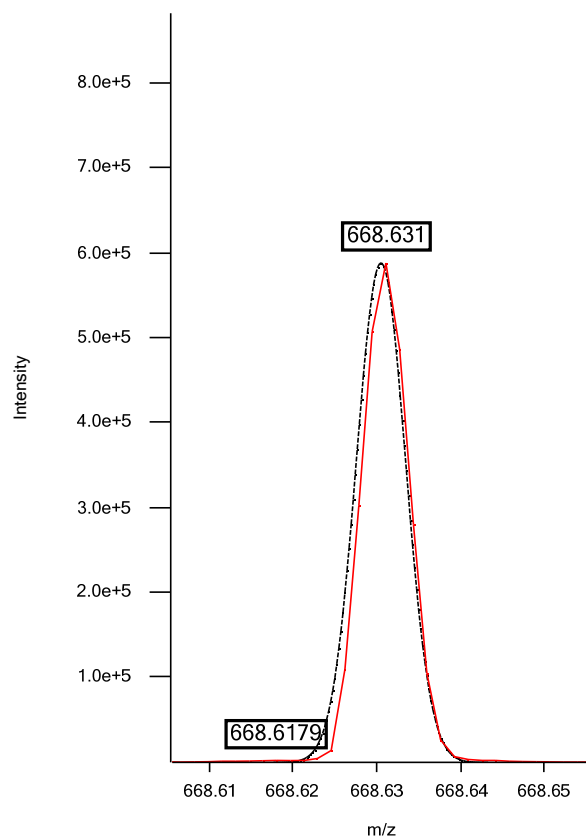


Isotope 3

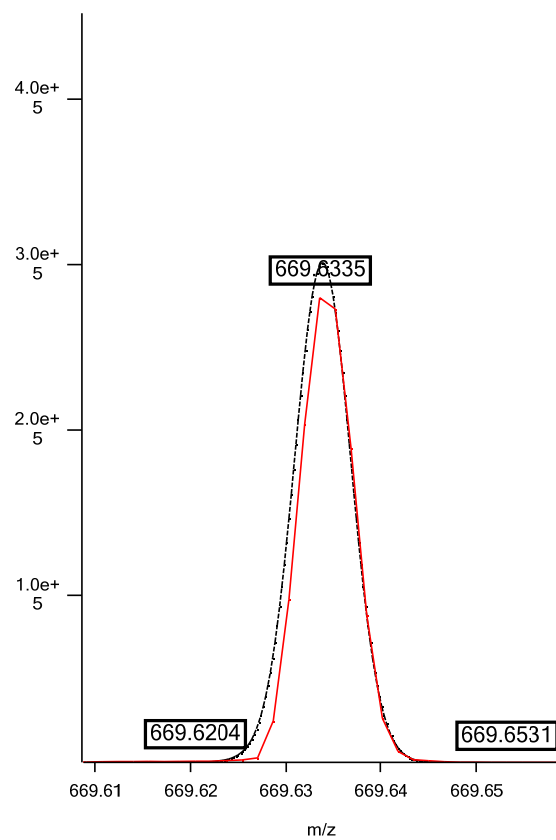


Positive ESI: CE 18:1; C₄₅H₈₂NO₂; theoretical *m/z* 668.6345, (M+NH₄)⁺; isotopic fit 0.0066

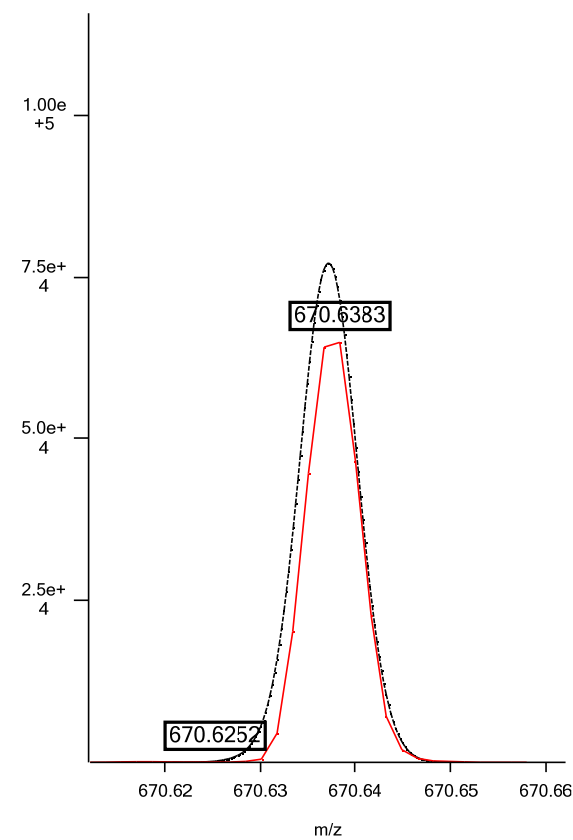
Isotope 1



Isotope 2

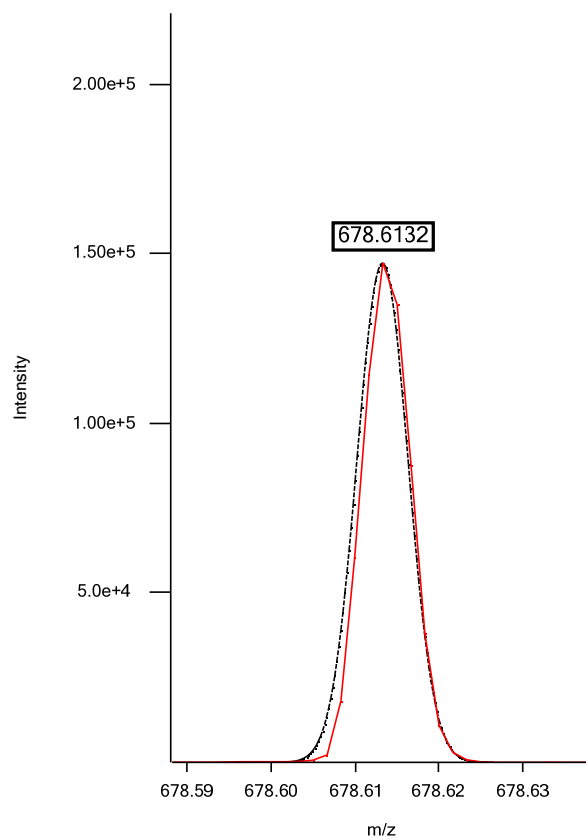


Isotope 3

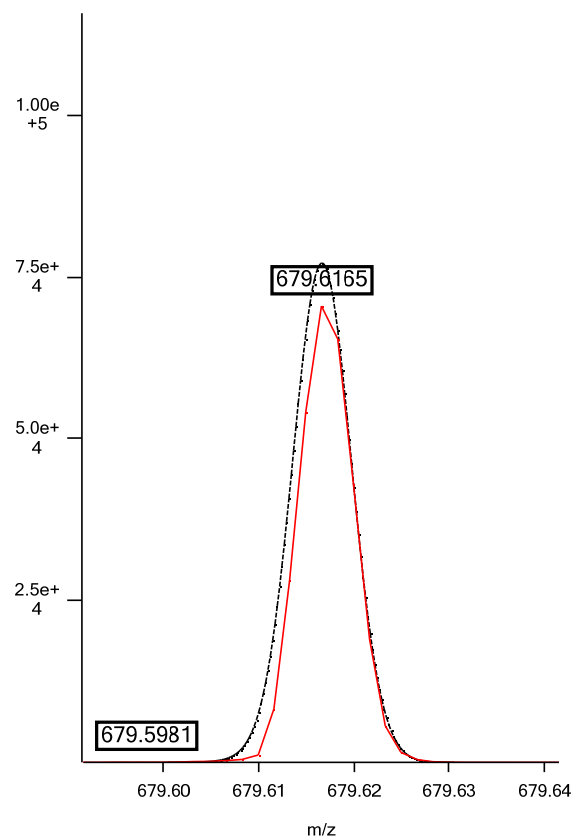


Positive ESI: CE 19:3; C₄₆H₈₀NO₂; theoretical *m/z* 678.6189, (M+NH₄)⁺; isotopic fit 0.0062

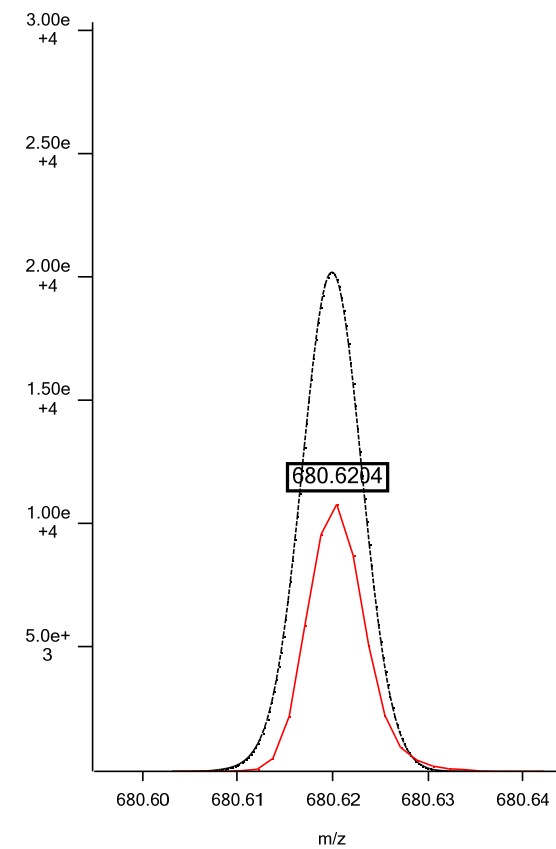
Isotope 1



Isotope 2

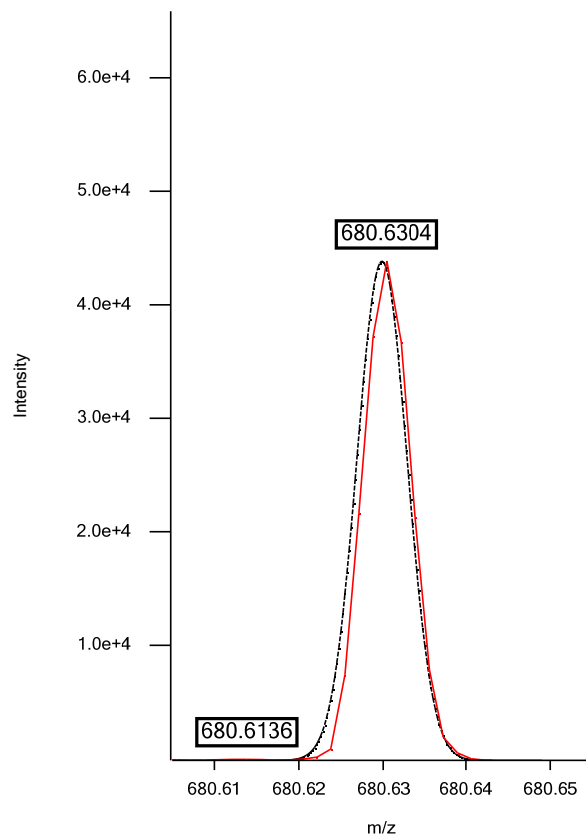


Isotope 3

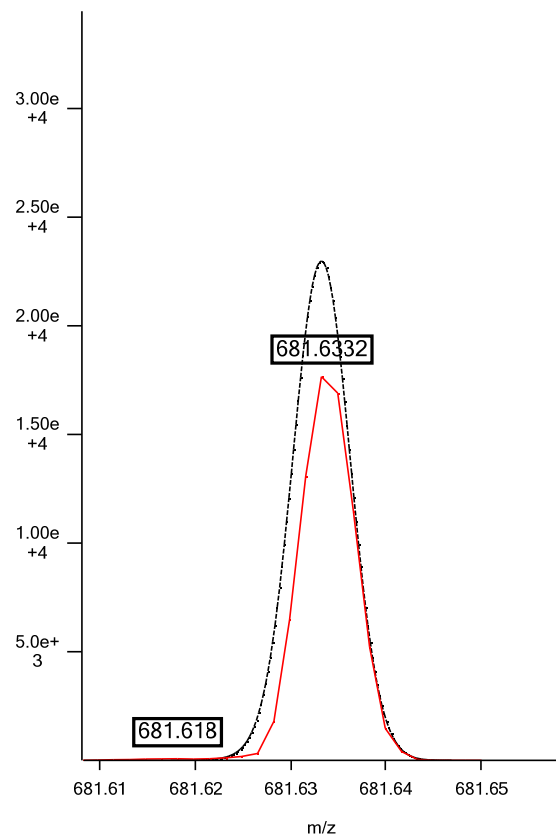


Positive ESI: CE 19:2; C₄₆H₈₂NO₂; theoretical *m/z* 680.6345, (M+NH₄)⁺; isotopic fit 0.0180

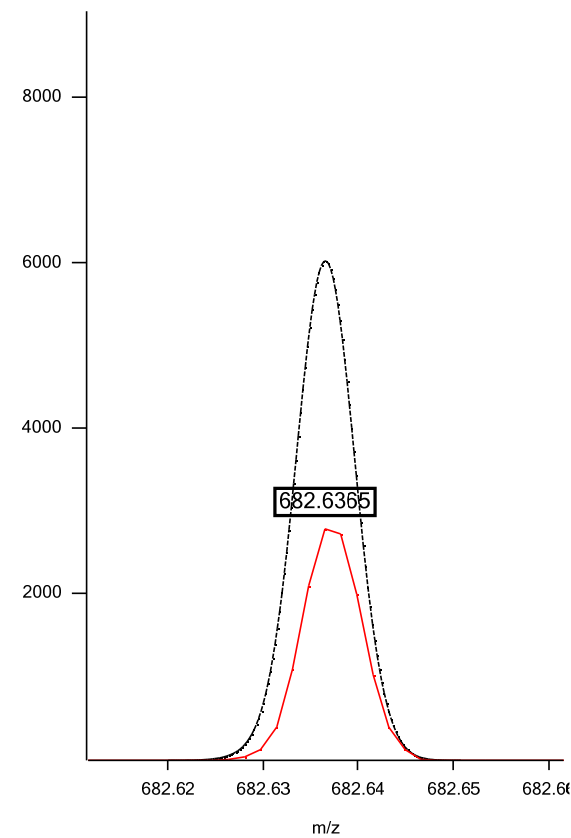
Isotope 1



Isotope 2

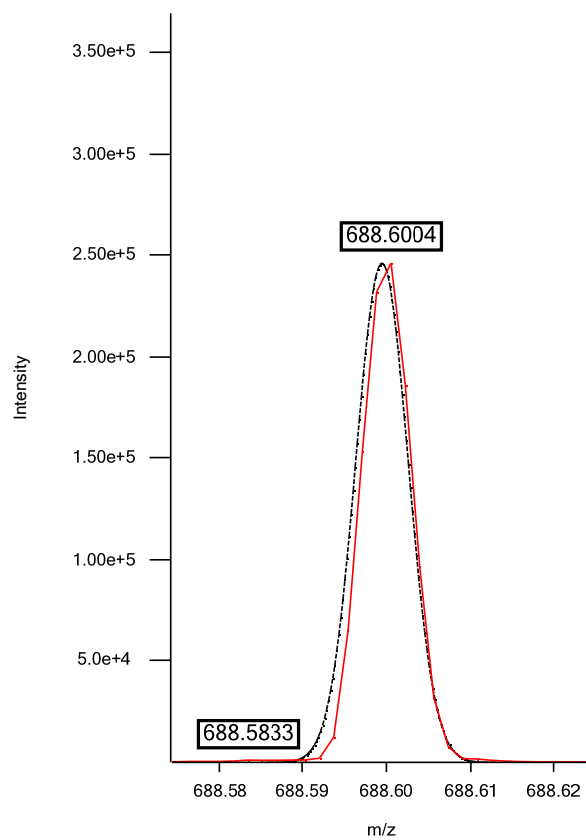


Isotope 3

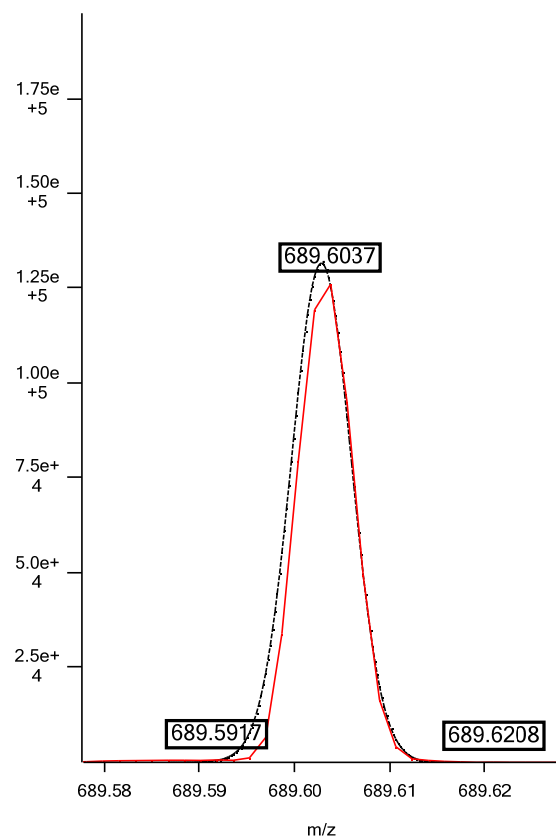


Positive ESI: CE 20:5; C₄₇H₇₈NO₂; theoretical *m/z* 688.6032, (M+NH₄)⁺; isotopic fit 0.0044

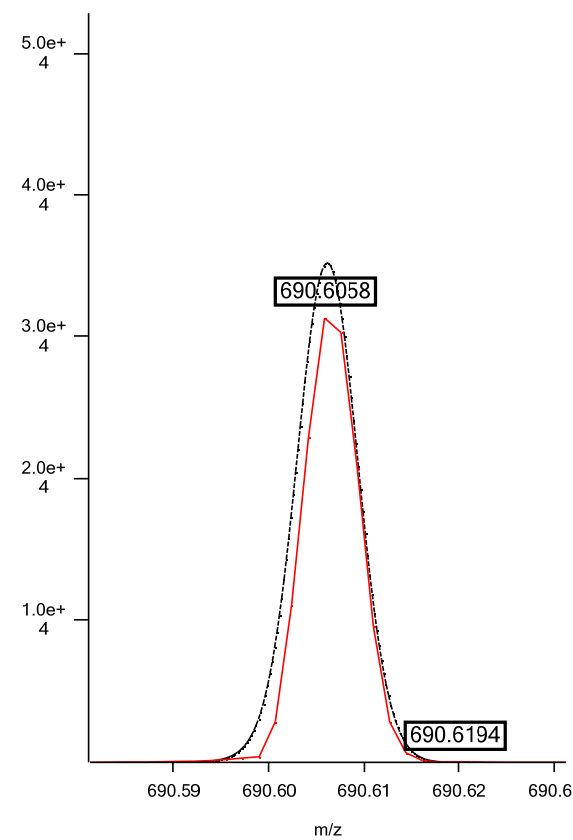
Isotope 1



Isotope 2

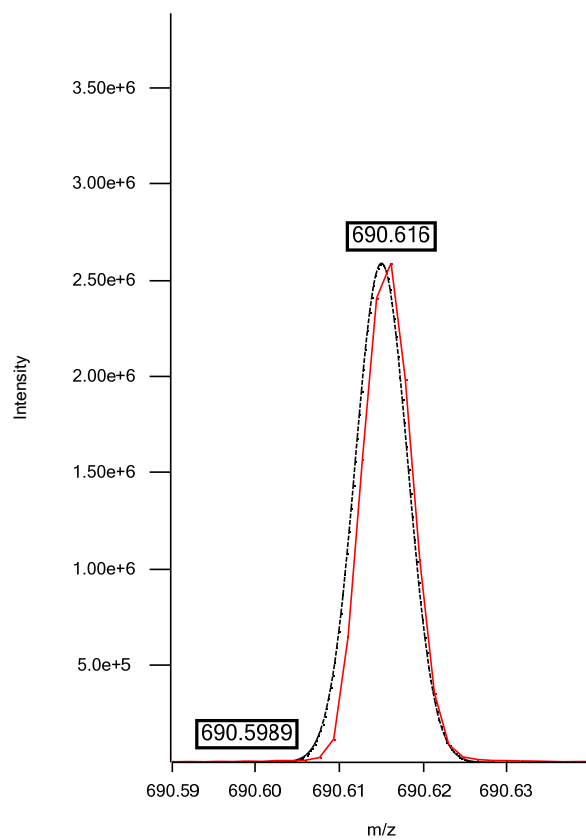


Isotope 3

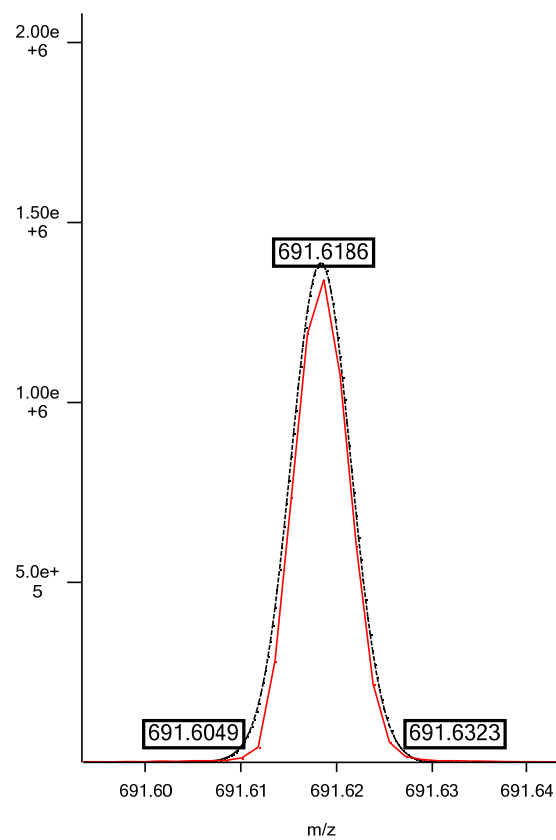


Positive ESI: CE 20:4; C₄₇H₈₀NO₂; theoretical *m/z* 690.6189, (M+NH₄)⁺; isotopic fit 0.0056

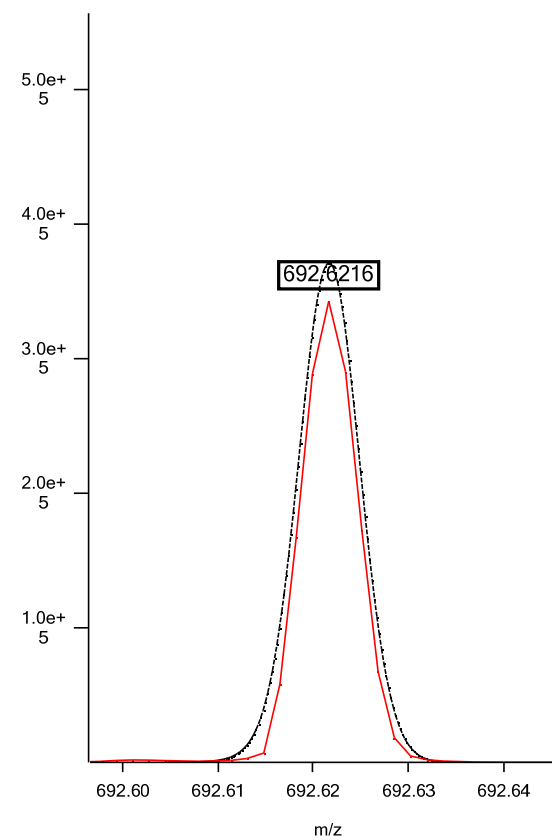
Isotope 1



Isotope 2

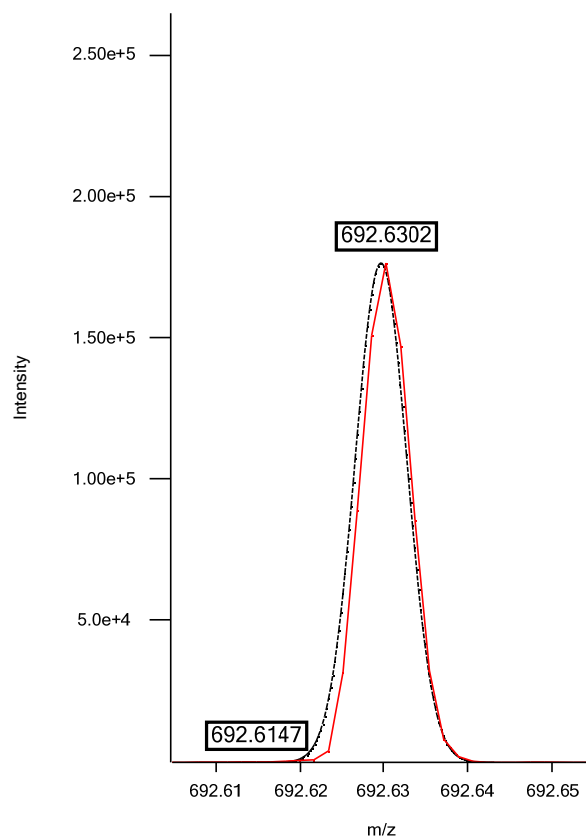


Isotope 3

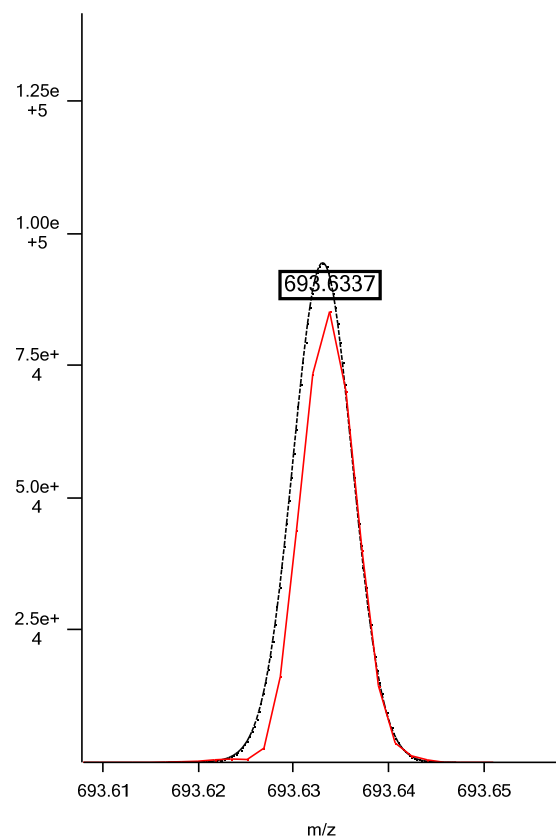


Positive ESI: CE 20:3; C₄₇H₈₂NO₂; theoretical *m/z* 692.6345, (M+NH₄)⁺; isotopic fit 0.0049

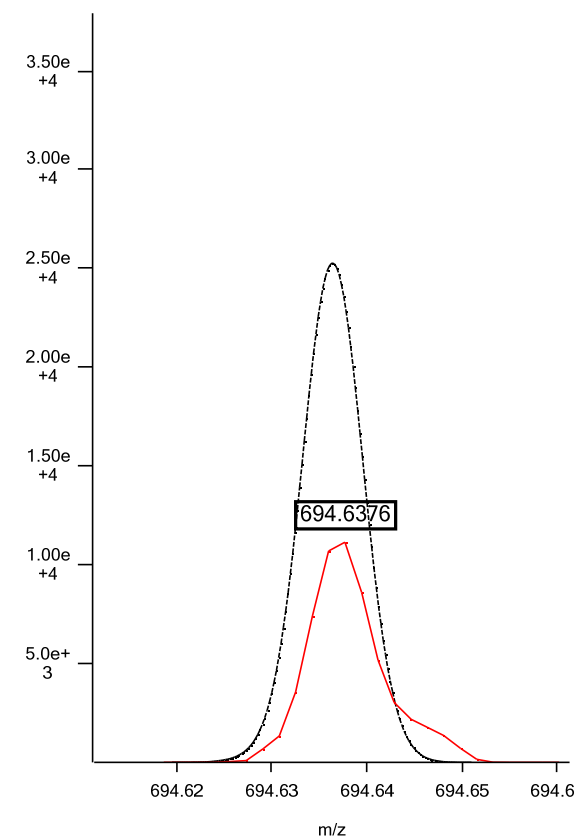
Isotope 1



Isotope 2

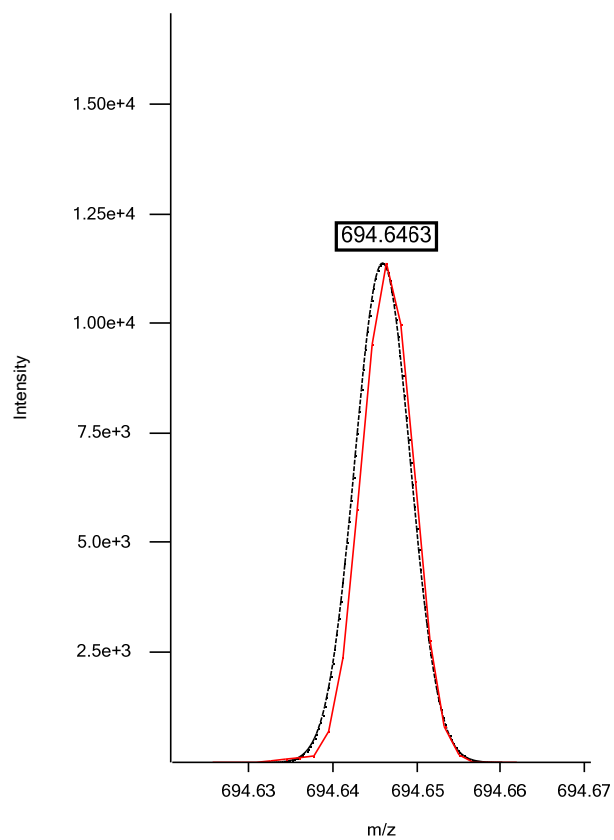


Isotope 3

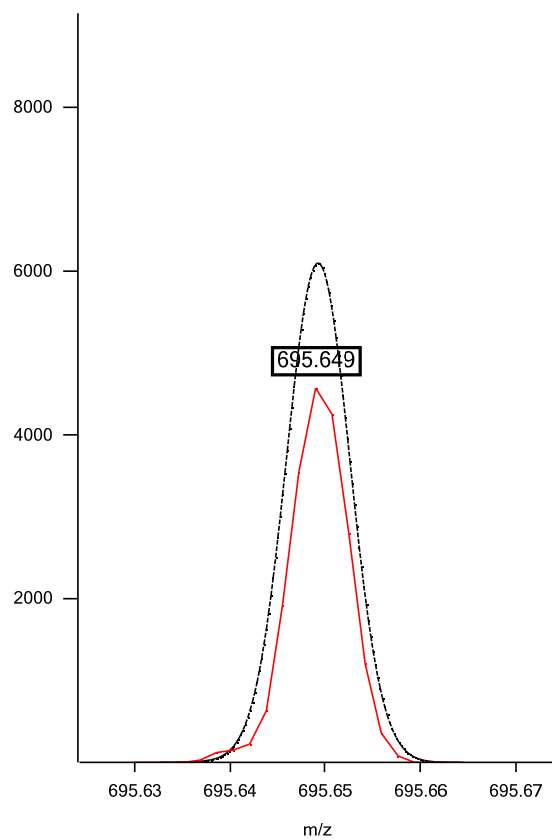


Positive ESI: CE 20:2; C₄₇H₈₄NO₂; theoretical m/z 694.6502, (M+NH₄)⁺; isotopic fit 0.0203

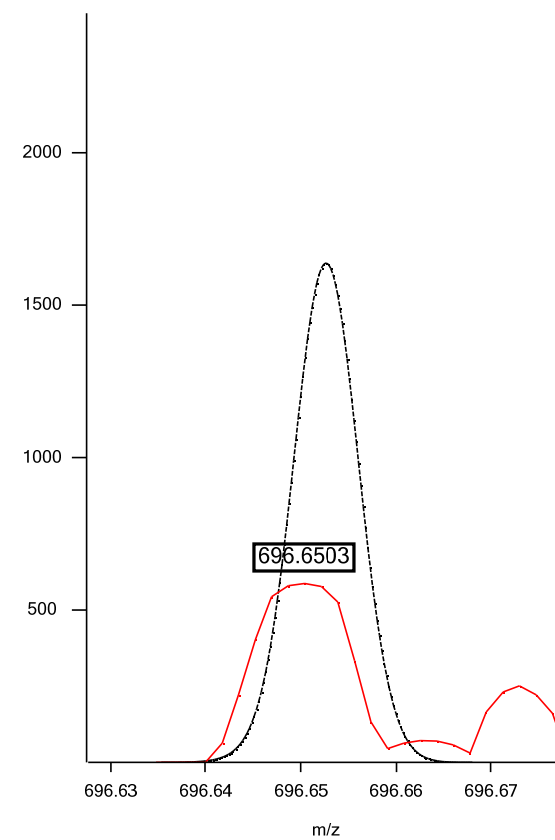
Isotope 1



Isotope 2

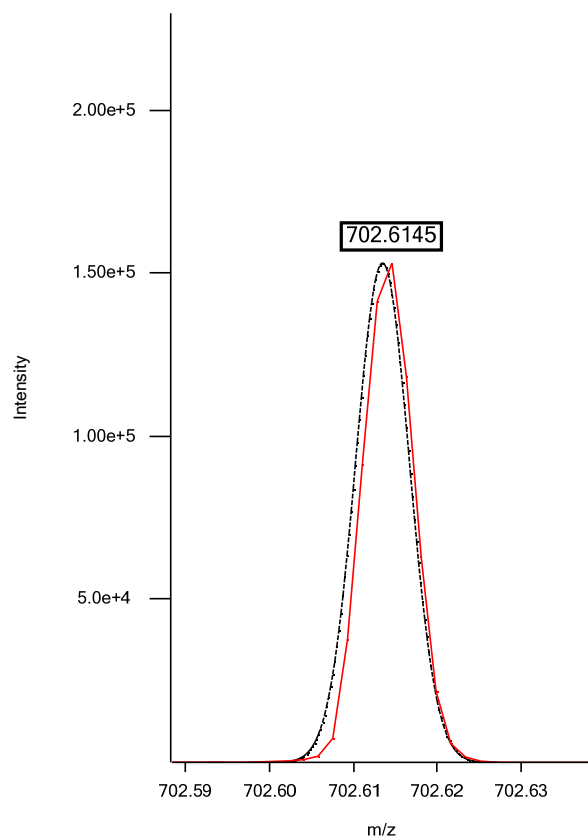


Isotope 3

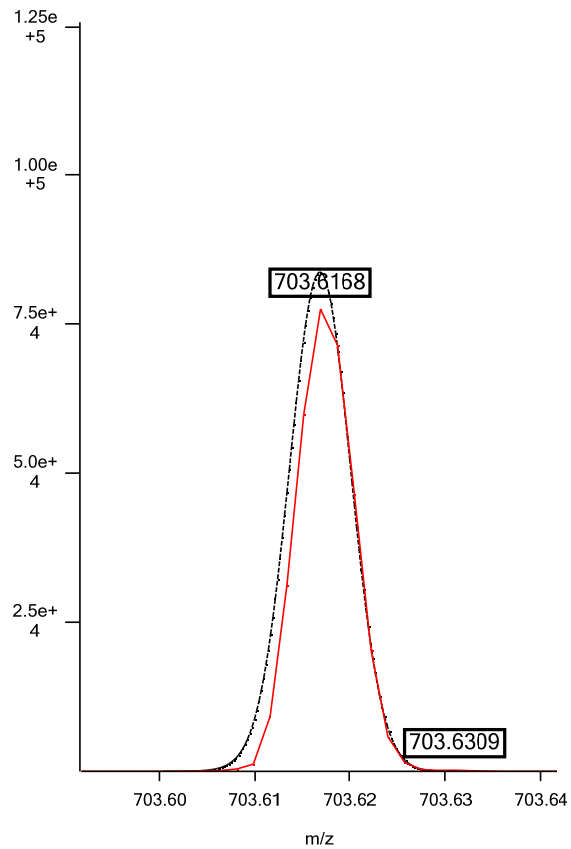


Positive ESI: CE 21:5; C₄₈H₈₀NO₂; theoretical m/z 702.6189, (M+NH₄)⁺; isotopic fit 0.0091

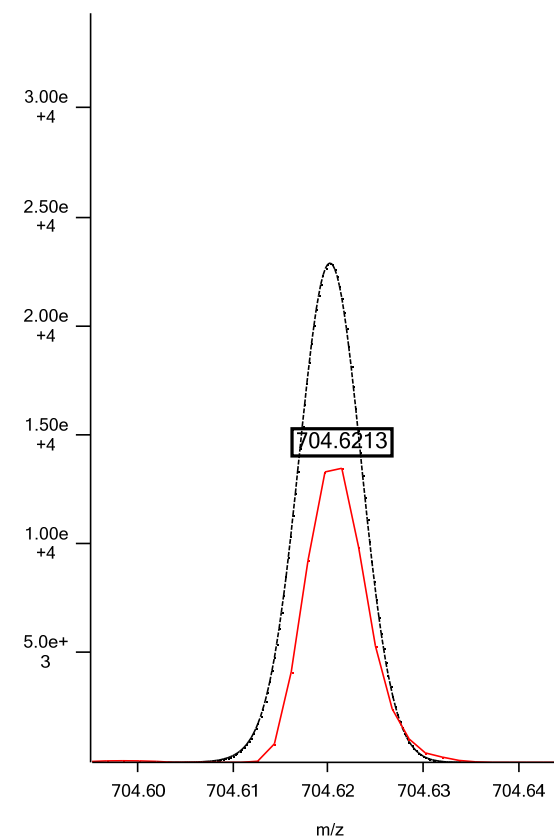
Isotope 1



Isotope 2

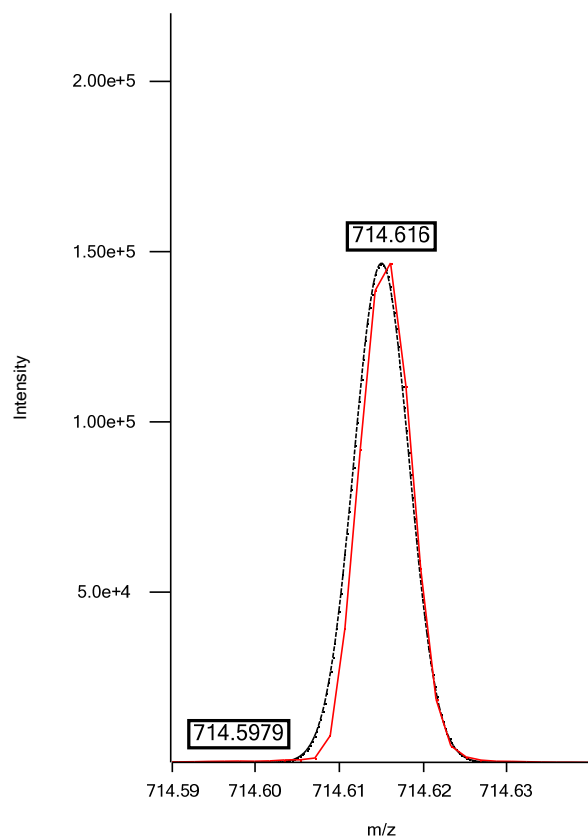


Isotope 3

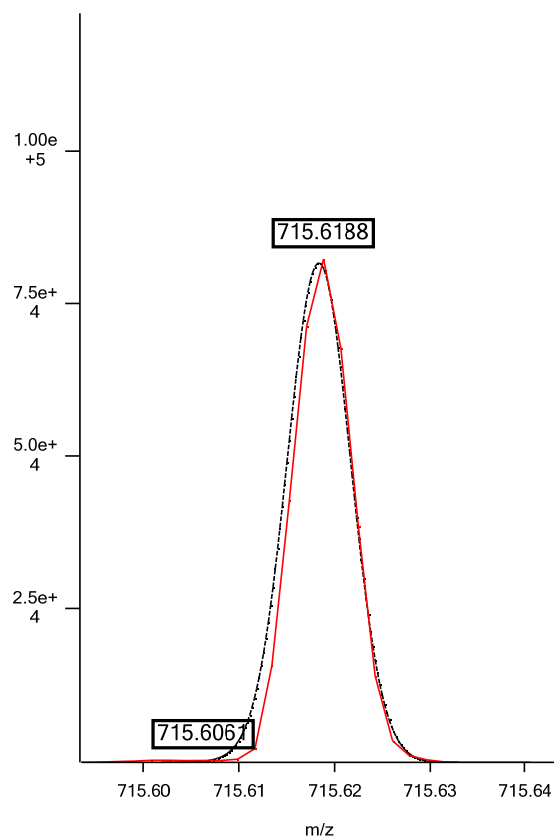


Positive ESI: CE 22:6; C₄₉H₈₀NO₂; theoretical m/z 714.6189, (M+NH₄)⁺; isotopic fit 0.0033

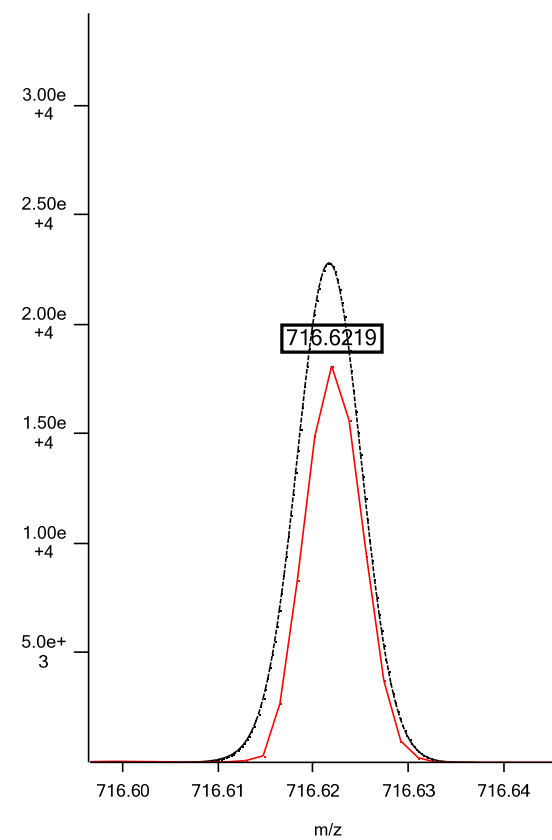
Isotope 1



Isotope 2

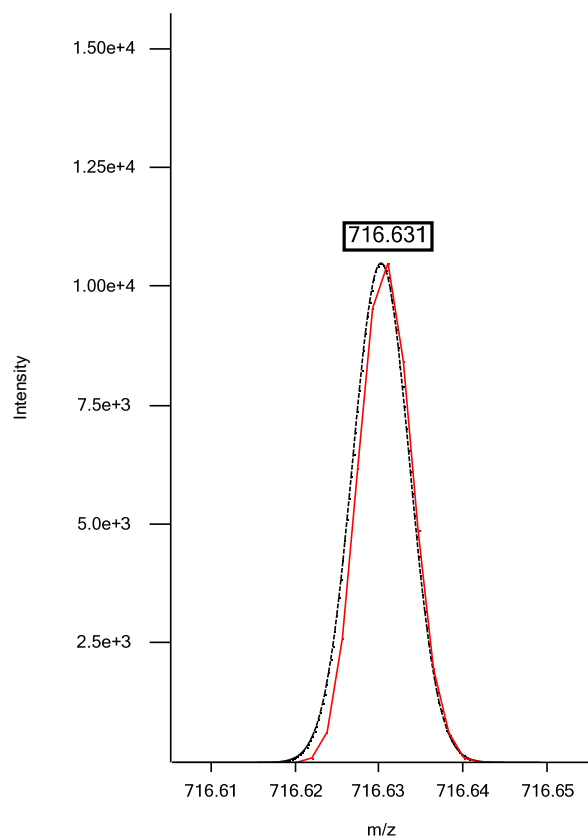


Isotope 3

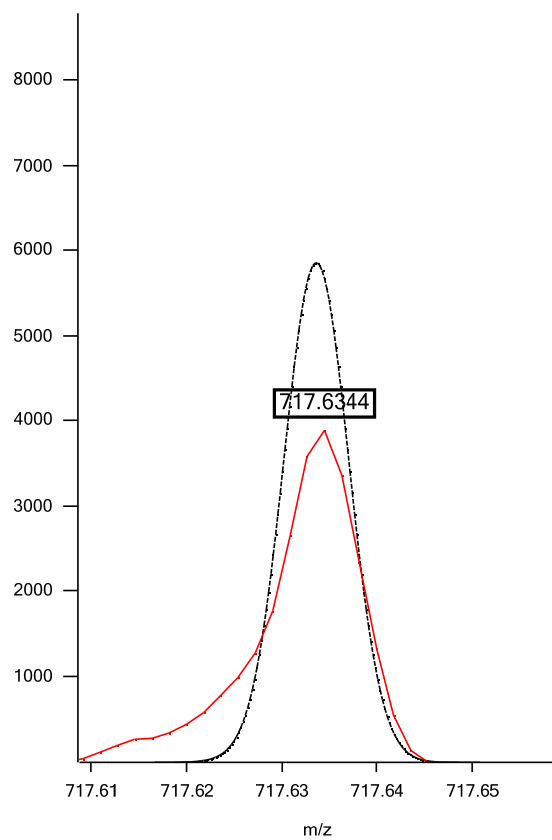


Positive ESI: CE 22:5; C₄₉H₈₂NO₂; theoretical m/z 716.6345, (M+NH₄)⁺; isotopic fit 0.0312

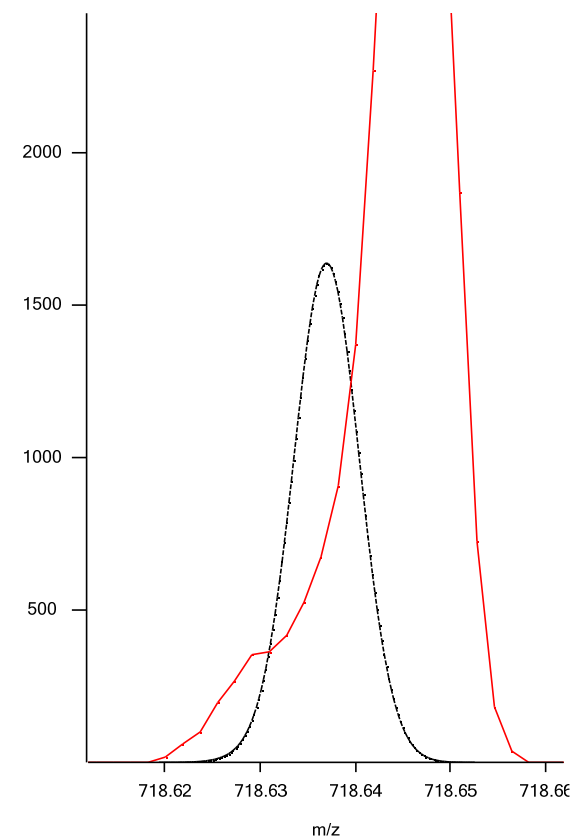
Isotope 1



Isotope 2

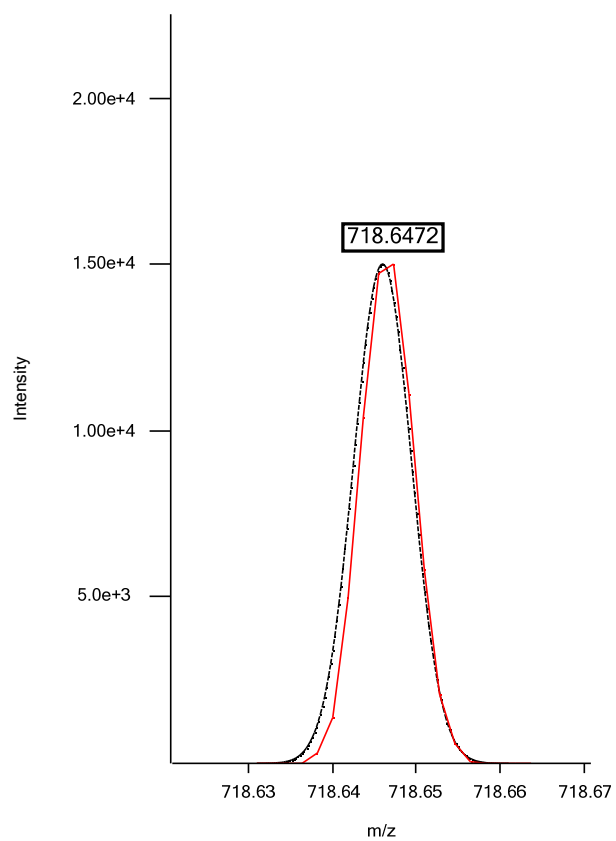


Isotope 3

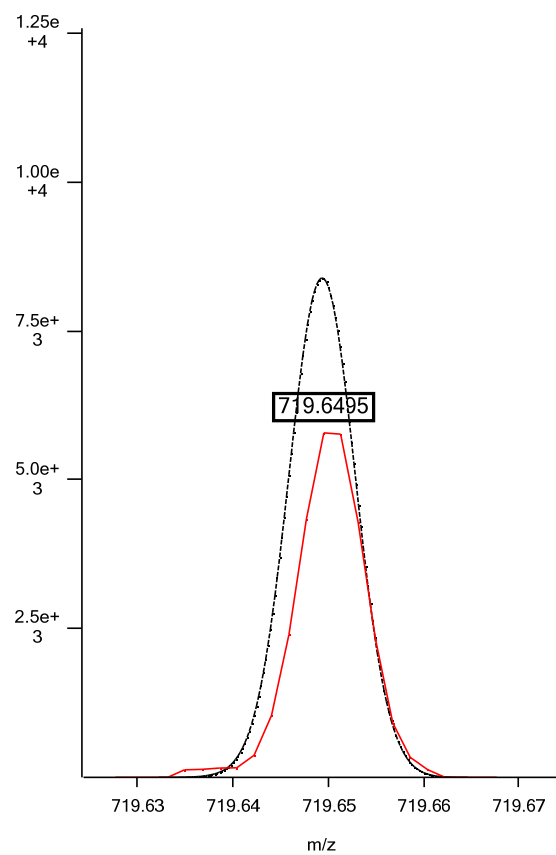


Positive ESI: CE 22:4; C₄₉H₈₄NO₂; theoretical m/z 718.6502, (M+NH₄)⁺; isotopic fit 0.0288

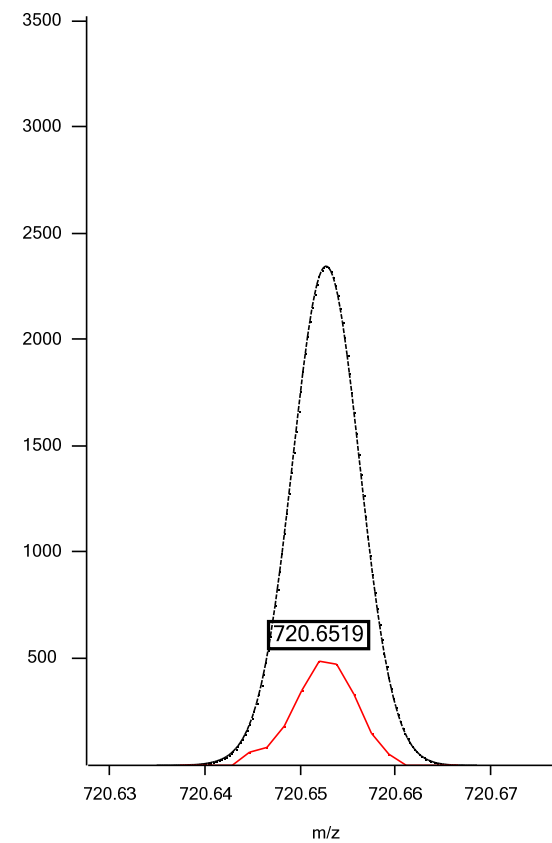
Isotope 1



Isotope 2



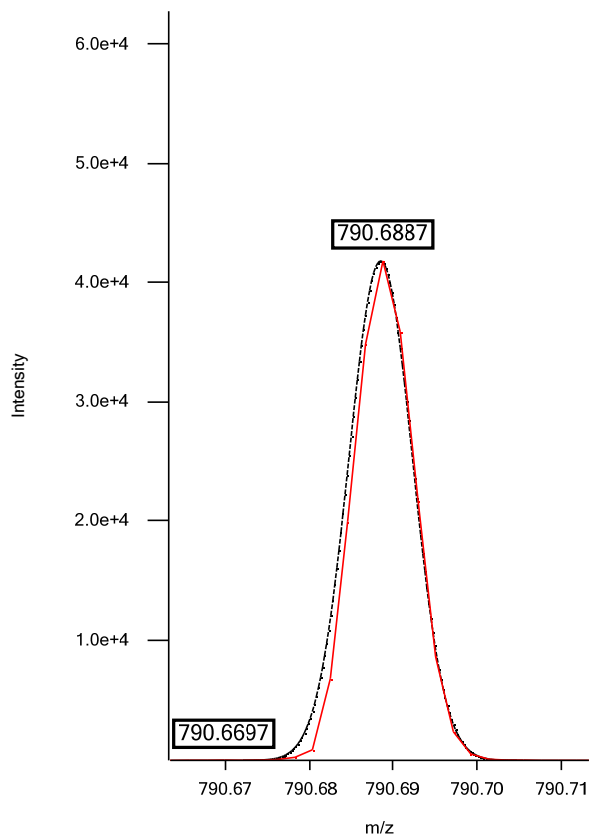
Isotope 3



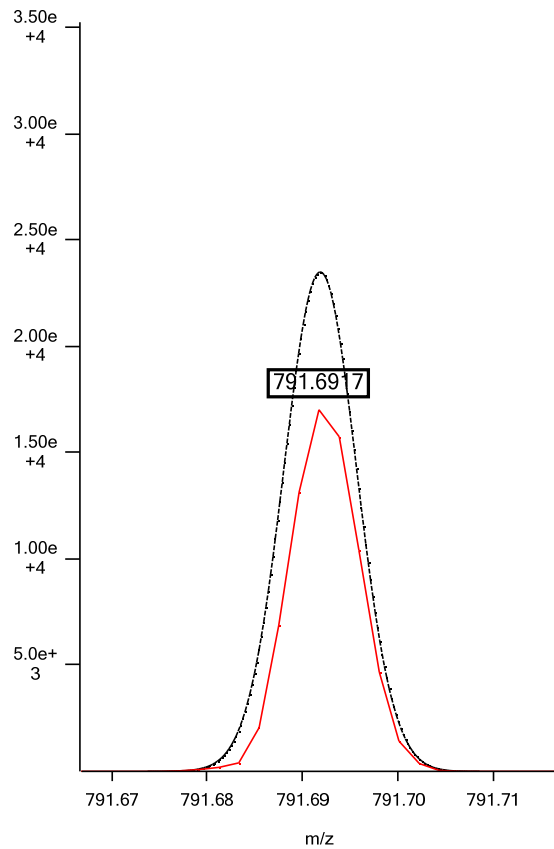
Triacylglycerols

Positive ESI: TAG 46:3; C₄₉H₉₂NO₆; theoretical *m/z* 790.6924, (M+NH₄)⁺; isotopic fit 0.0242

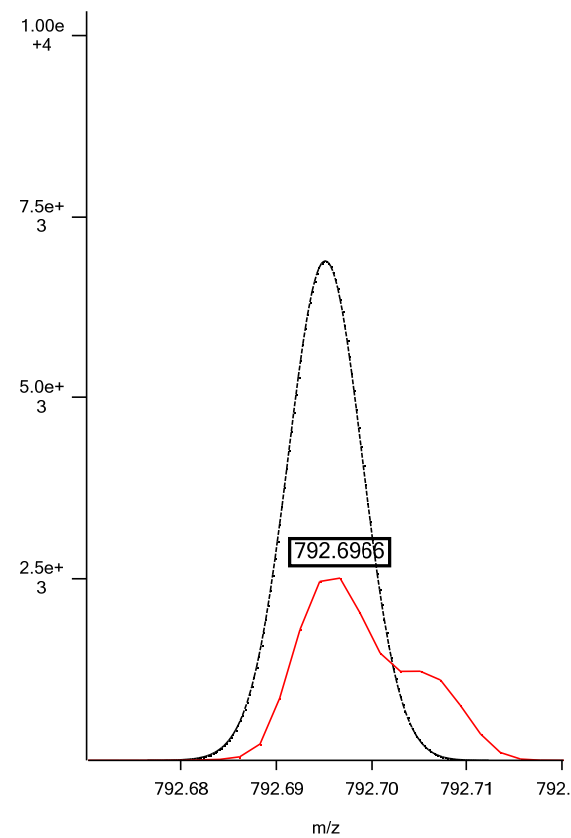
Isotope 1



Isotope 2

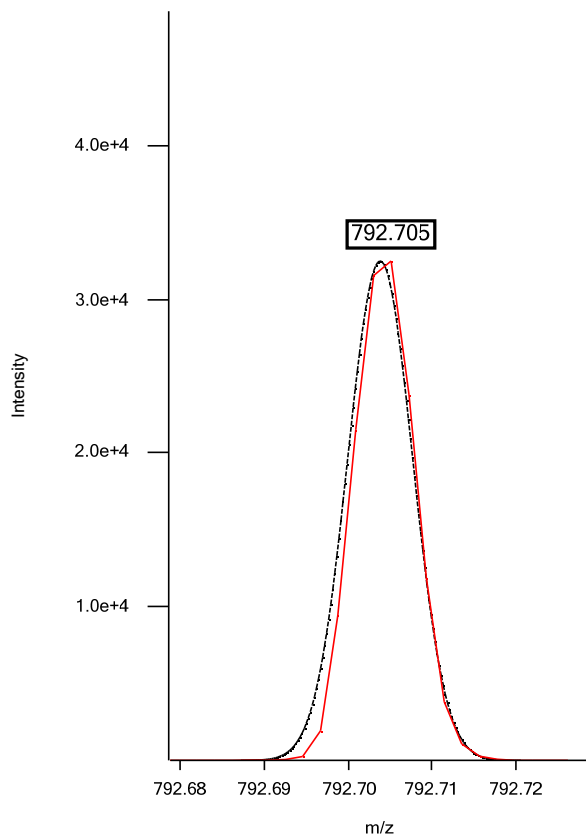


Isotope 3

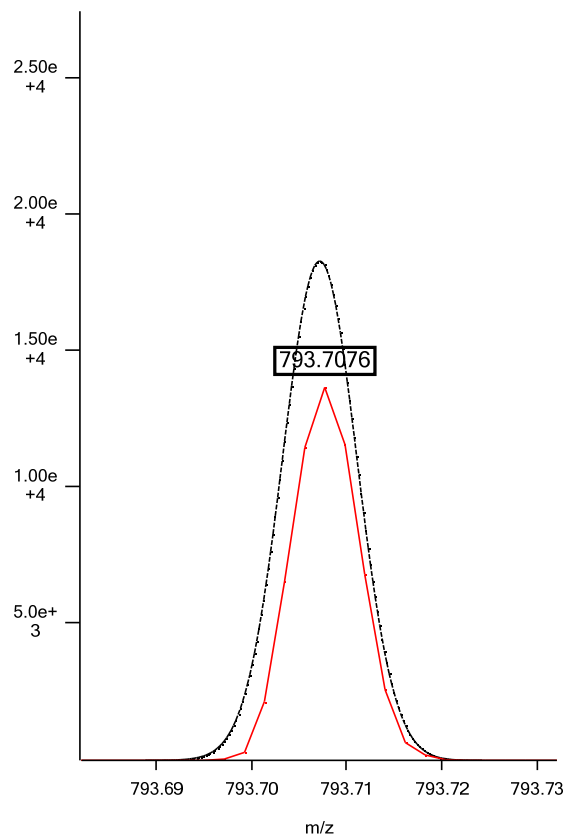


Positive ESI: TAG 46:2; C₄₉H₉₄NO₆; theoretical *m/z* 792.7081, (M+NH₄)⁺; isotopic fit 0.0259

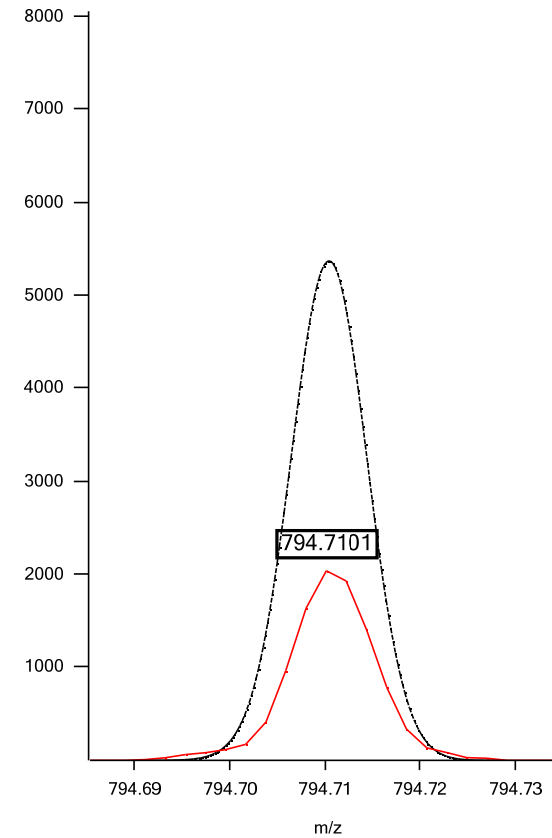
Isotope 1



Isotope 2

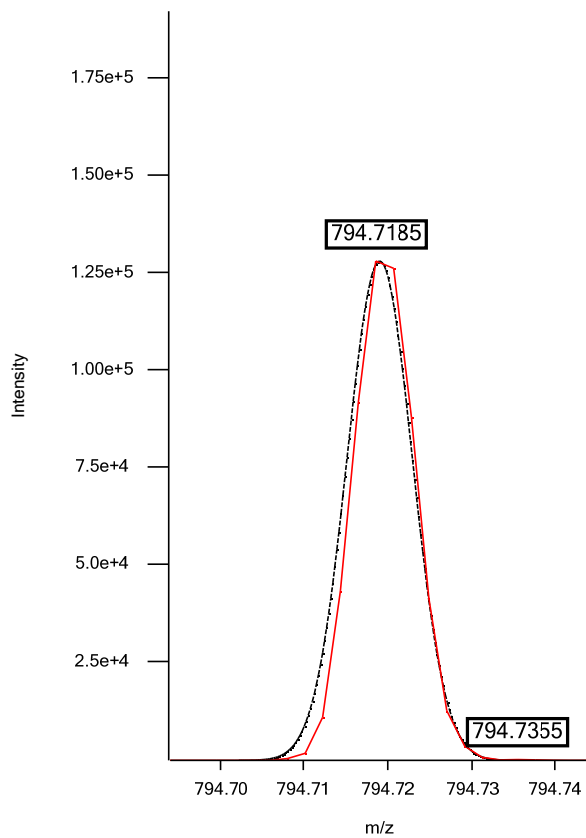


Isotope 3

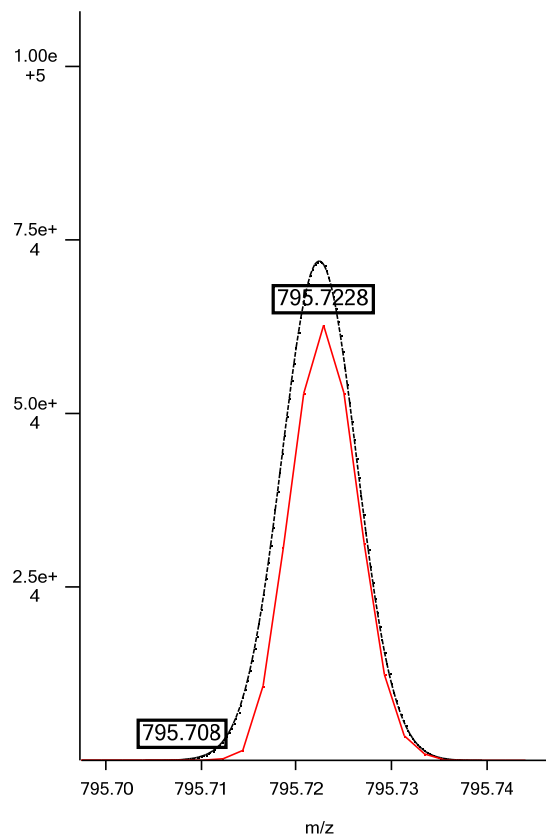


Positive ESI: TAG 46:1; C₄₉H₉₆NO₆; theoretical *m/z* 794.7237, (M+NH₄)⁺; isotopic fit 0.0096

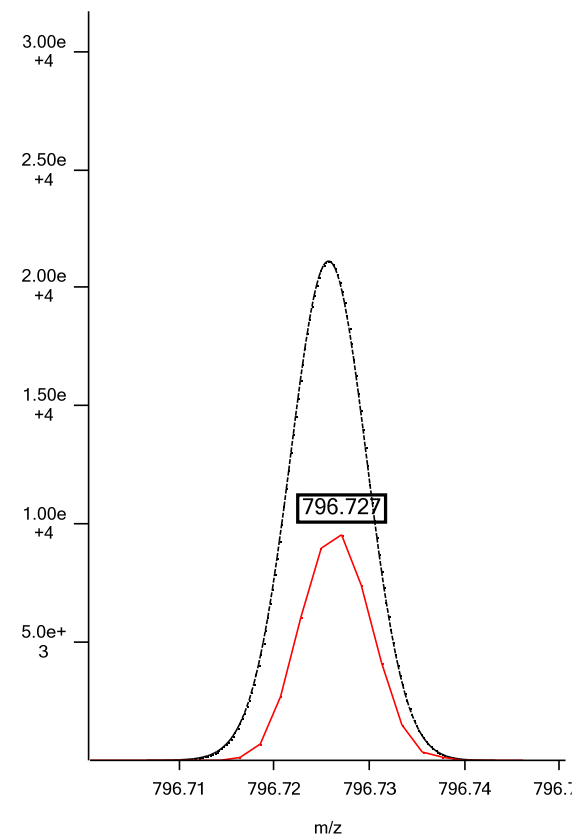
Isotope 1



Isotope 2

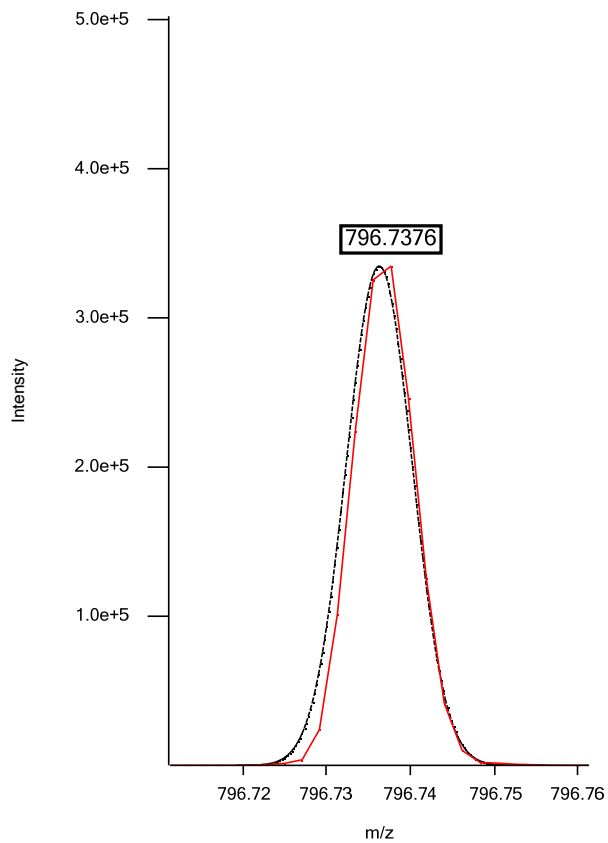


Isotope 3

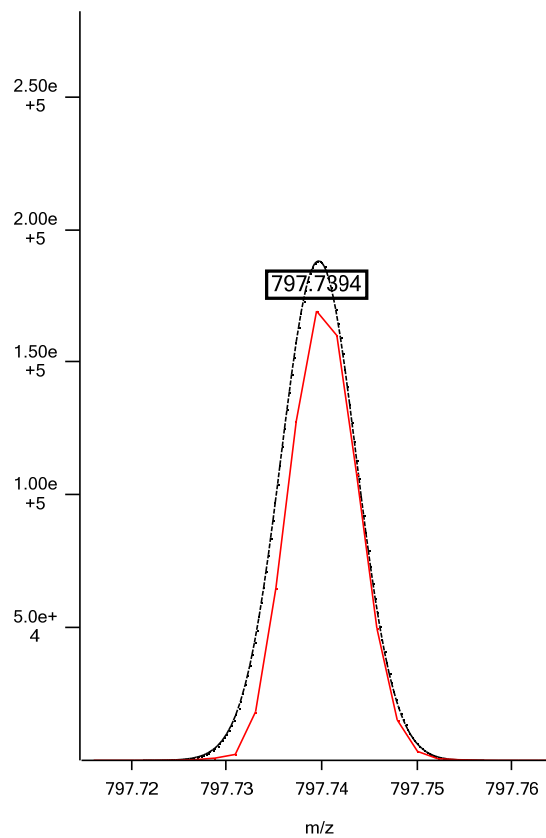


Positive ESI: TAG 46:0; C₄₉H₉₈NO₆; theoretical *m/z* 796.7394, (M+NH₄)⁺; isotopic fit 0.0065

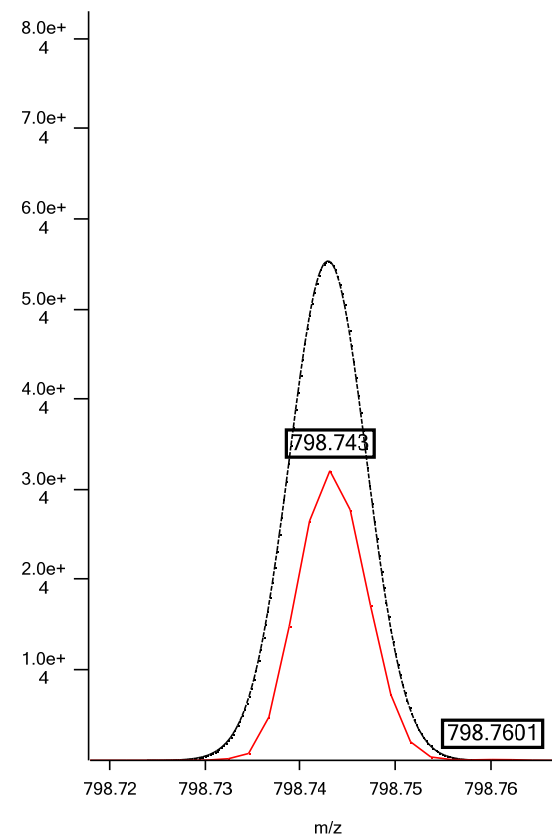
Isotope 1



Isotope 2

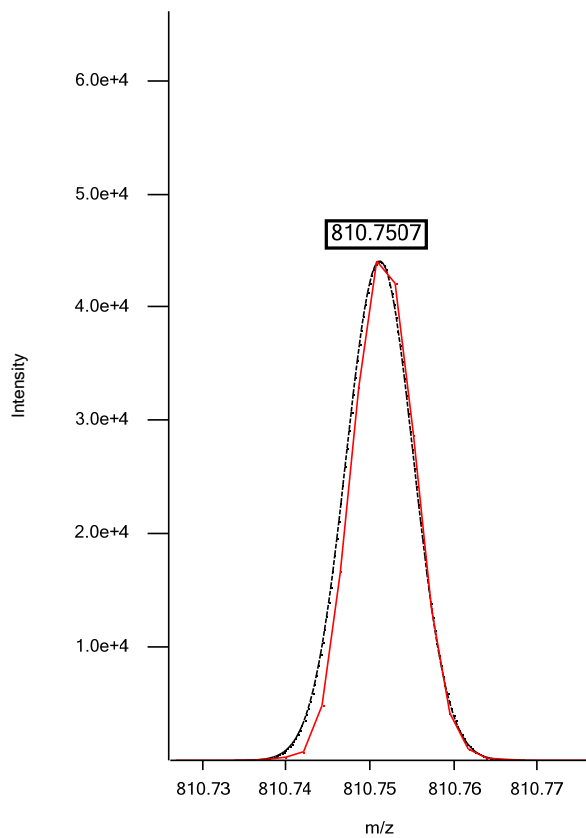


Isotope 3

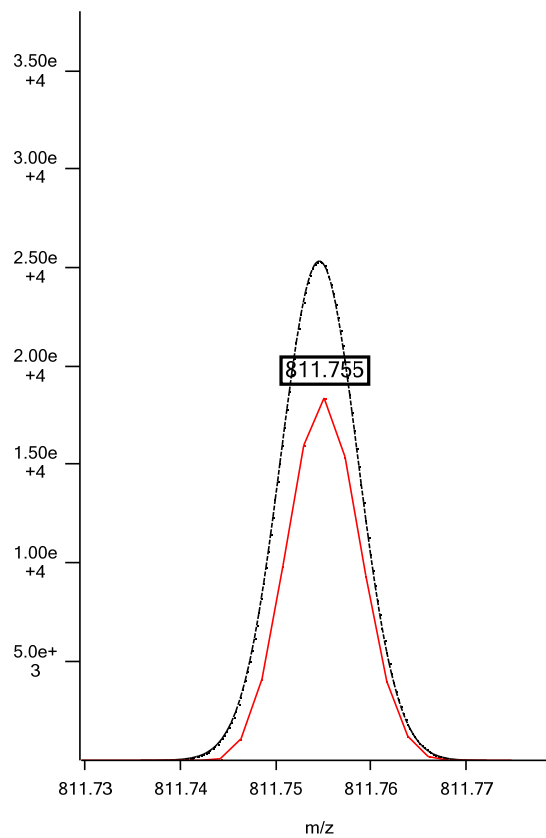


Positive ESI: TAG 47:0; C₅₀H₁₀₀NO₆; theoretical *m/z* 810.7550, (M+NH₄)⁺; isotopic fit 0.0248

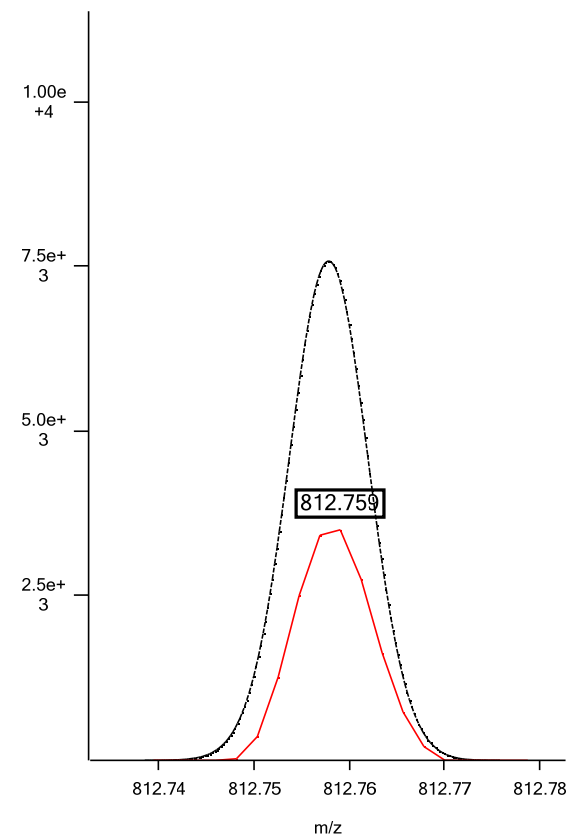
Isotope 1



Isotope 2

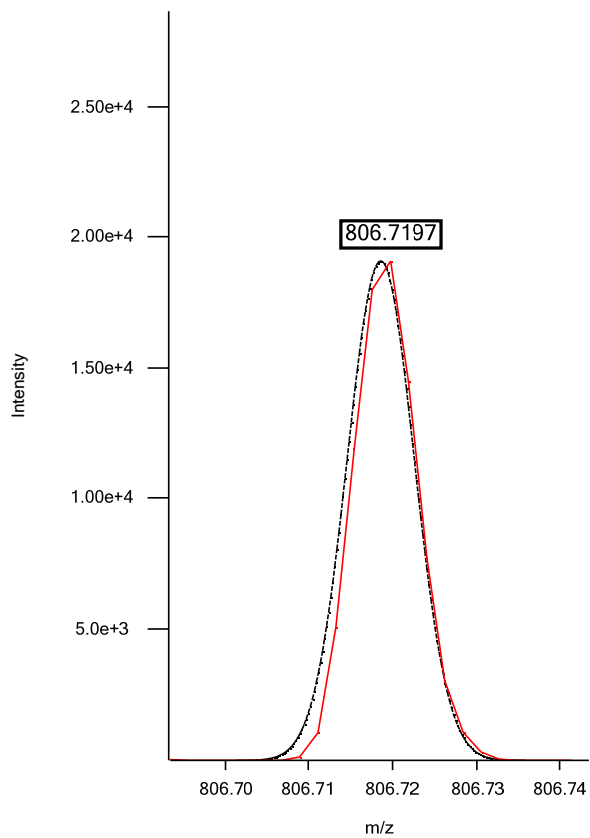


Isotope 3

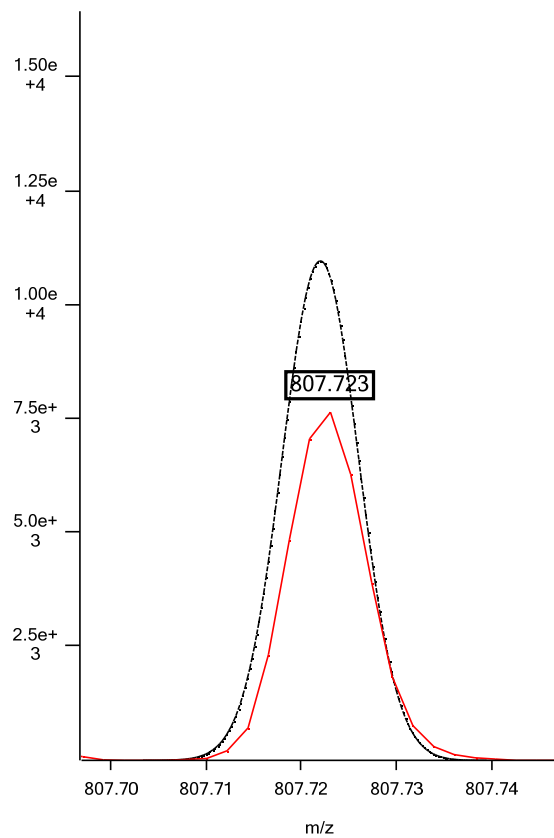


Positive ESI: TAG 47:2; C₅₀H₉₆NO₆; theoretical m/z 806.7237, (M+NH₄)⁺; isotopic fit 0.0266

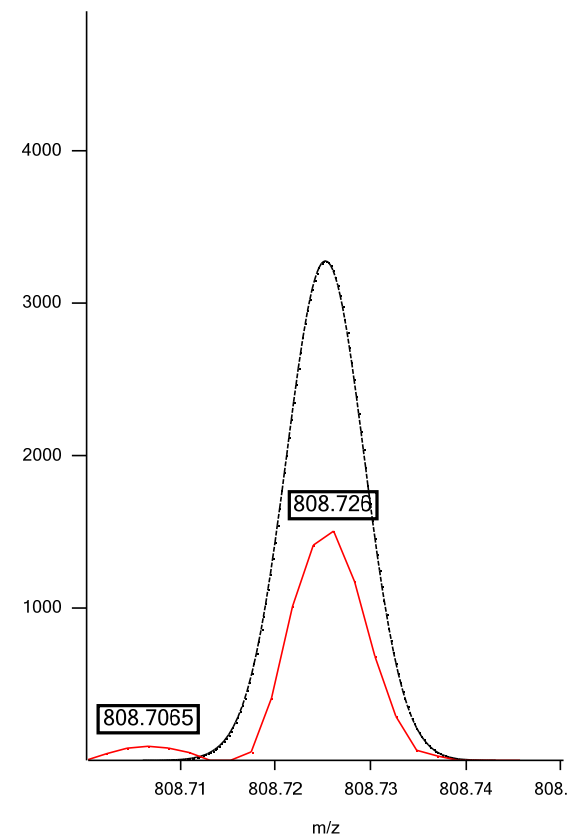
Isotope 1



Isotope 2

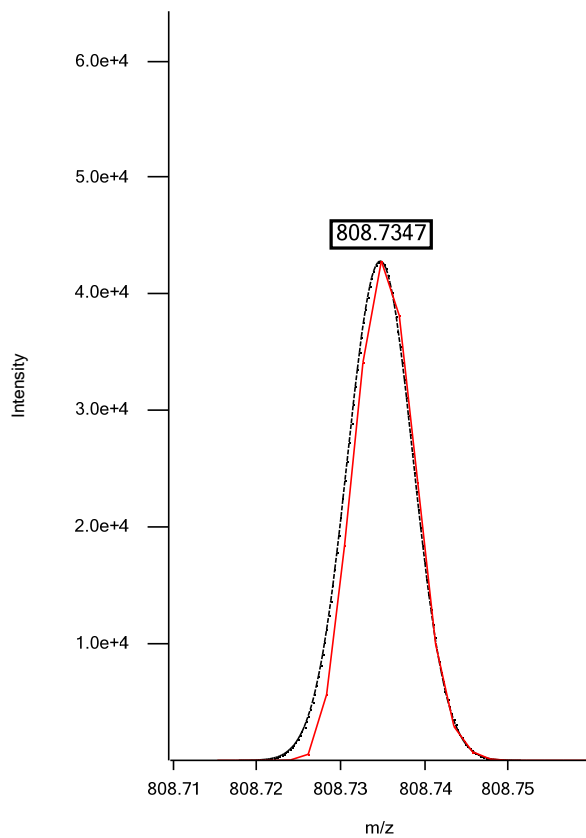


Isotope 3

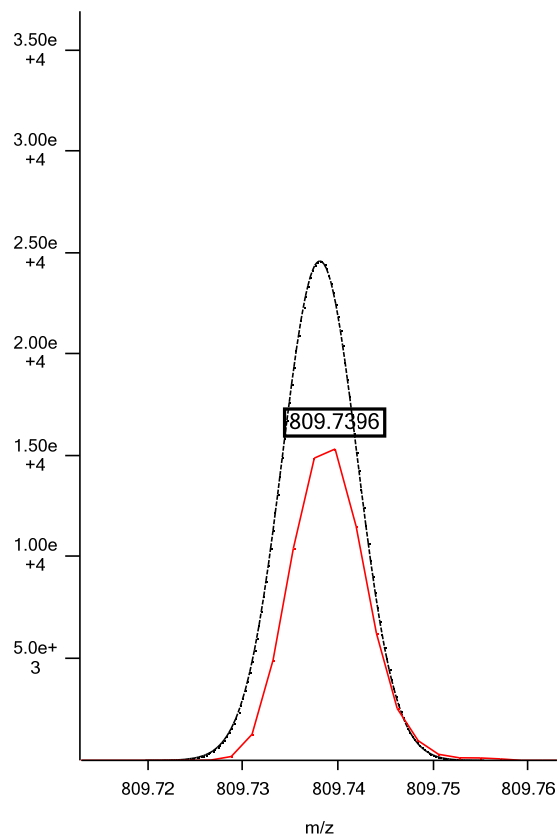


Positive ESI: TAG 47:1; C₅₀H₉₈NO₆; theoretical m/z 808.7394, (M+NH₄)⁺; isotopic fit 0.0415

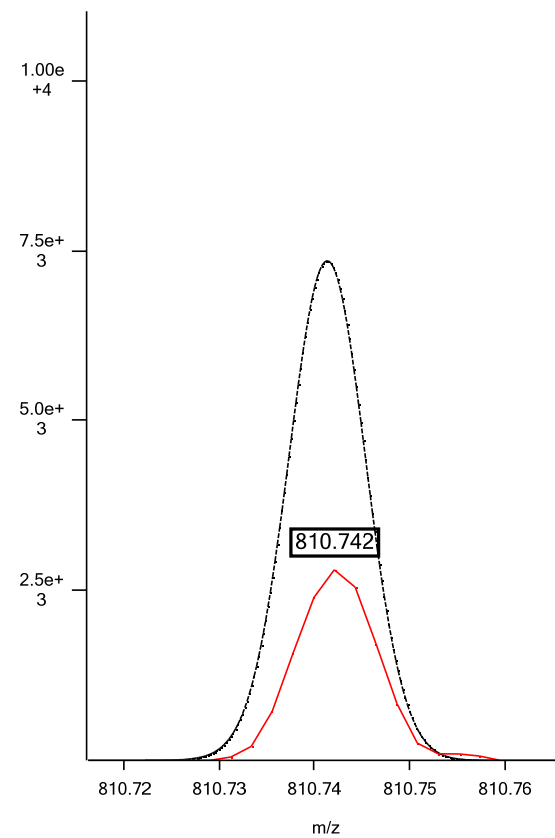
Isotope 1



Isotope 2

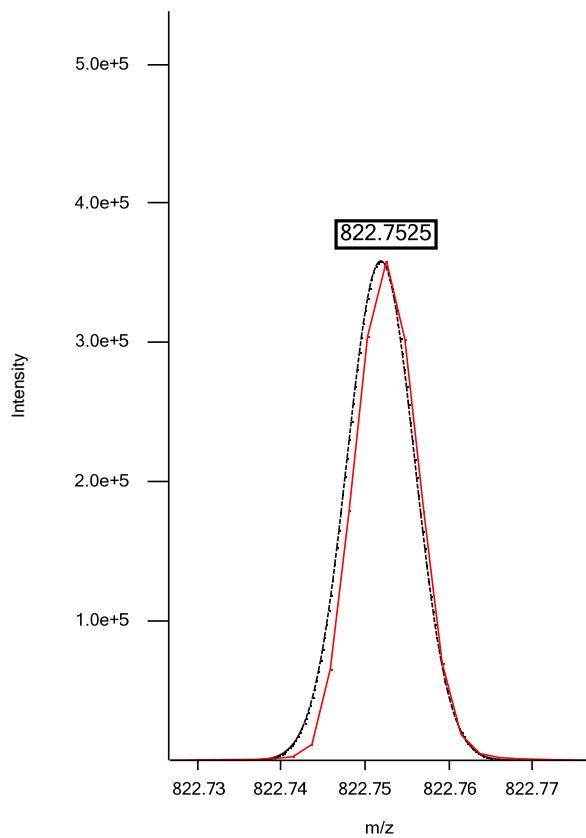


Isotope 3

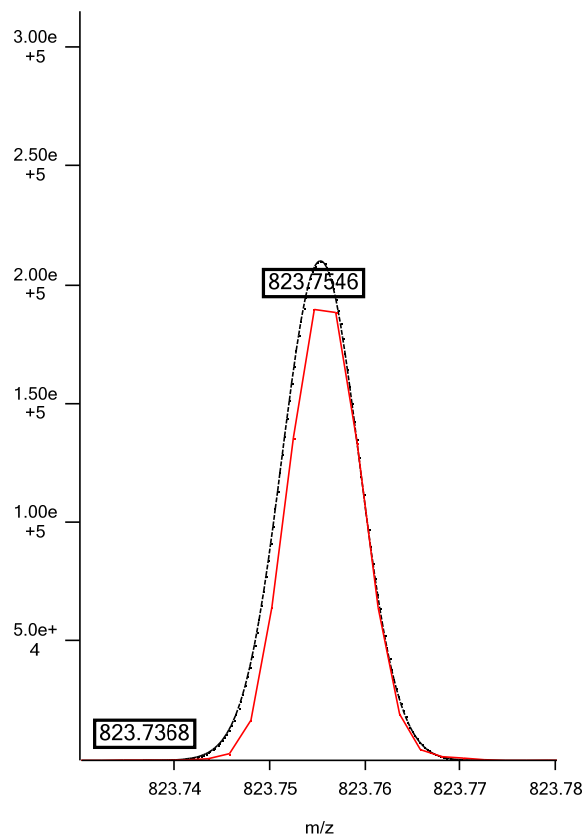


Positive ESI: TAG 48:1; $C_{51}H_{100}NO_6$; theoretical m/z 822.7550, $(M+NH_4)^+$; isotopic fit 0.0057

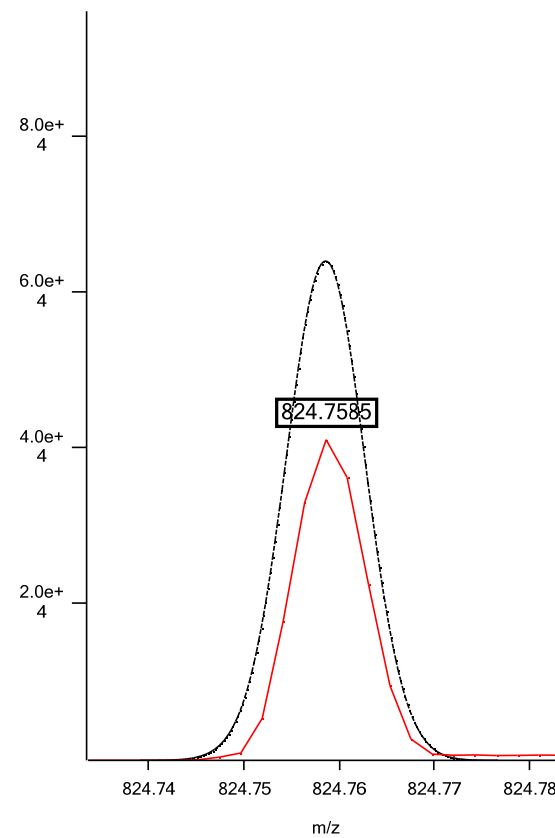
Isotope 1



Isotope 2

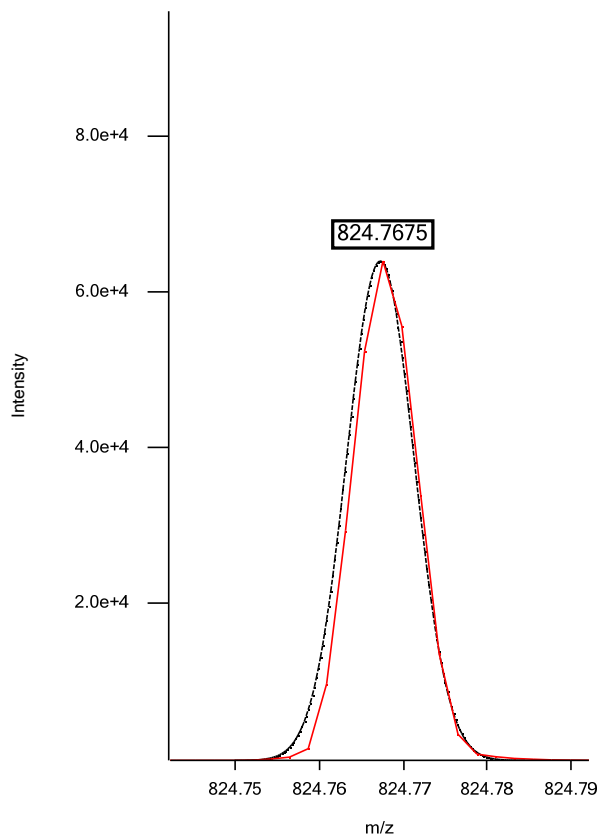


Isotope 3

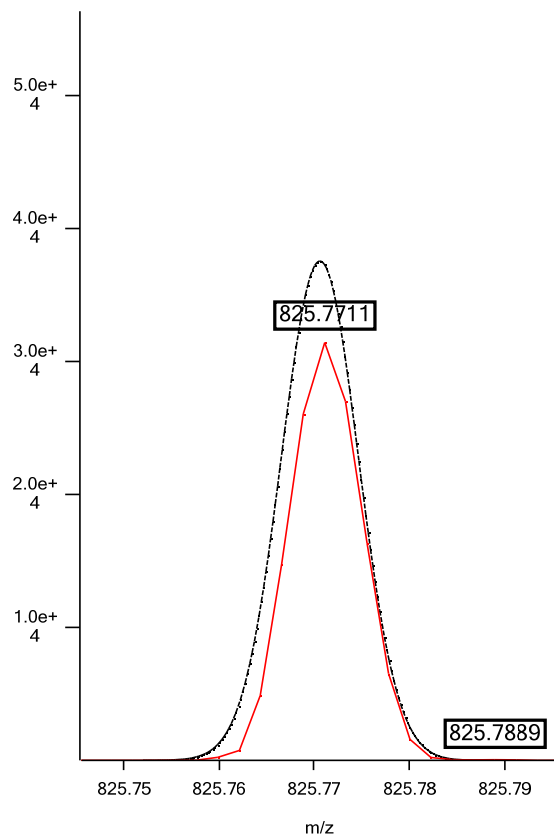


Positive ESI: TAG 48:0; C₅₁H₁₀₂NO₆; theoretical *m/z* 824.7707, (M+NH₄)⁺; isotopic fit 0.0162

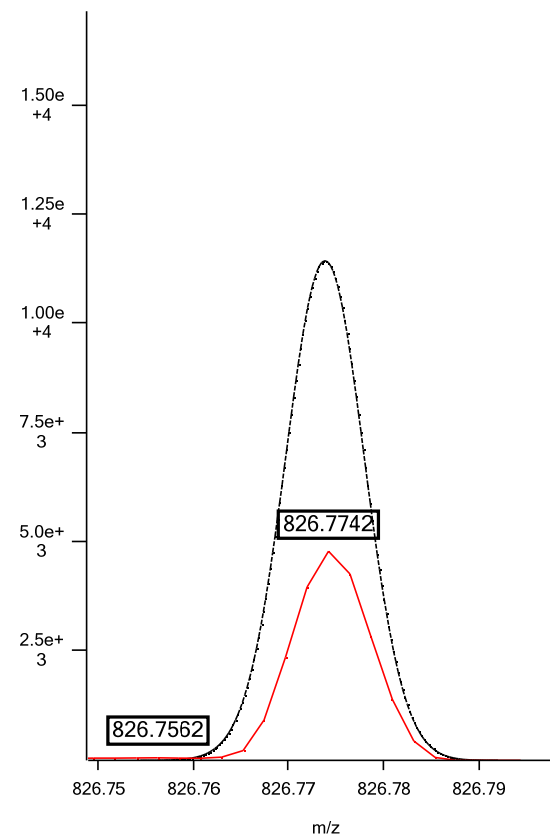
Isotope 1



Isotope 2

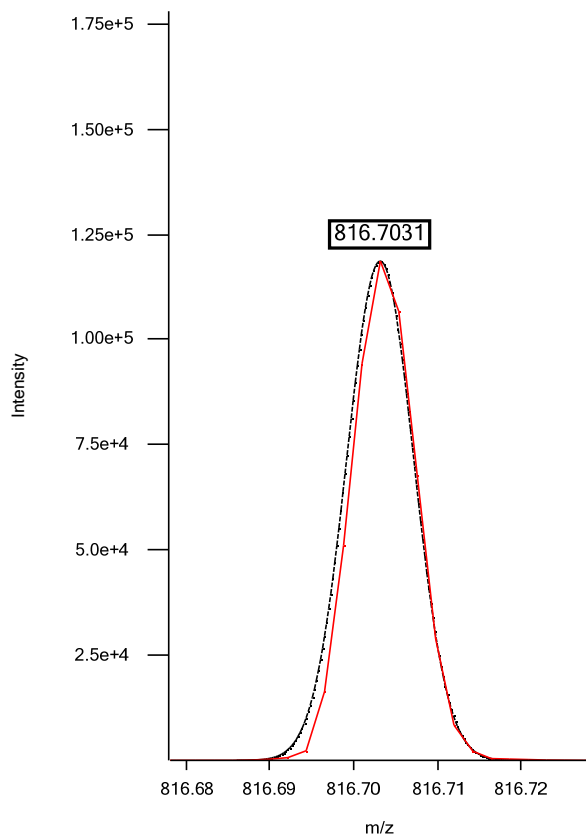


Isotope 3

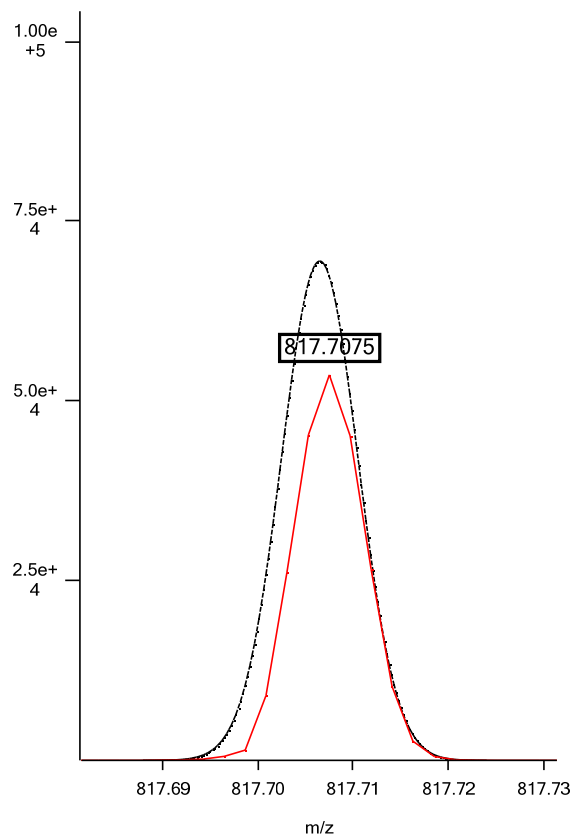


Positive ESI: TAG 48:4; C₅₁H₉₄NO₆; theoretical m/z 816.7081, (M+NH₄)⁺; isotopic fit 0.0188

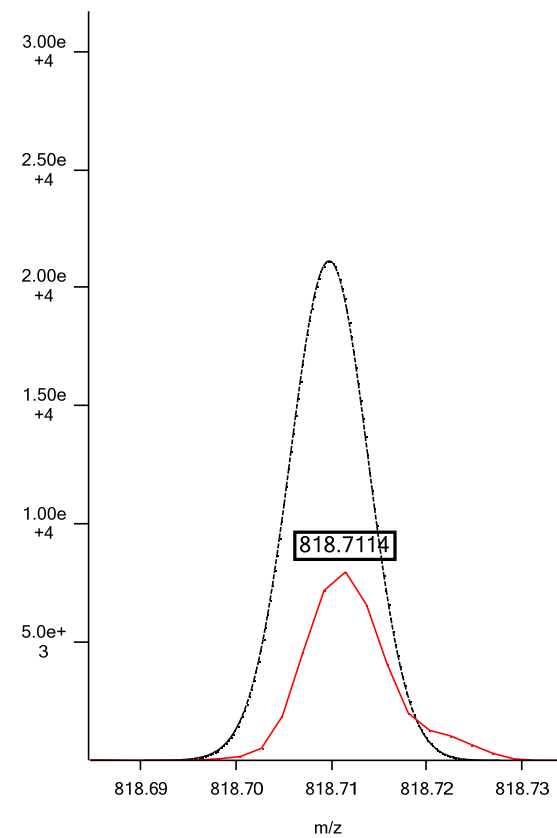
Isotope 1



Isotope 2

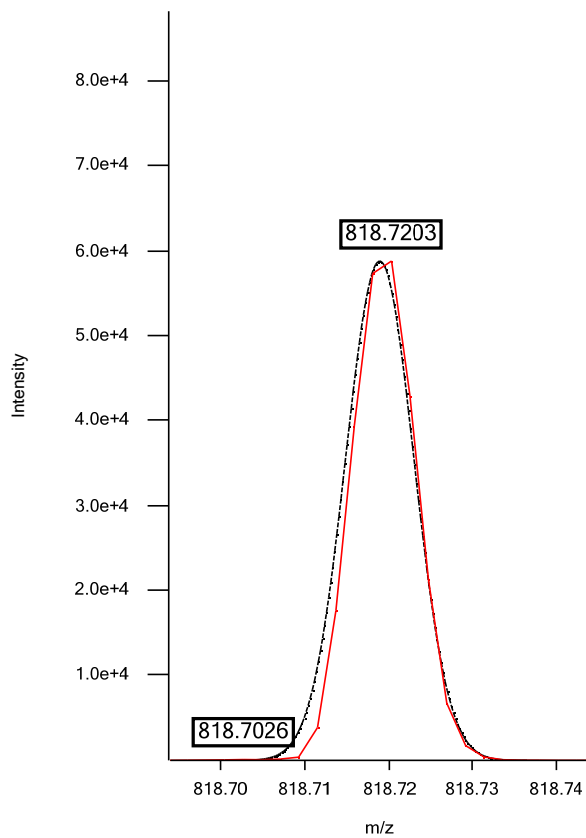


Isotope 3

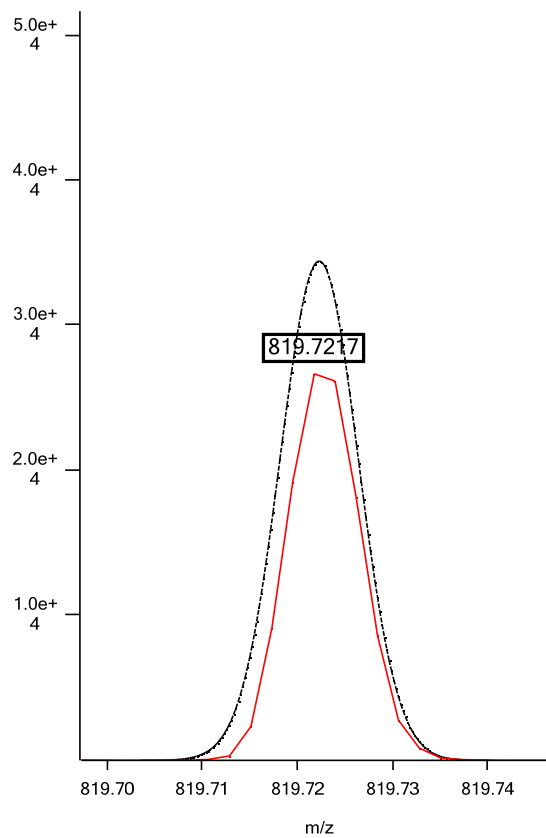


Positive ESI: TAG 48:3; C₅₁H₉₆NO₆; theoretical m/z 818.7238, (M+NH₄)⁺; isotopic fit 0.0169

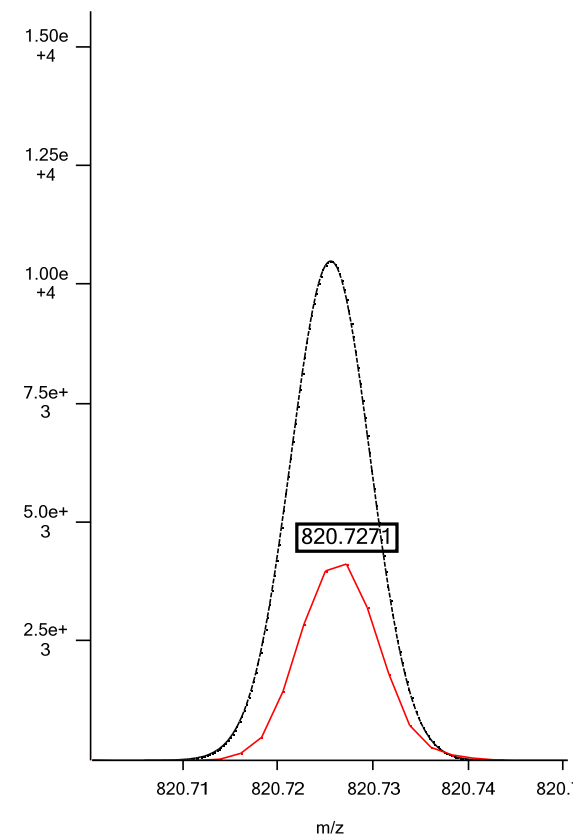
Isotope 1



Isotope 2

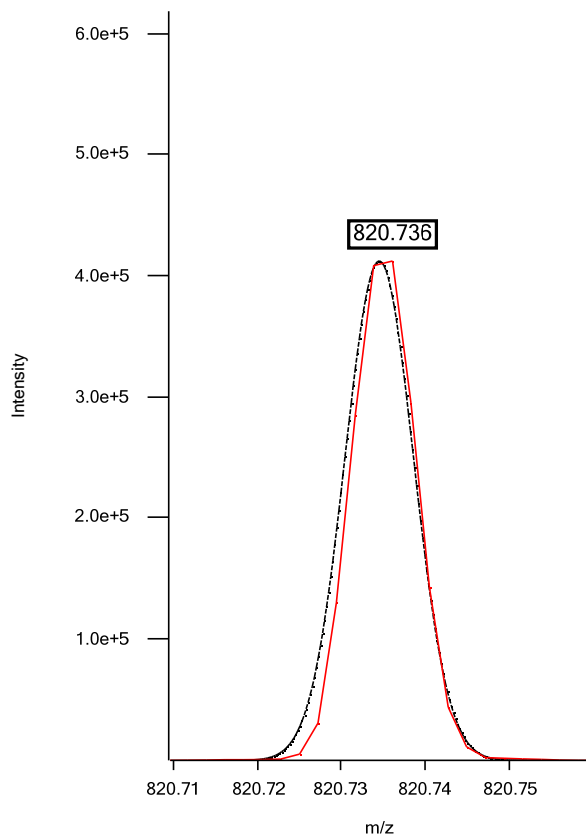


Isotope 3

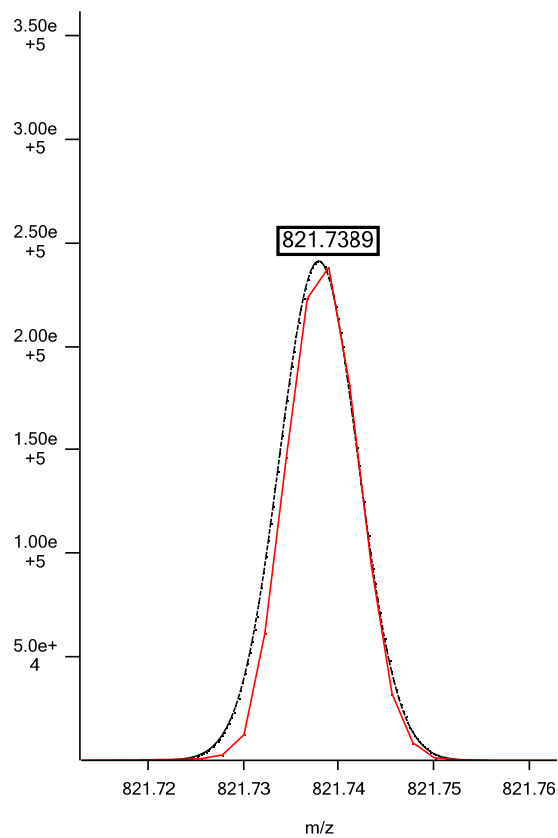


Positive ESI: TAG 48:2; C₅₁H₉₈NO₆; theoretical m/z 820.7394, (M+NH₄)⁺; isotopic fit 0.0029

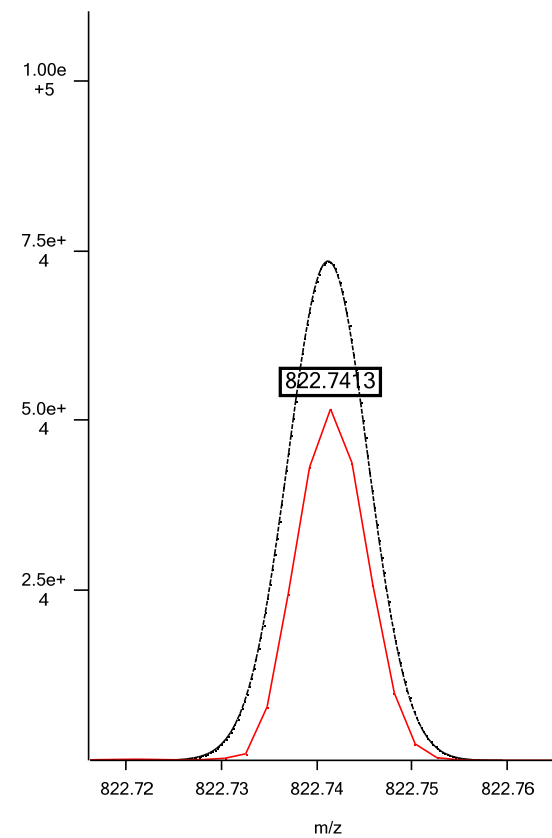
Isotope 1



Isotope 2

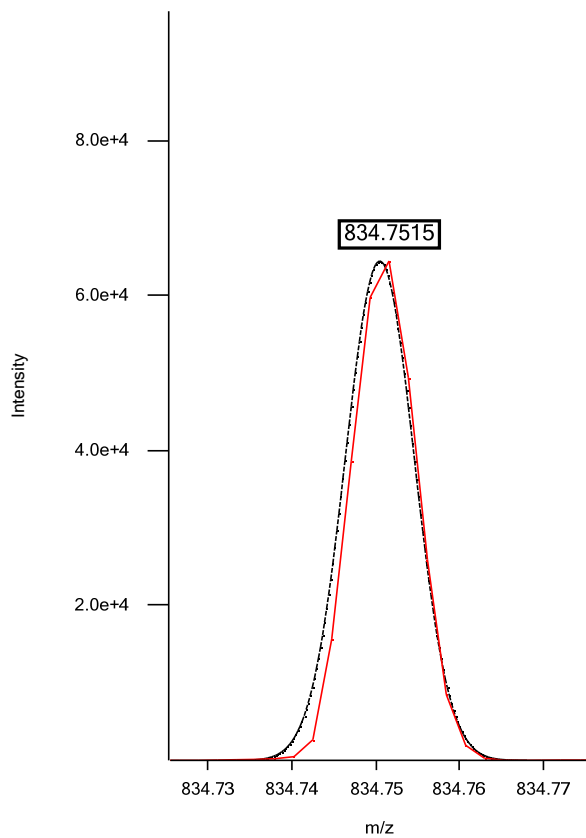


Isotope 3

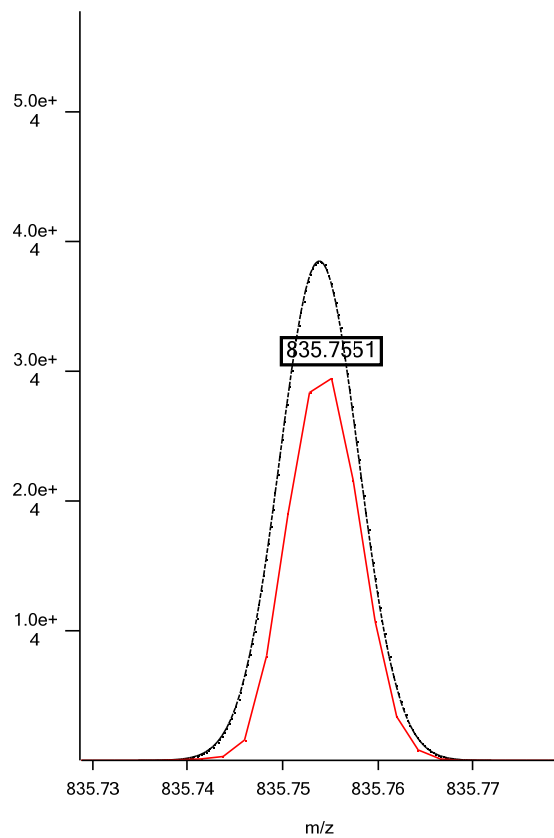


Positive ESI: TAG 49:2; C₅₂H₁₀₀NO₆; theoretical m/z 834.7550, (M+NH₄)⁺; isotopic fit 0.0180

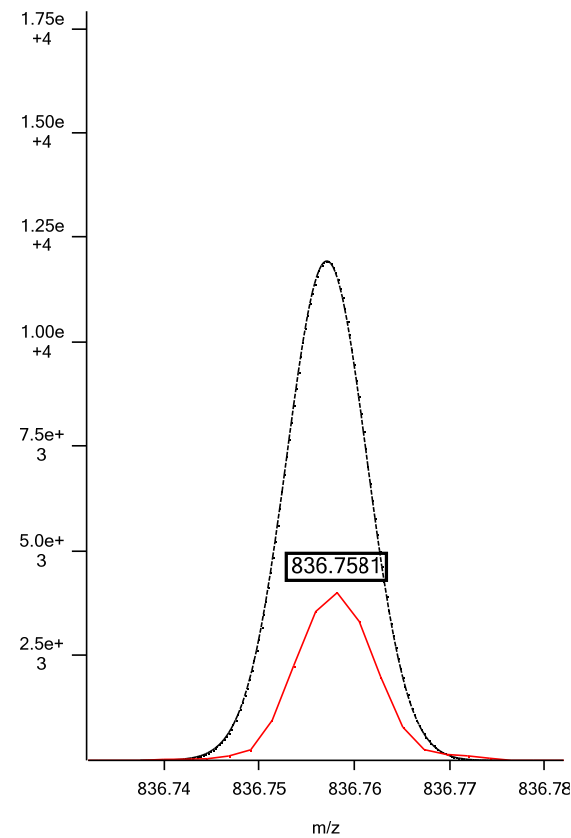
Isotope 1



Isotope 2

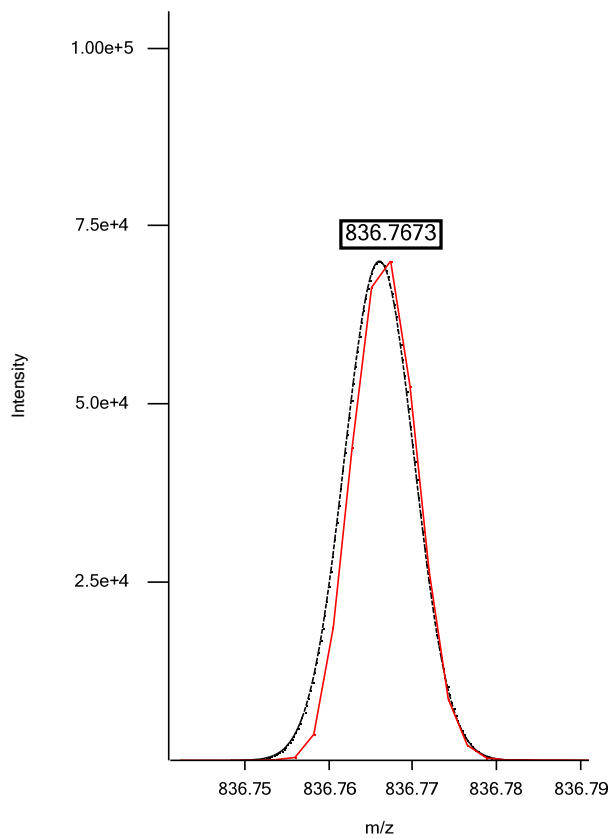


Isotope 3

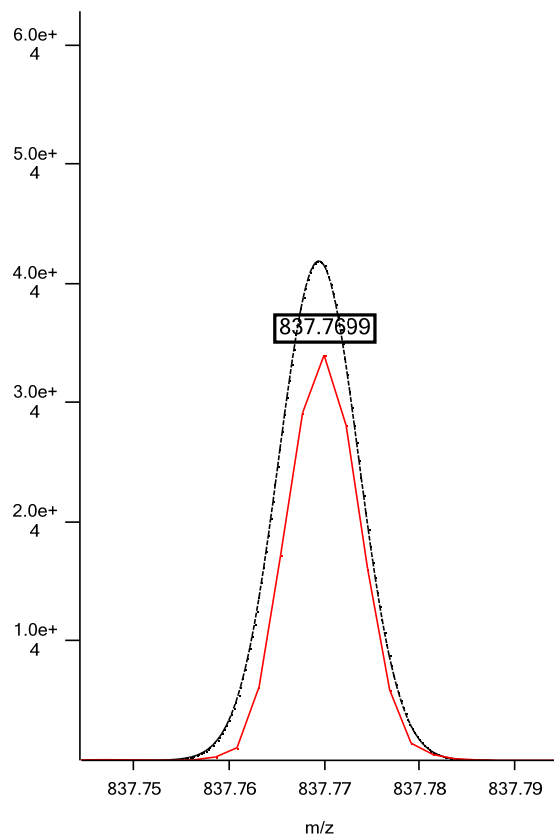


Positive ESI: TAG 49:1; C₅₂H₁₀₂NO₆; theoretical *m/z* 836.7707, (M+NH₄)⁺; isotopic fit 0.0162

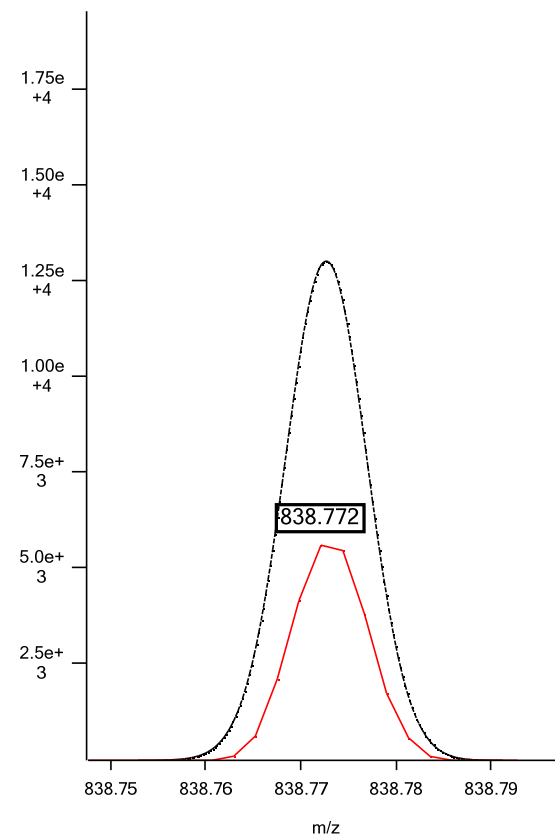
Isotope 1



Isotope 2

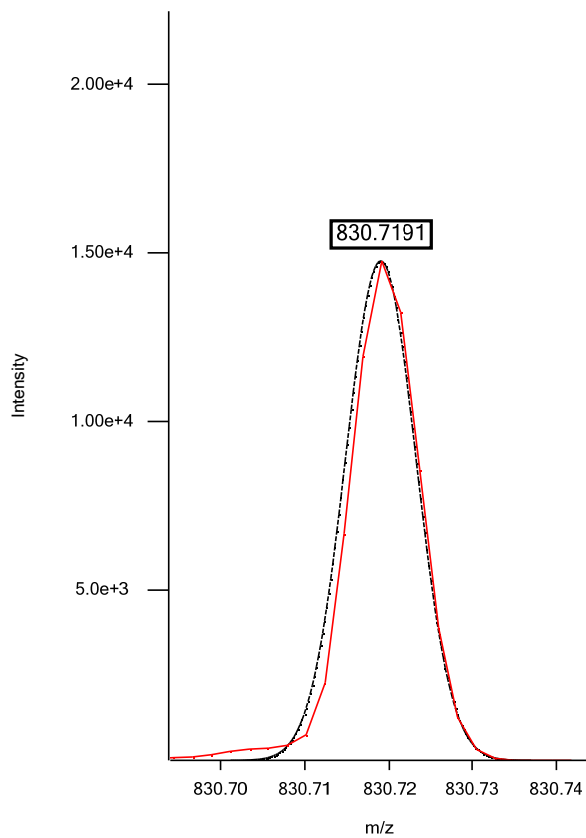


Isotope 3

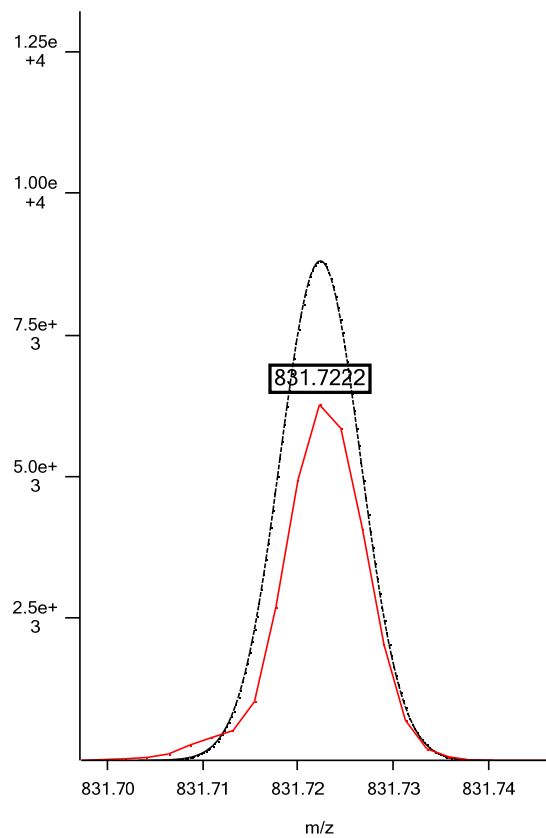


Positive ESI: TAG 49:4; C₅₂H₉₆NO₆; theoretical m/z 830.7237, (M+NH₄)⁺; isotopic fit 0.0258

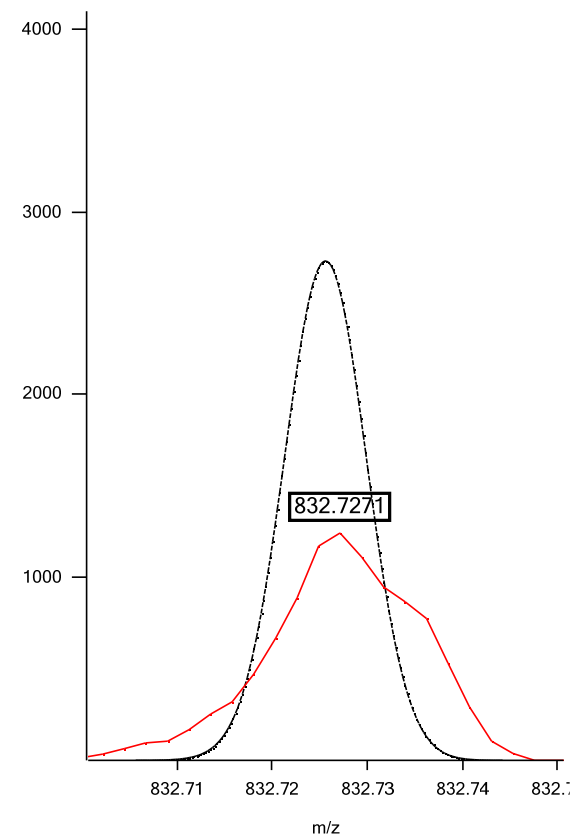
Isotope 1



Isotope 2

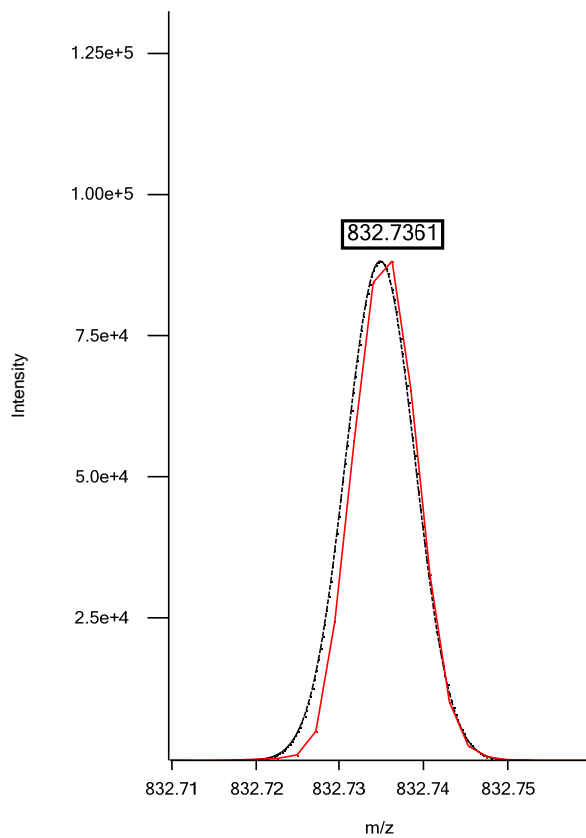


Isotope 3

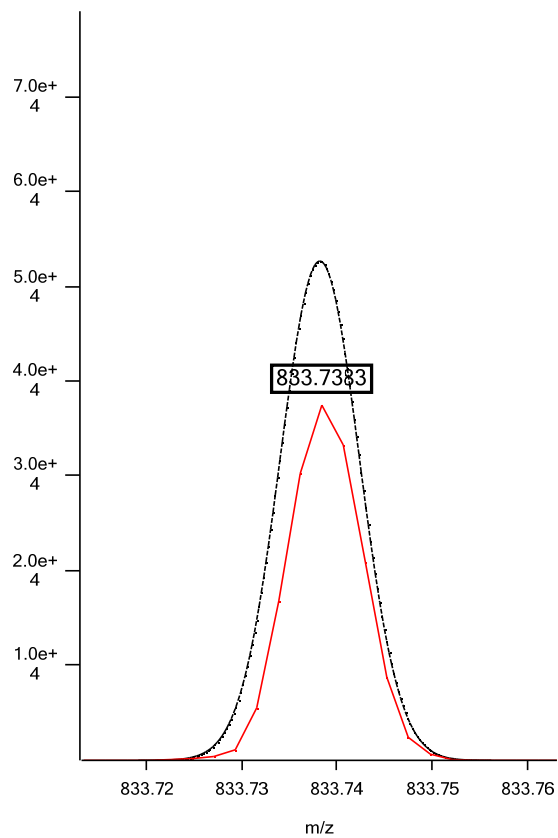


Positive ESI: TAG 49:3; C₅₂H₉₈NO₆; theoretical *m/z* 832.7394, (M+NH₄)⁺; isotopic fit 0.0272

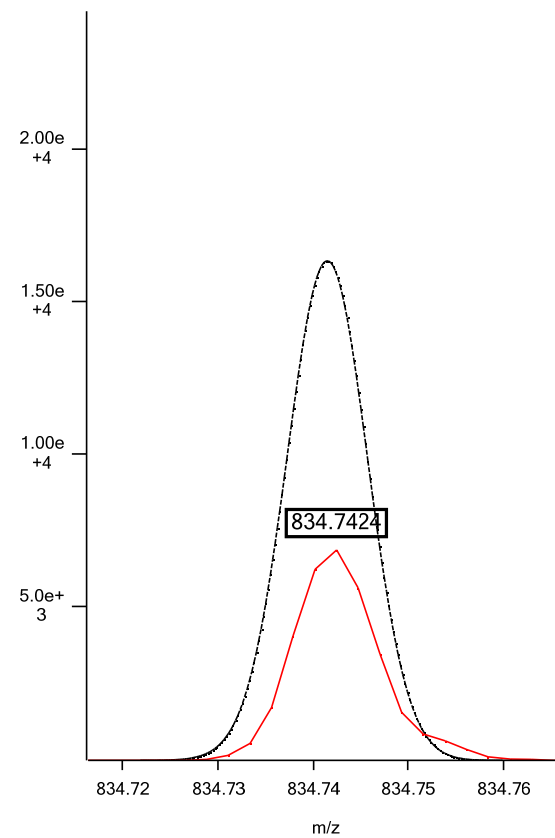
Isotope 1



Isotope 2

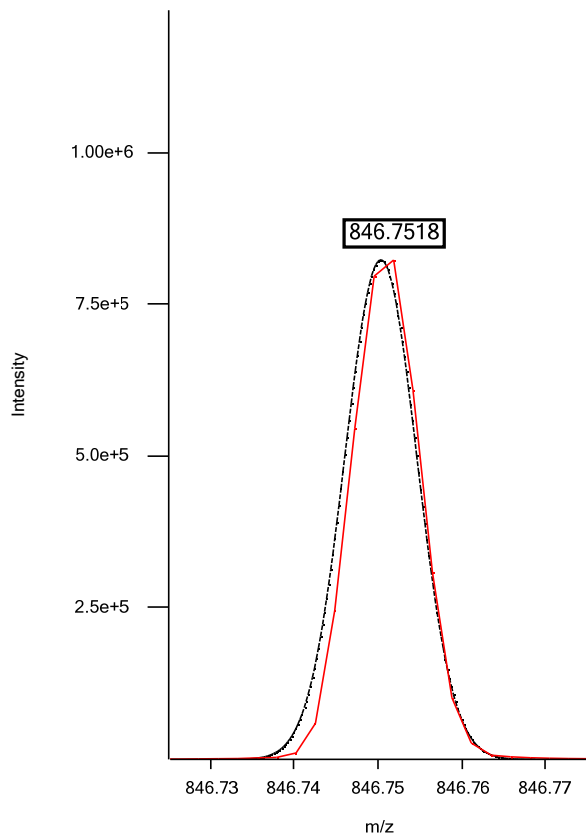


Isotope 3

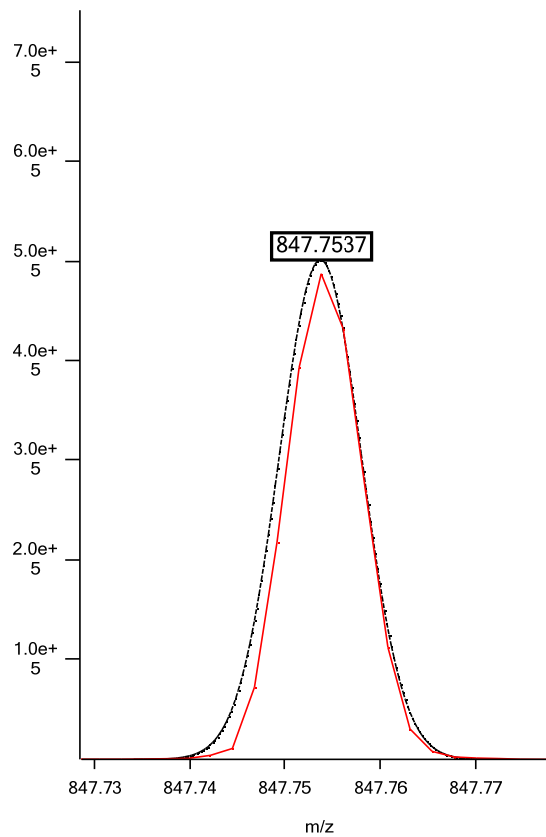


Positive ESI: TAG 50:3; C₅₃H₁₀₀NO₆; theoretical *m/z* 846.7551, (M+NH₄)⁺; isotopic fit 0.0043

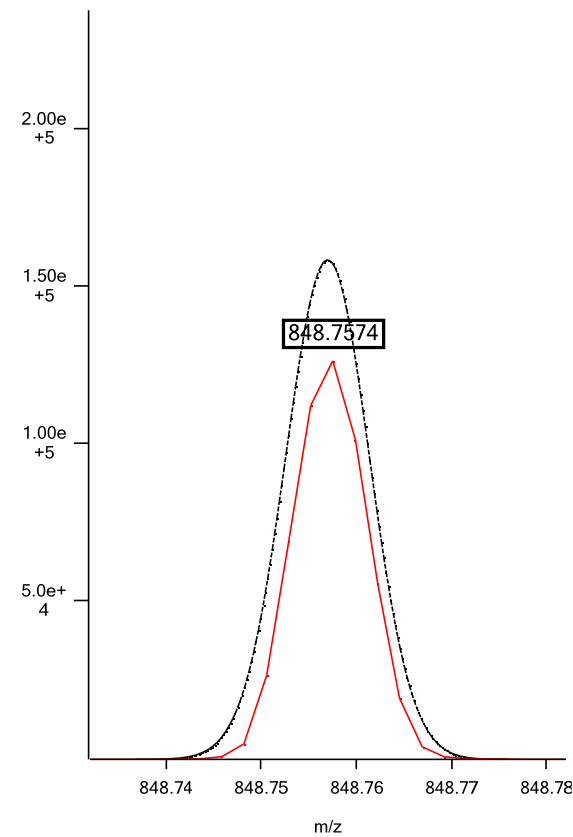
Isotope 1



Isotope 2

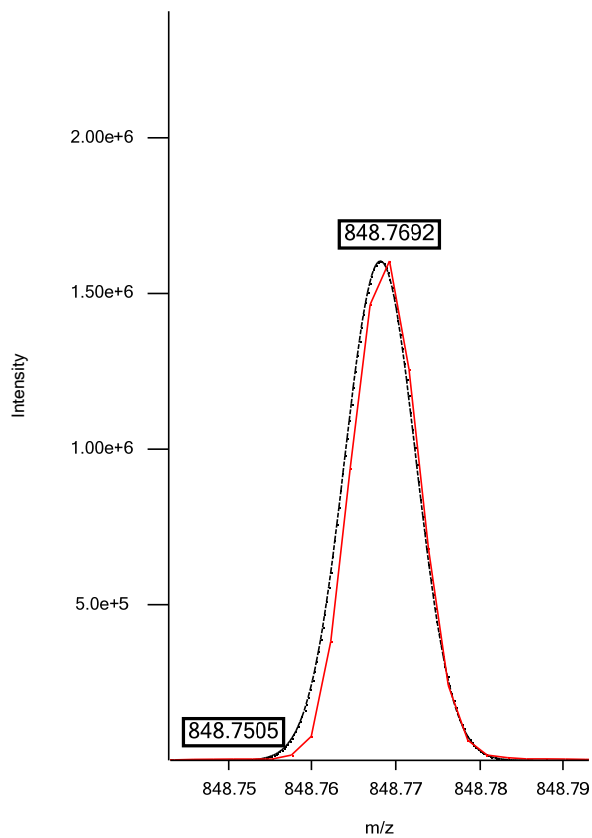


Isotope 3

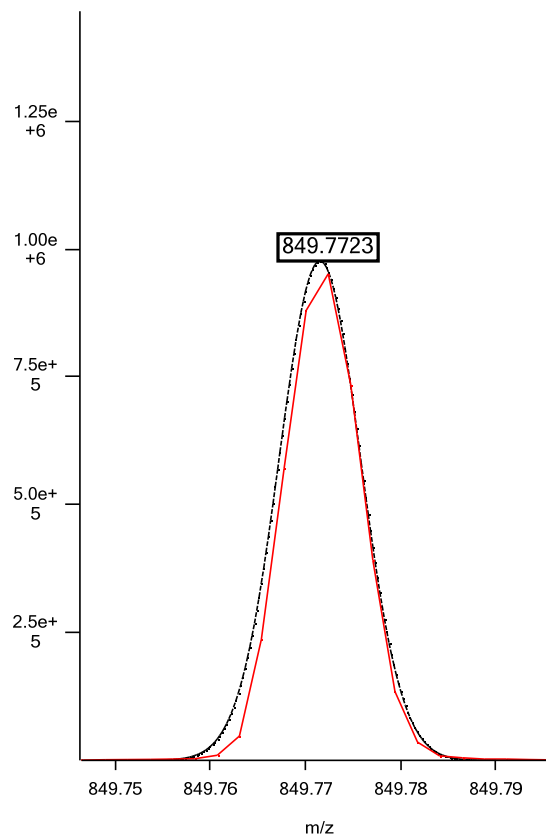


Positive ESI: TAG 50:2; C₅₃H₁₀₂NO₆; theoretical *m/z* 848.7707, (M+NH₄)⁺; isotopic fit 0.0033

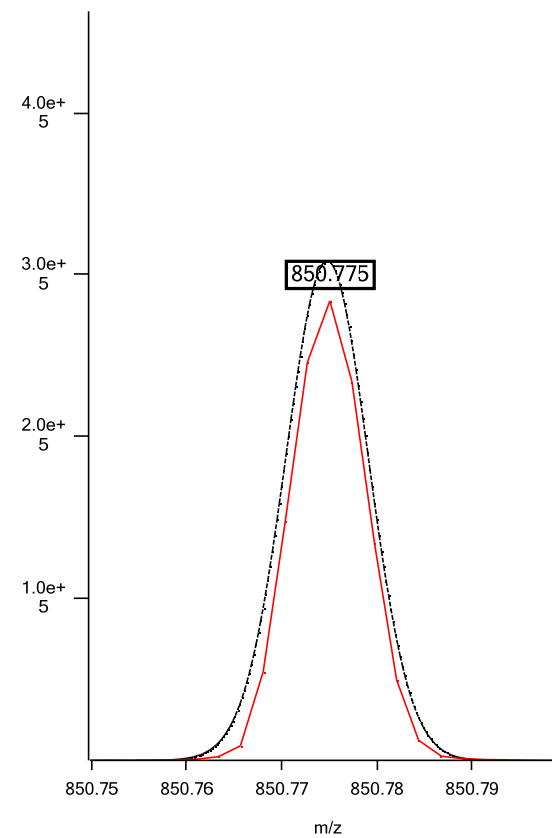
Isotope 1



Isotope 2

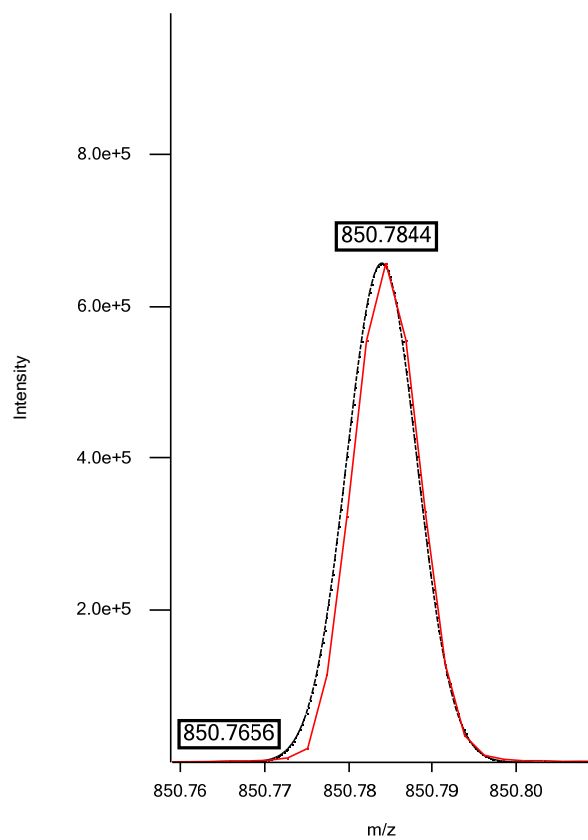


Isotope 3

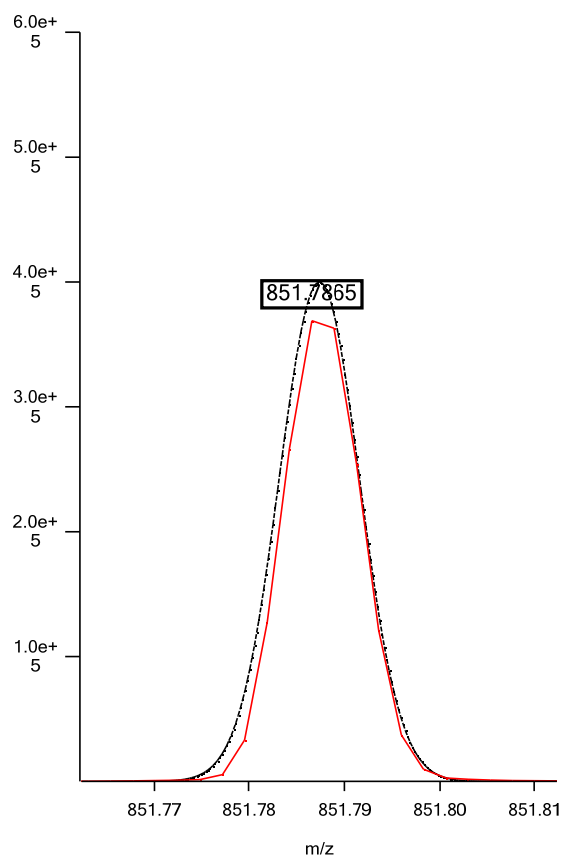


Positive ESI: TAG 50:1; $C_{53}H_{104}NO_6$; theoretical m/z 850.7864, $(M+NH_4)^+$; isotopic fit 0.0033

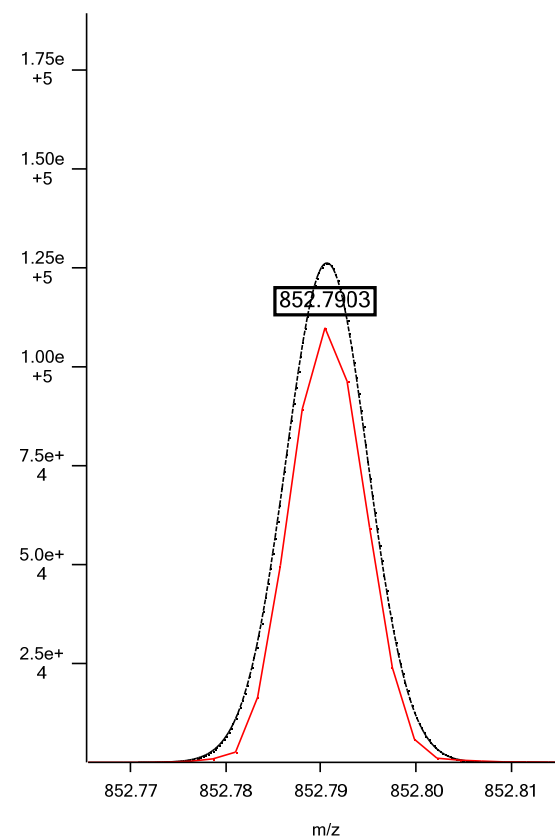
Isotope 1



Isotope 2

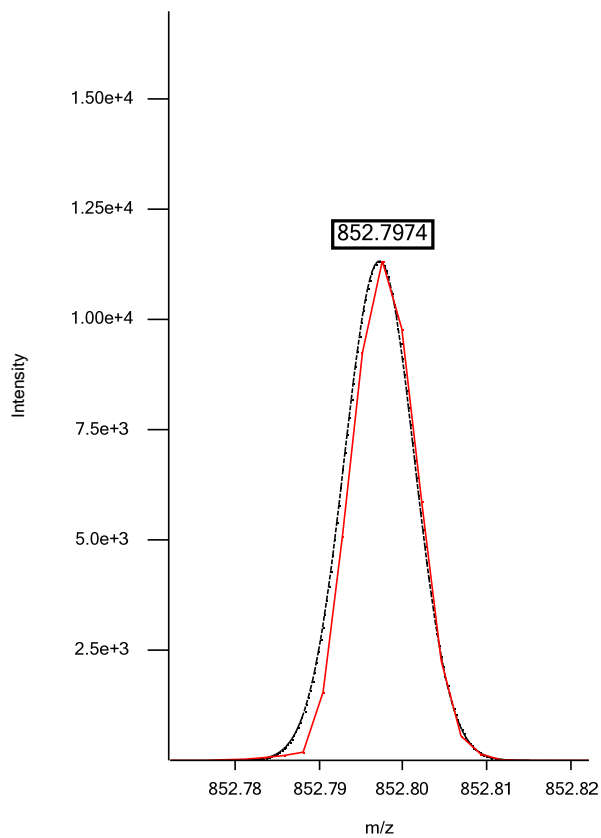


Isotope 3

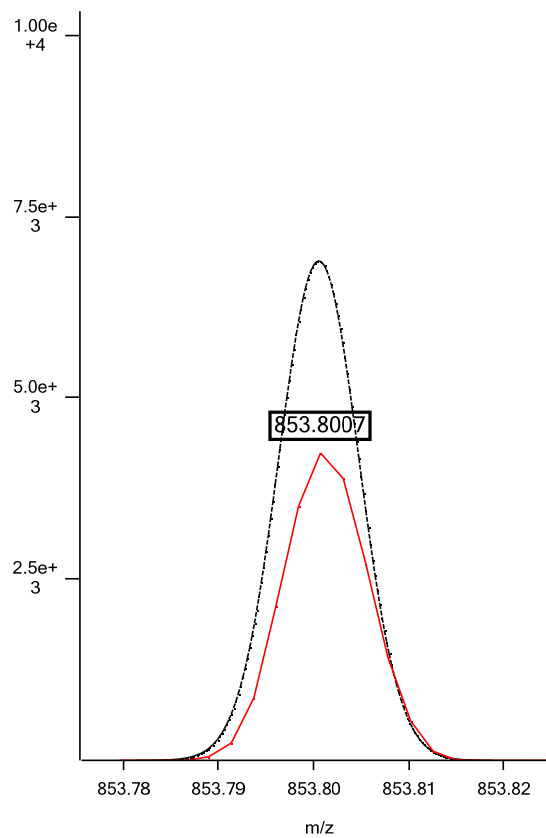


Positive ESI: TAG 50:0; C₅₃H₁₀₆NO₆; theoretical *m/z* 852.8020, (M+NH₄)⁺; isotopic fit 0.0409

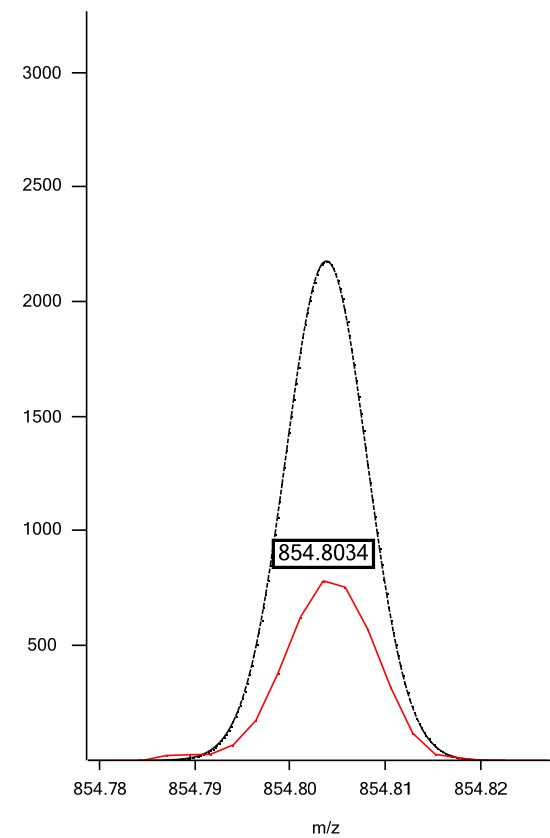
Isotope 1



Isotope 2

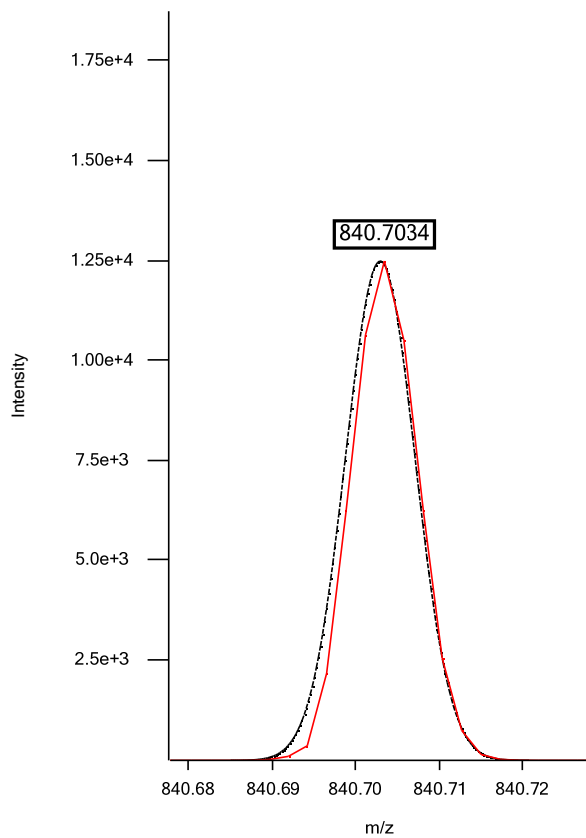


Isotope 3

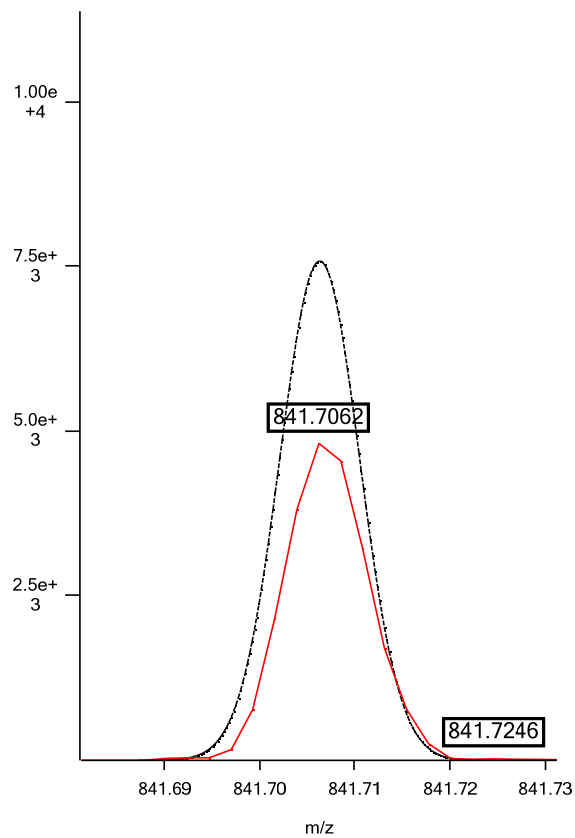


Positive ESI: TAG 50:6; C₅₃H₉₄NO₆; theoretical *m/z* 840.7081, (M+NH₄)⁺; isotopic fit 0.0375

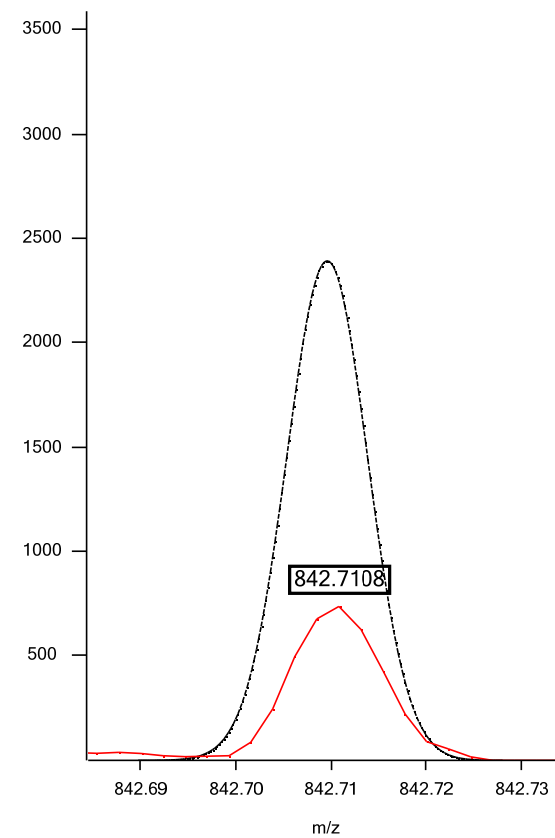
Isotope 1



Isotope 2

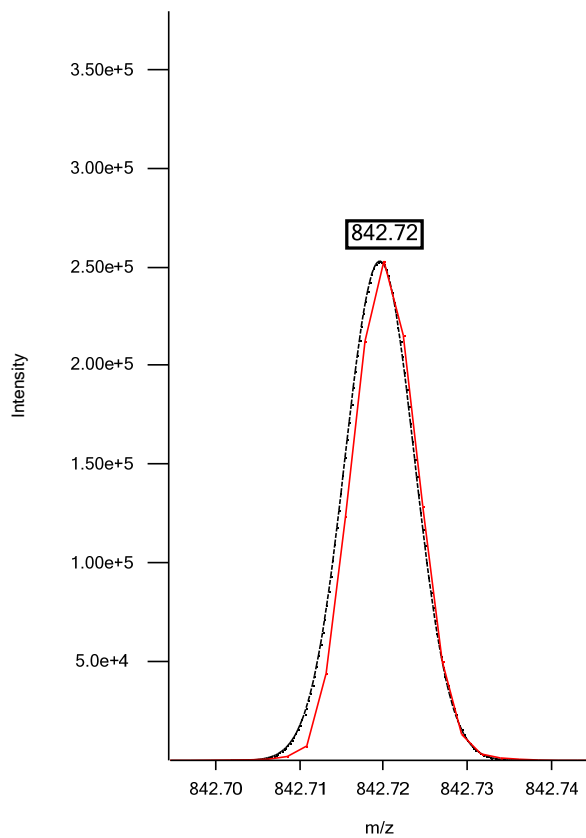


Isotope 3

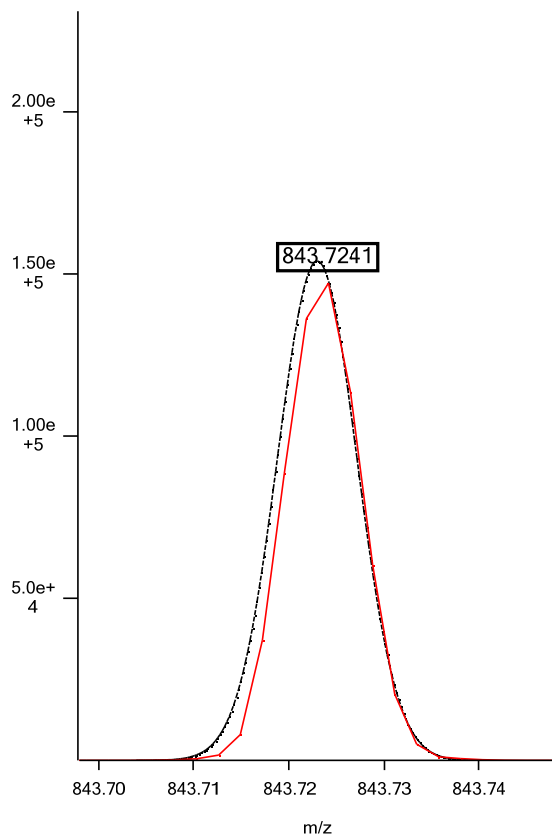


Positive ESI: TAG 50:5; C₅₃H₉₆NO₆; theoretical m/z 842.7237, (M+NH₄)⁺; isotopic fit 0.0052

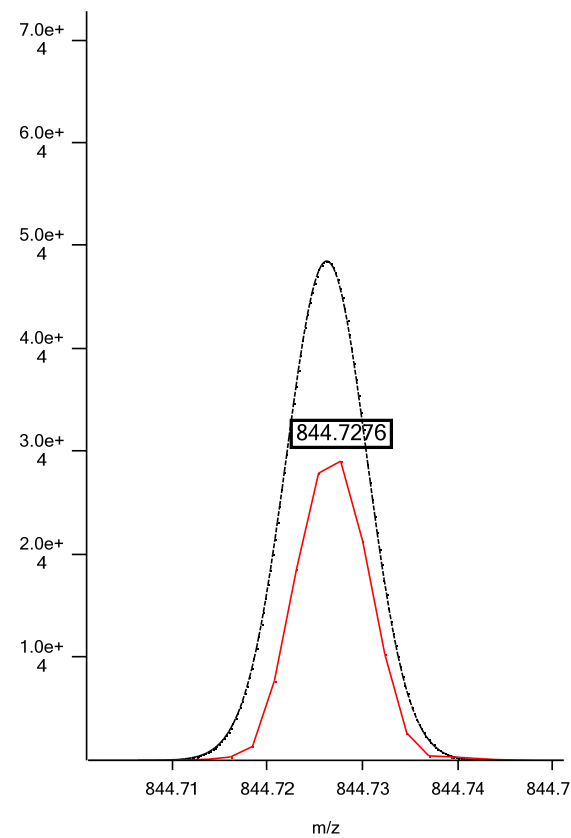
Isotope 1



Isotope 2

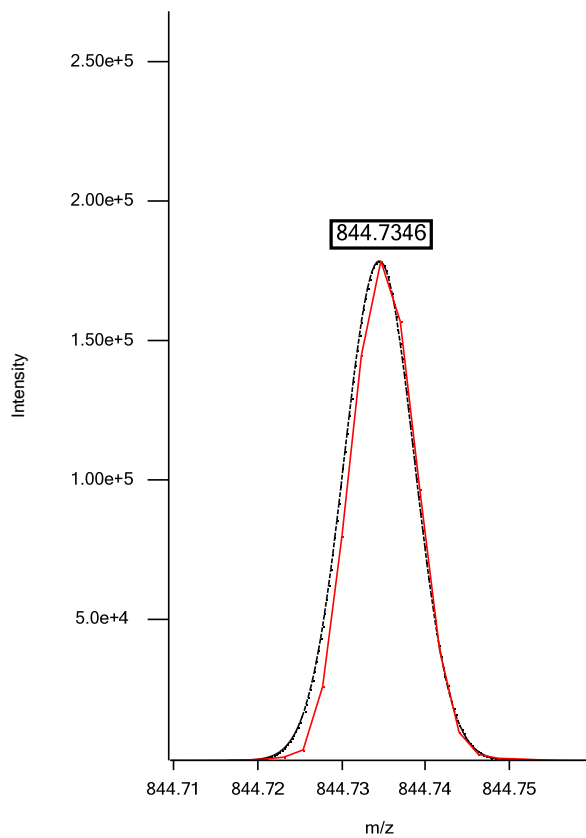


Isotope 3

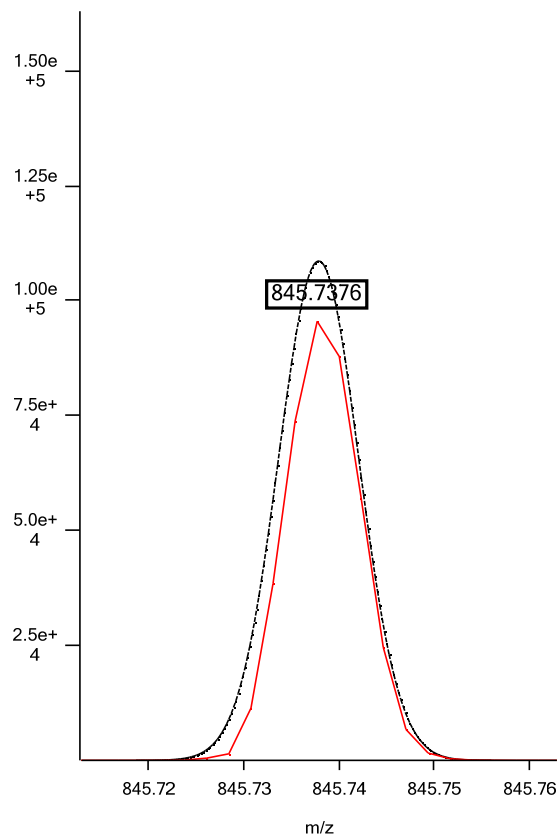


Positive ESI: TAG 50:4; C₅₃H₉₈NO₆; theoretical *m/z* 844.7394, (M+NH₄)⁺; isotopic fit 0.0117

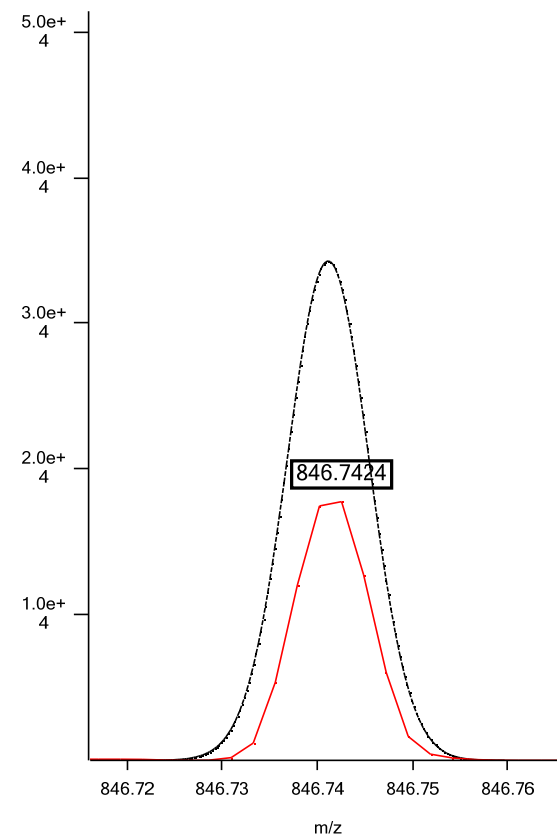
Isotope 1



Isotope 2

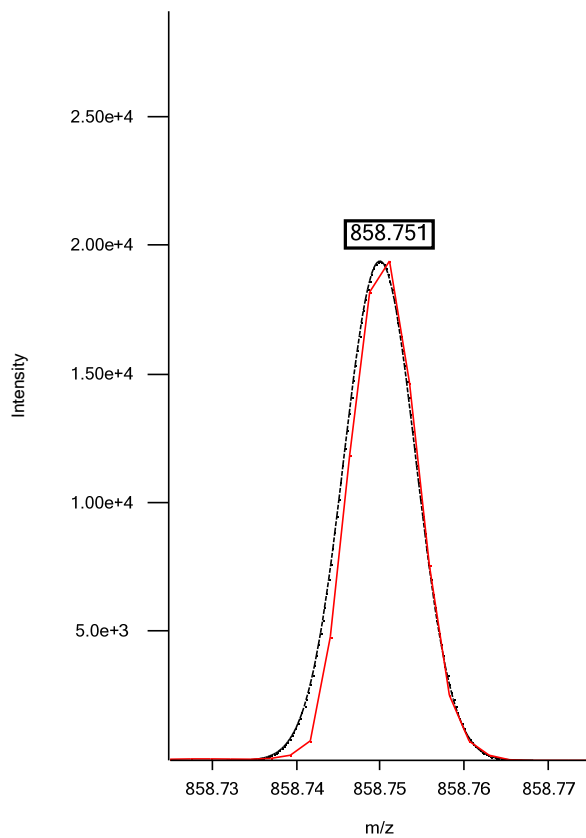


Isotope 3

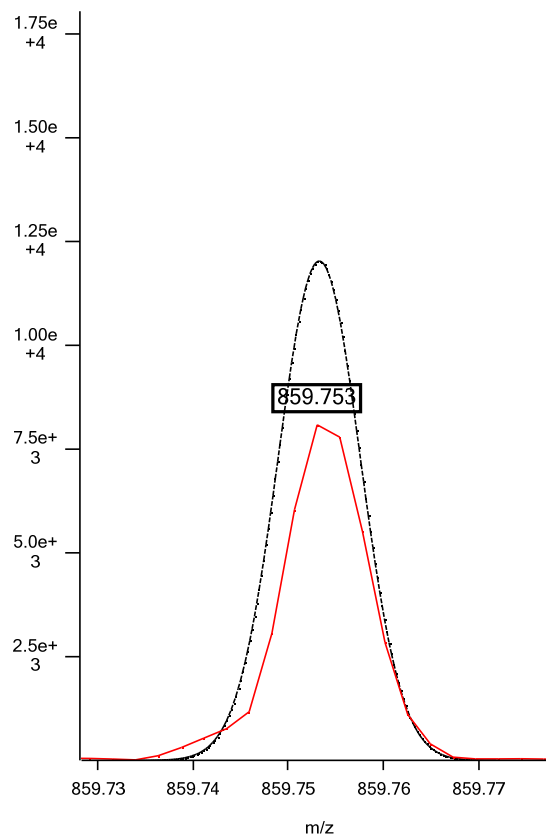


Positive ESI: TAG 51:4; C₅₄H₁₀₀NO₆; theoretical m/z 858.7550, (M+NH₄)⁺; isotopic fit 0.0338

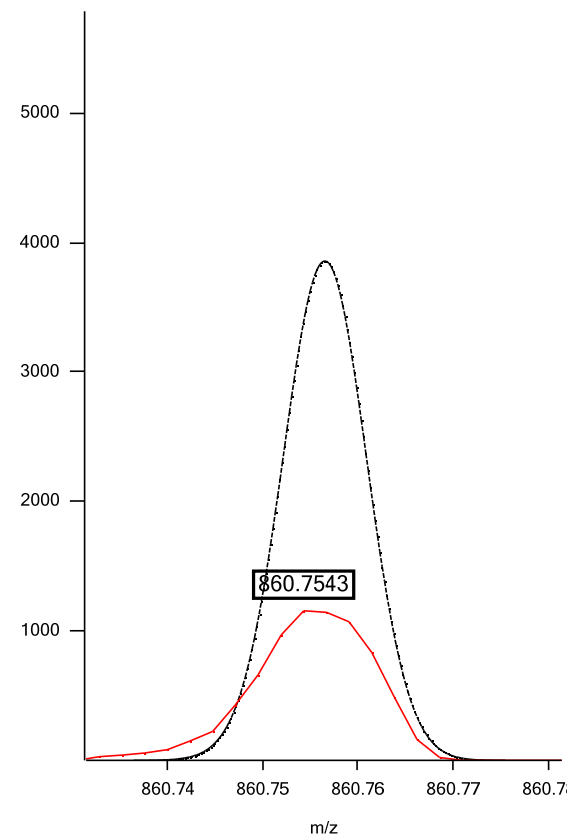
Isotope 1



Isotope 2

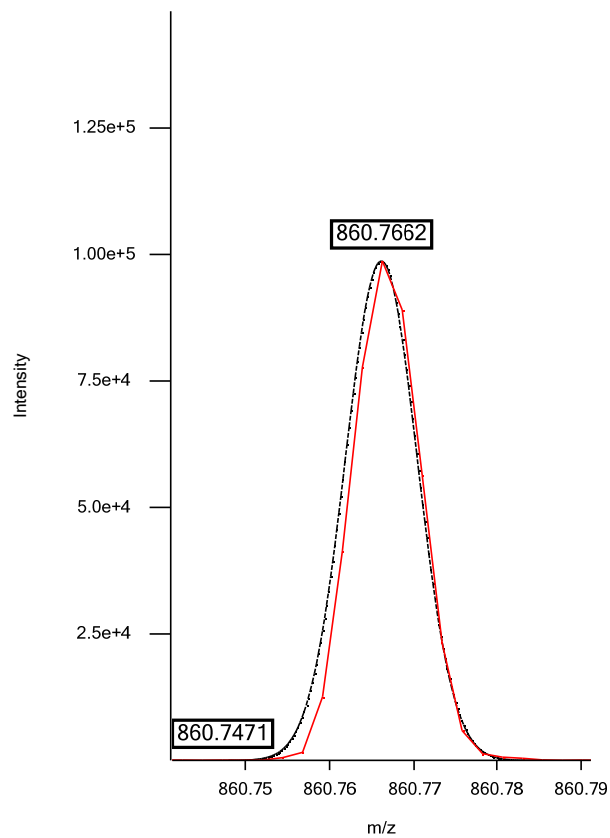


Isotope 3

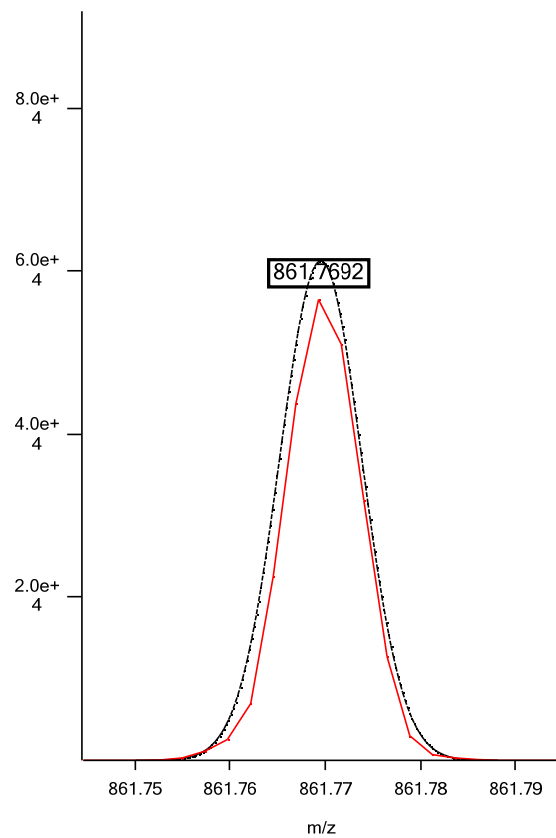


Positive ESI: TAG 51:3; C₅₄H₁₀₂NO₆; theoretical m/z 860.7707, (M+NH₄)⁺; isotopic fit 0.0096

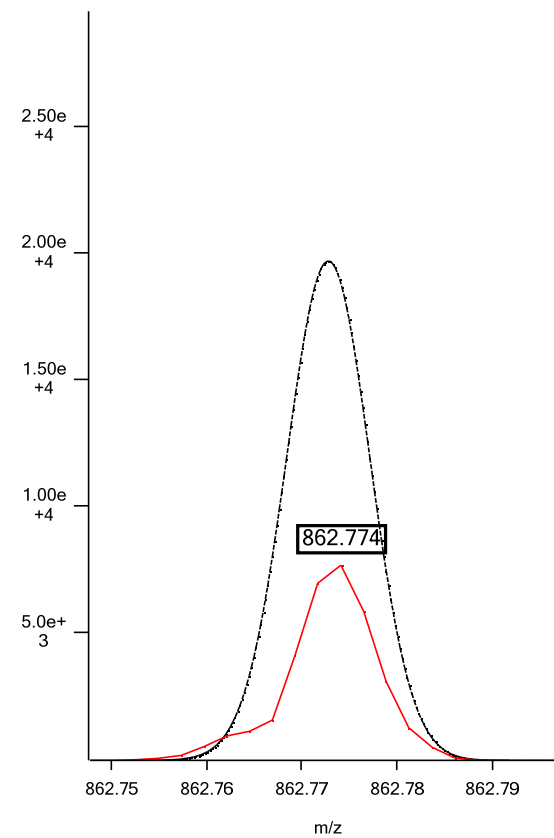
Isotope 1



Isotope 2

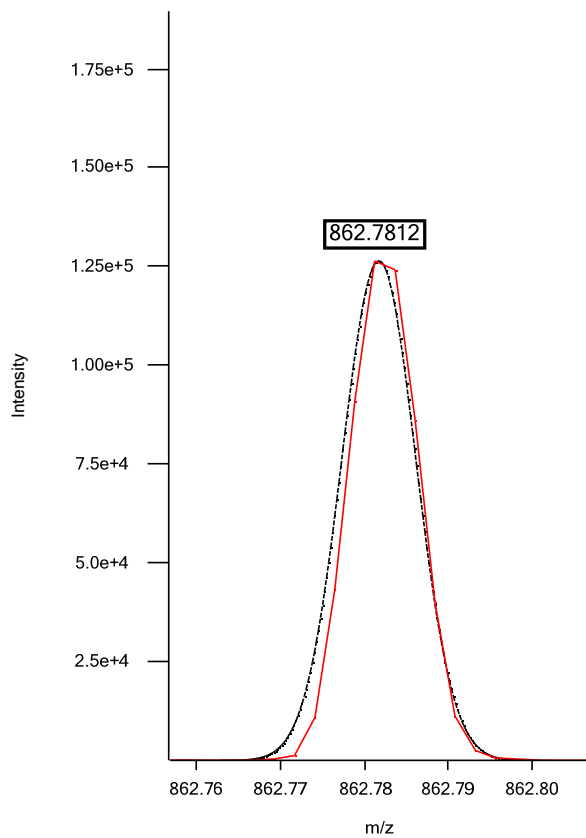


Isotope 3

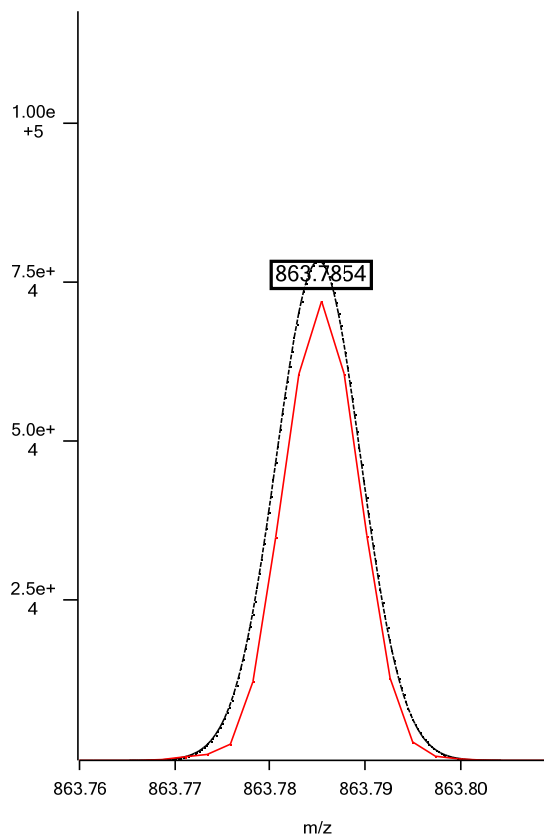


Positive ESI: TAG 51:2; C₅₄H₁₀₄NO₆; theoretical *m/z* 862.7863, (M+NH₄)⁺; isotopic fit 0.0085

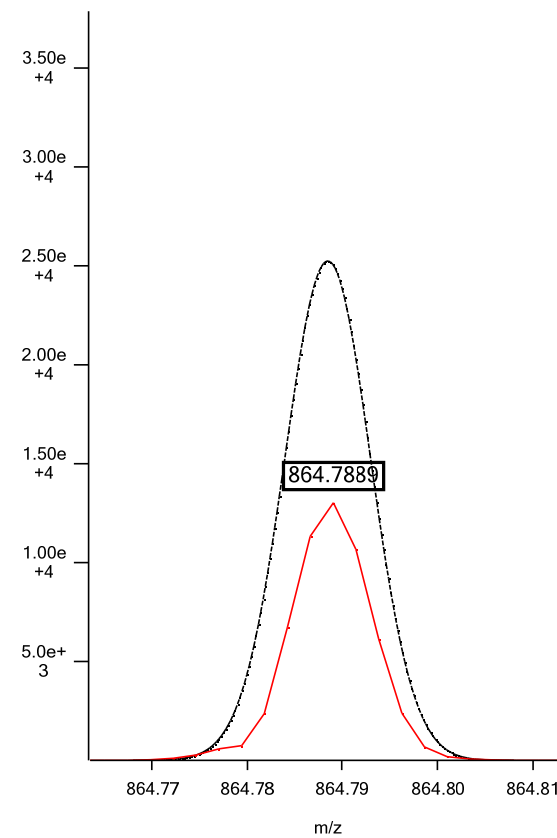
Isotope 1



Isotope 2

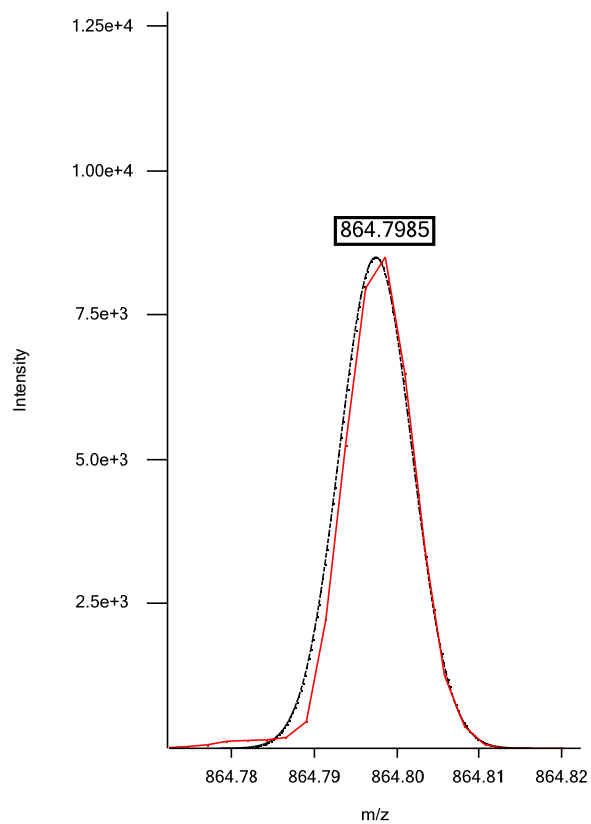


Isotope 3

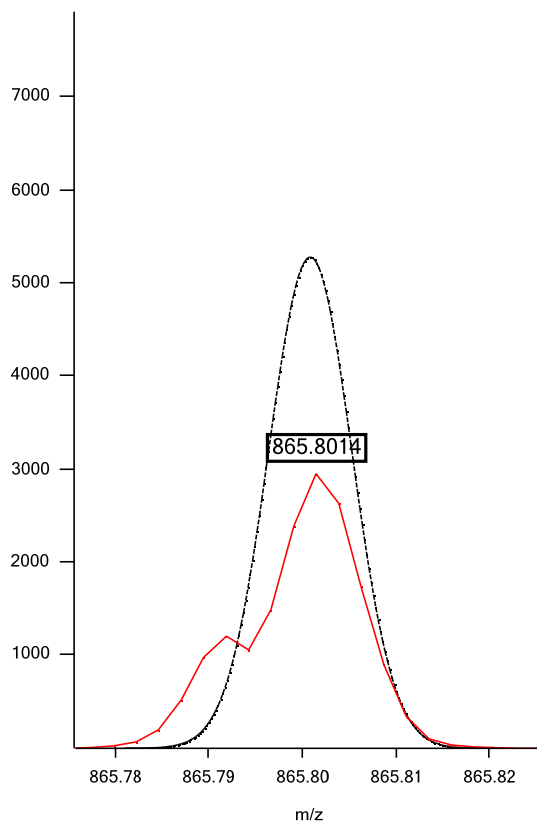


Positive ESI: TAG 51:1; C₅₄H₁₀₆NO₆; theoretical *m/z* 864.8020, (M+NH₄)⁺; isotopic fit 0.0581

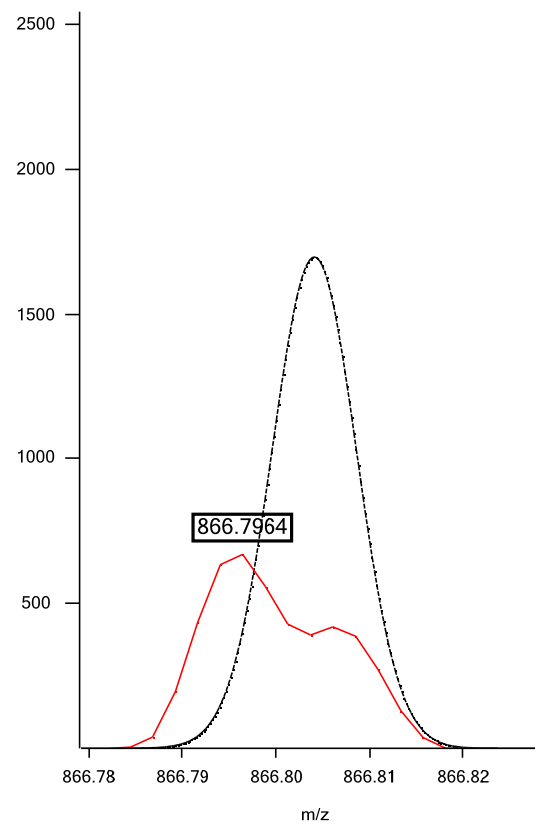
Isotope 1



Isotope 2

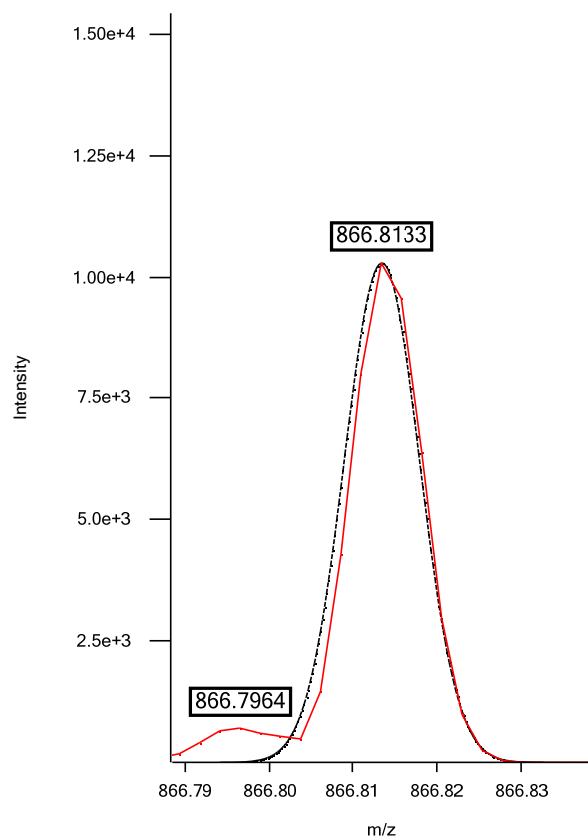


Isotope 3

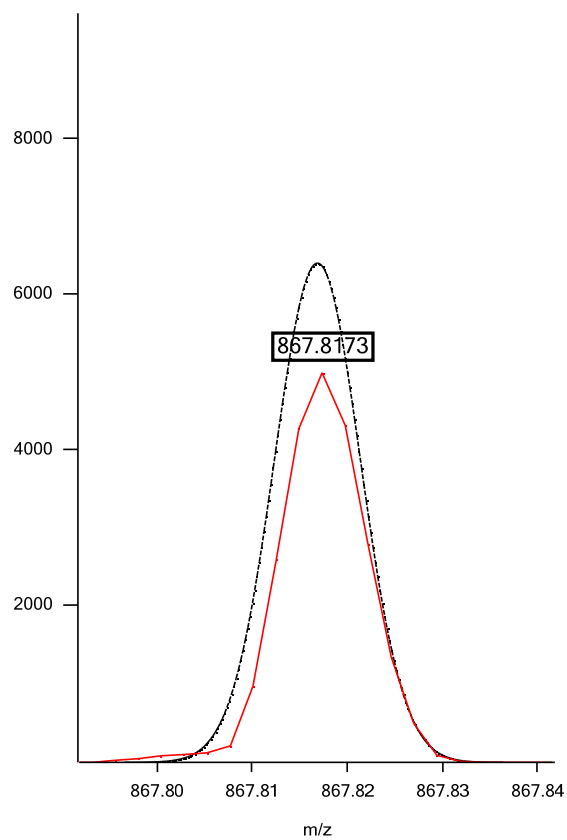


Positive ESI: TAG 51:0; C₅₄H₁₀₈NO₆; theoretical *m/z* 866.8176, (M+NH₄)⁺; isotopic fit 0.0173

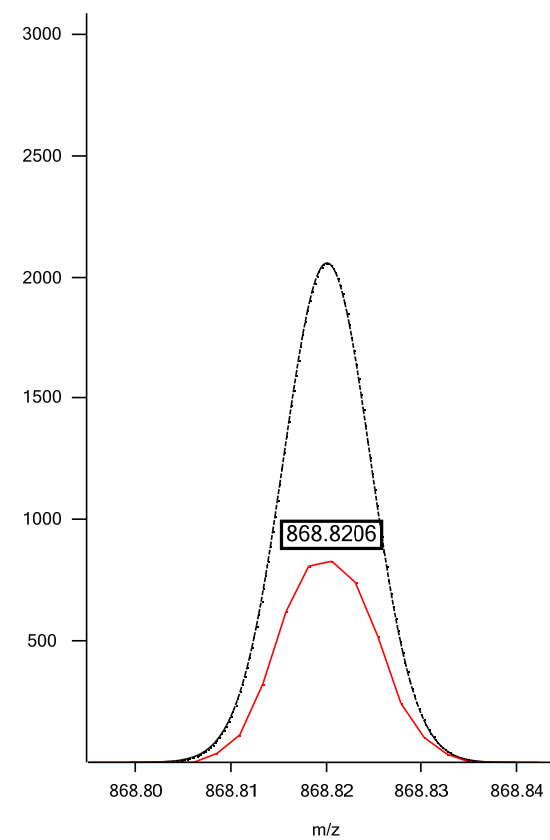
Isotope 1



Isotope 2

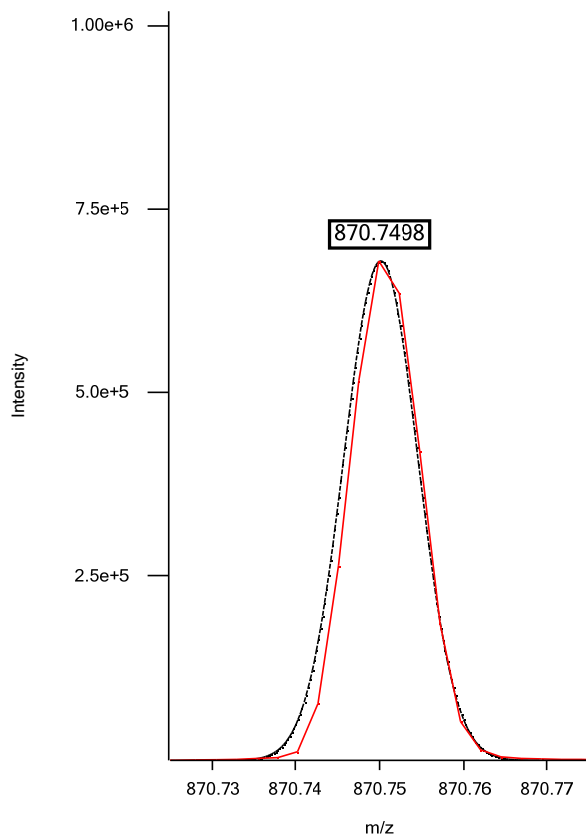


Isotope 3

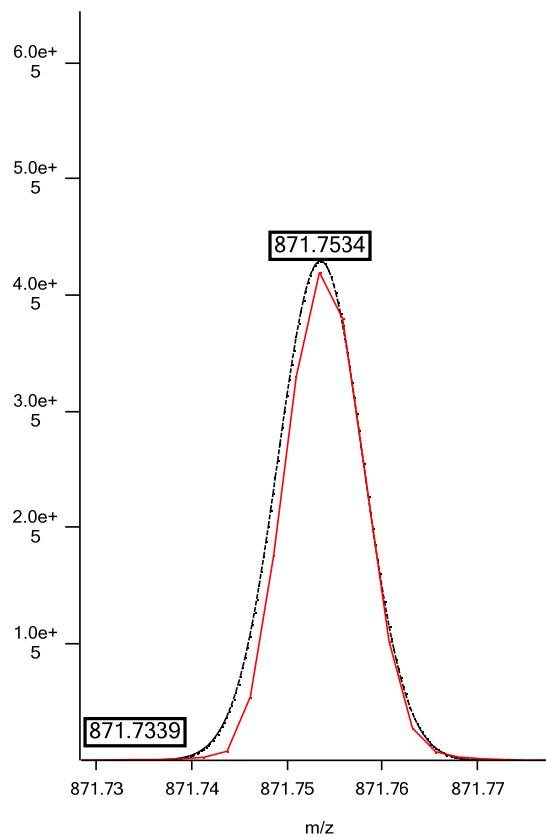


Positive ESI: TAG 52:5; C₅₅H₁₀₀NO₆; theoretical *m/z* 870.7551, (M+NH₄)⁺; isotopic fit 0.0029

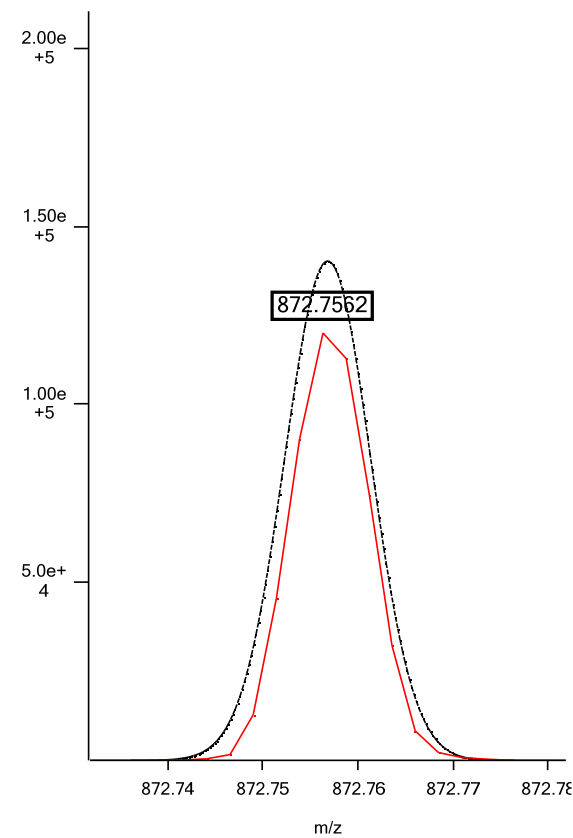
Isotope 1



Isotope 2

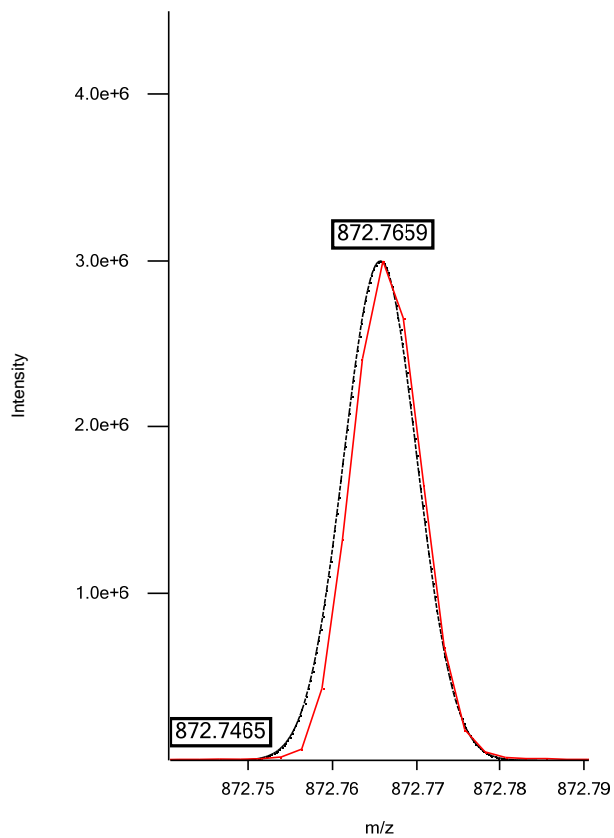


Isotope 3

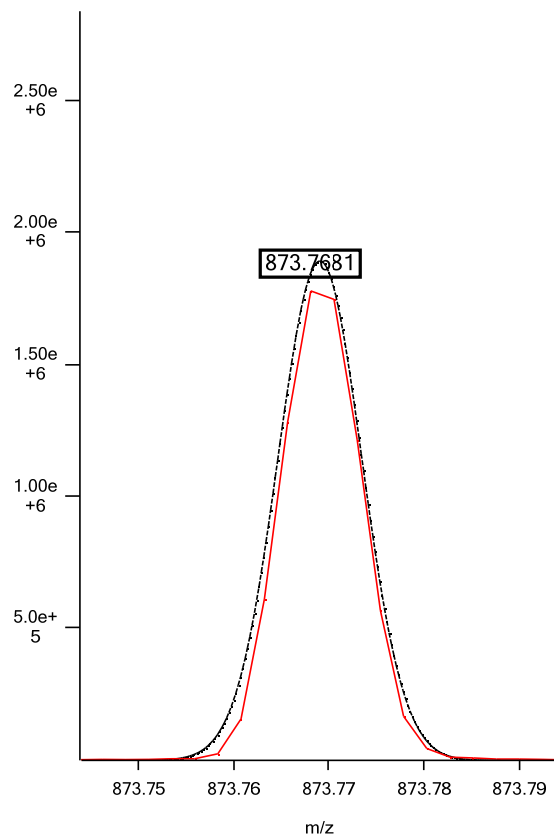


Positive ESI: TAG 52:4; C₅₅H₁₀₂NO₆; theoretical *m/z* 872.7707, (M+NH₄)⁺; isotopic fit 0.0043

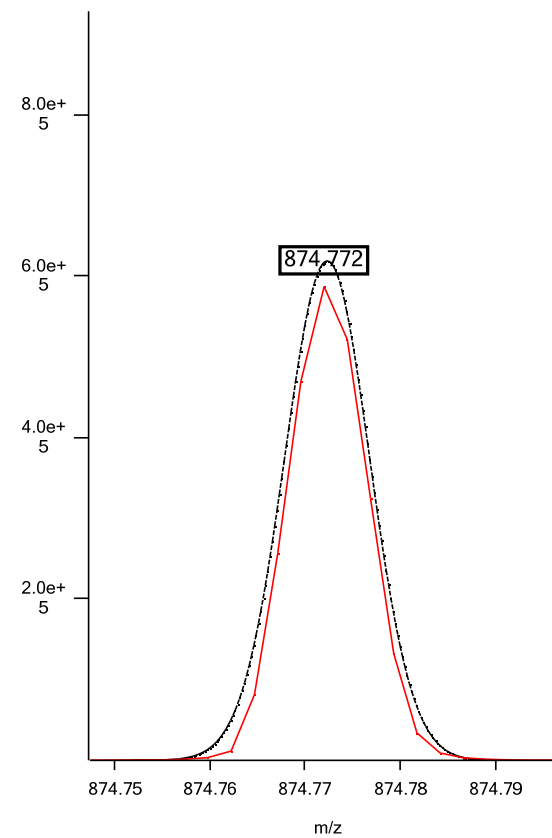
Isotope 1



Isotope 2

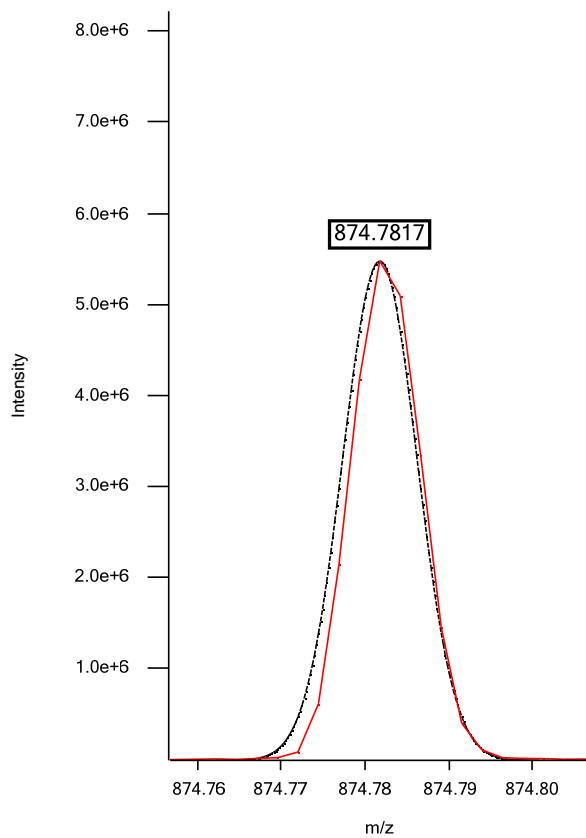


Isotope 3

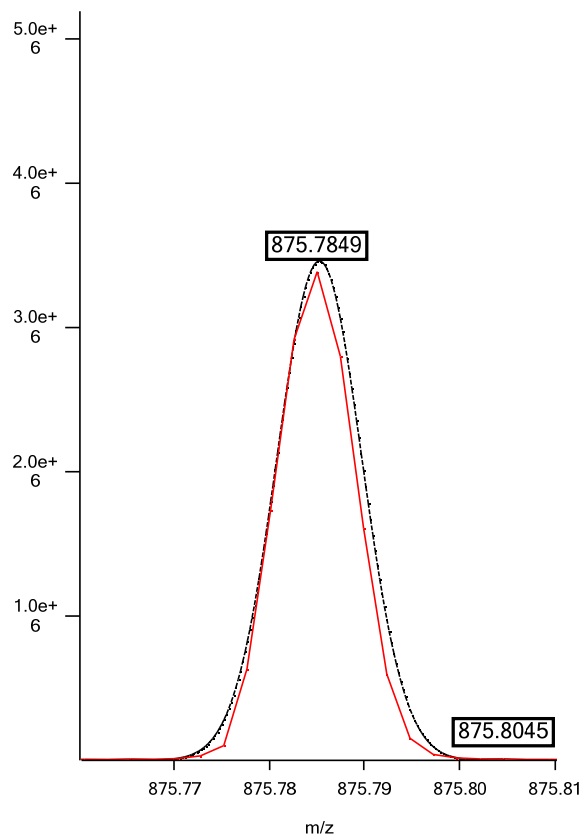


Positive ESI: TAG 52:3; C₅₅H₁₀₄NO₆; theoretical *m/z* 874.7864, (M+NH₄)⁺; isotopic fit 0.0101

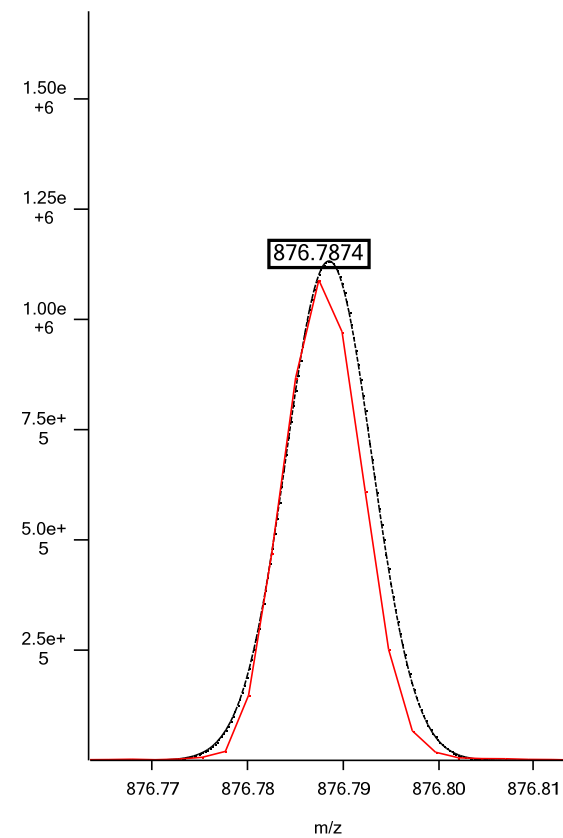
Isotope 1



Isotope 2

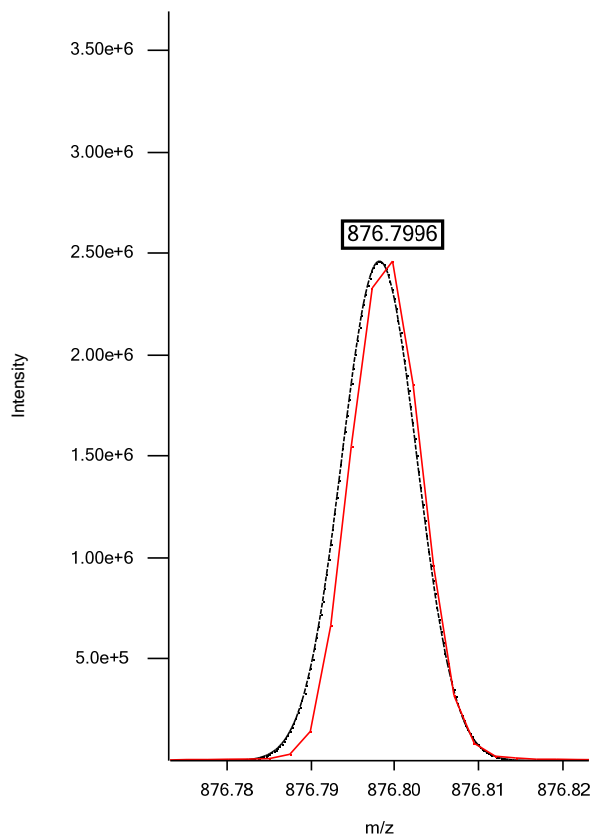


Isotope 3

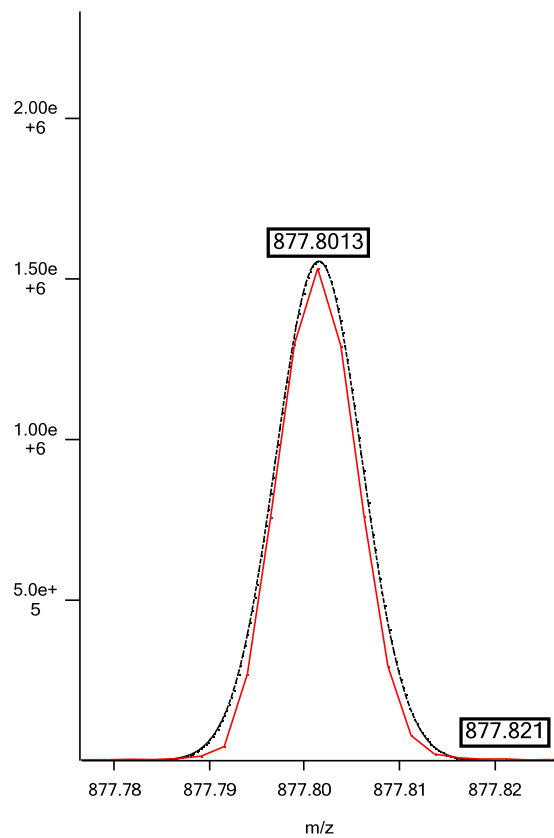


Positive ESI: TAG 52:2; C₅₅H₁₀₆NO₆; theoretical *m/z* 876.8020, (M+NH₄)⁺; isotopic fit 0.0087

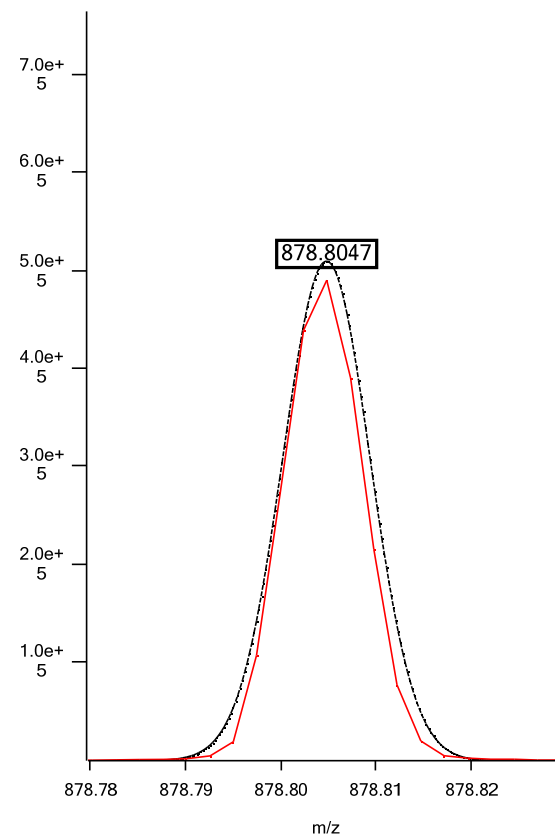
Isotope 1



Isotope 2

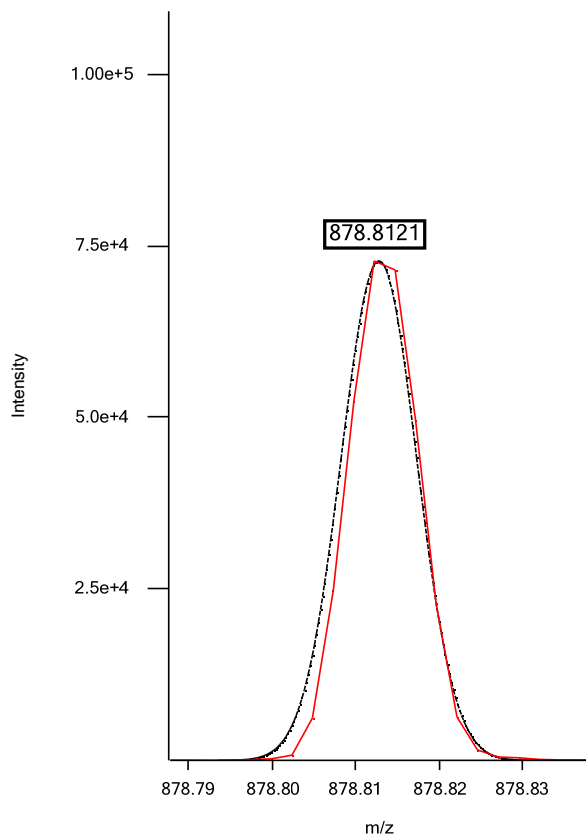


Isotope 3

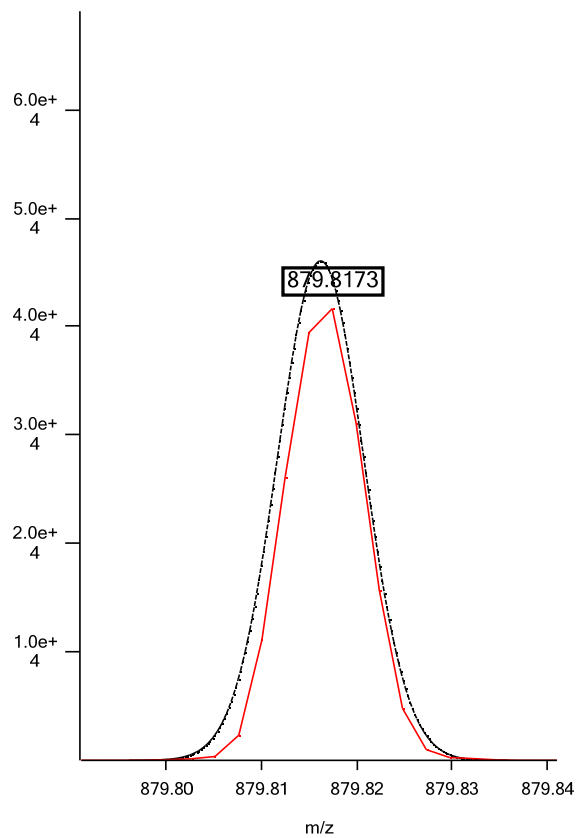


Positive ESI: TAG 52:1; C₅₅H₁₀₈NO₆; theoretical m/z 878.8176, (M+NH₄)⁺; isotopic fit 0.0080

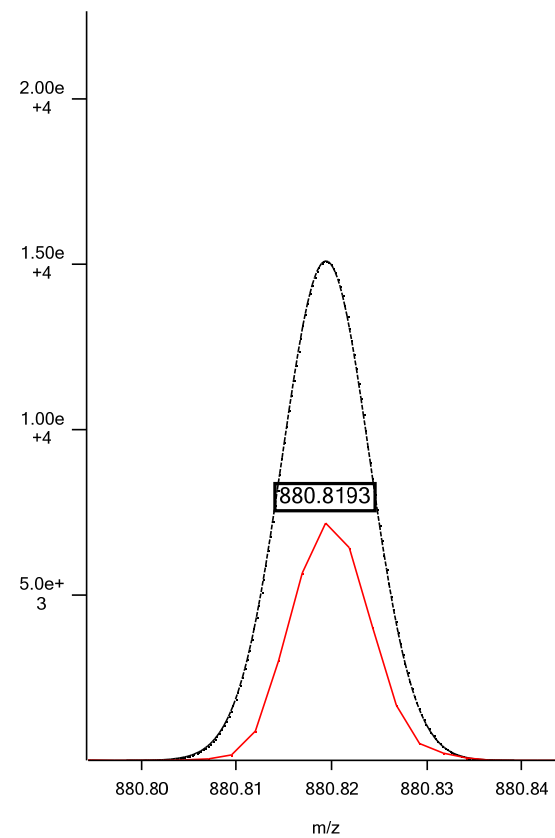
Isotope 1



Isotope 2

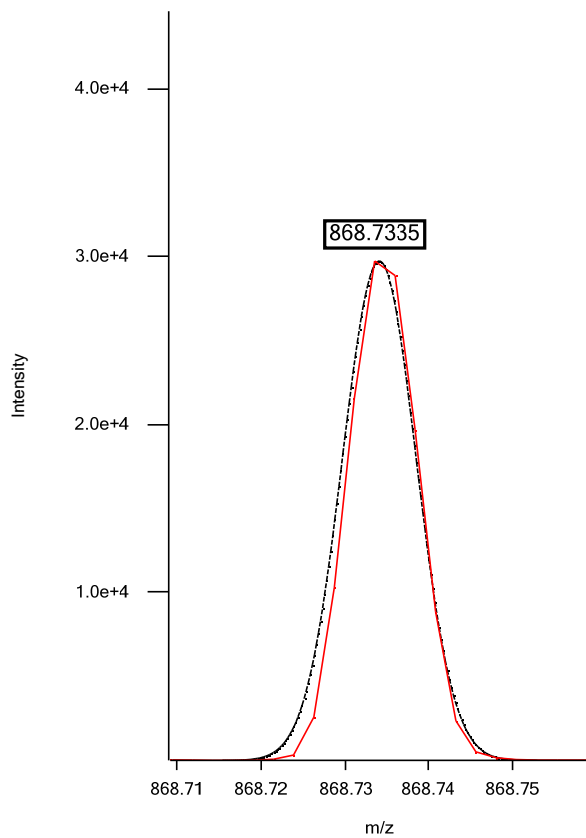


Isotope 3

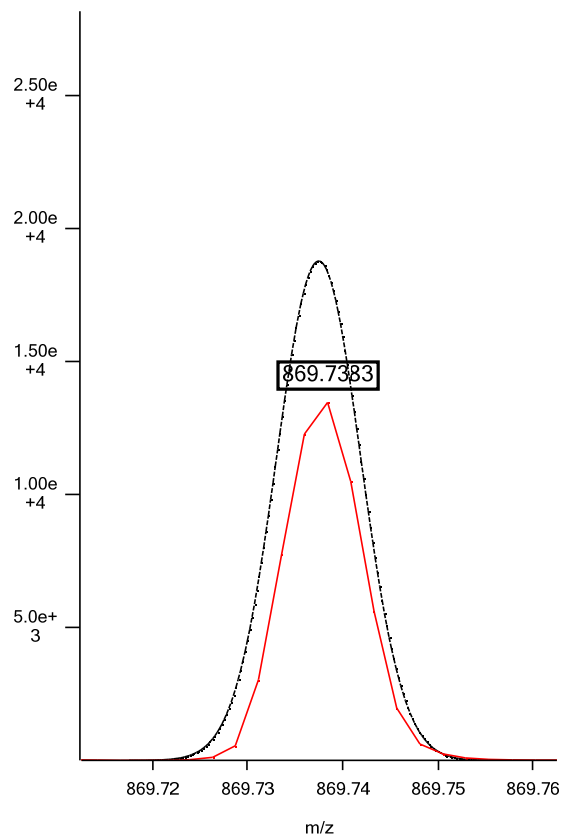


Positive ESI: TAG 52:6; C₅₅H₉₈NO₆; theoretical m/z 868.7394, (M+NH₄)⁺; isotopic fit 0.0281

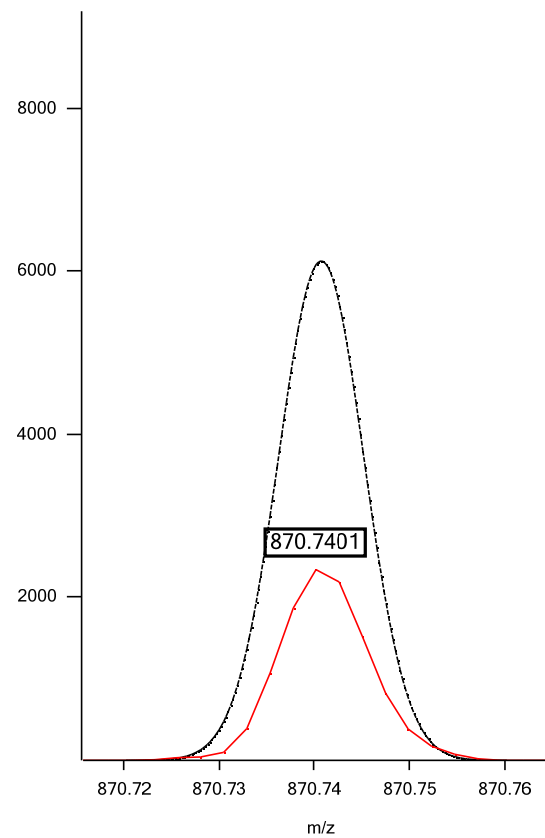
Isotope 1



Isotope 2

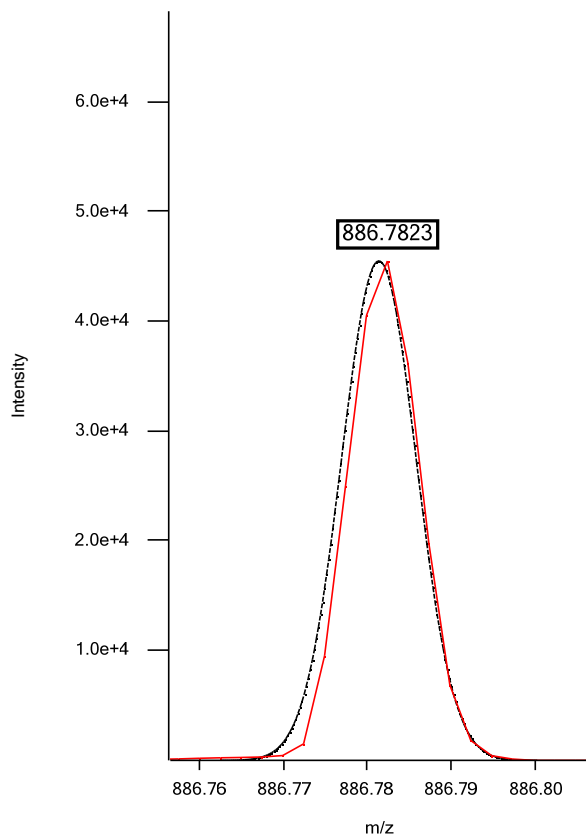


Isotope 3

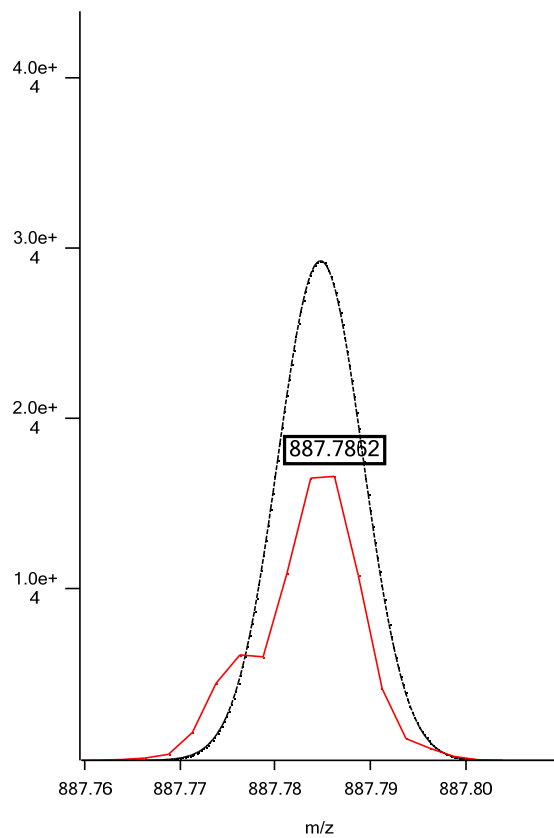


Positive ESI: TAG 53:4; C₅₆H₁₀₄NO₆; theoretical *m/z* 886.7863, (M+NH₄)⁺; isotopic fit 0.0583

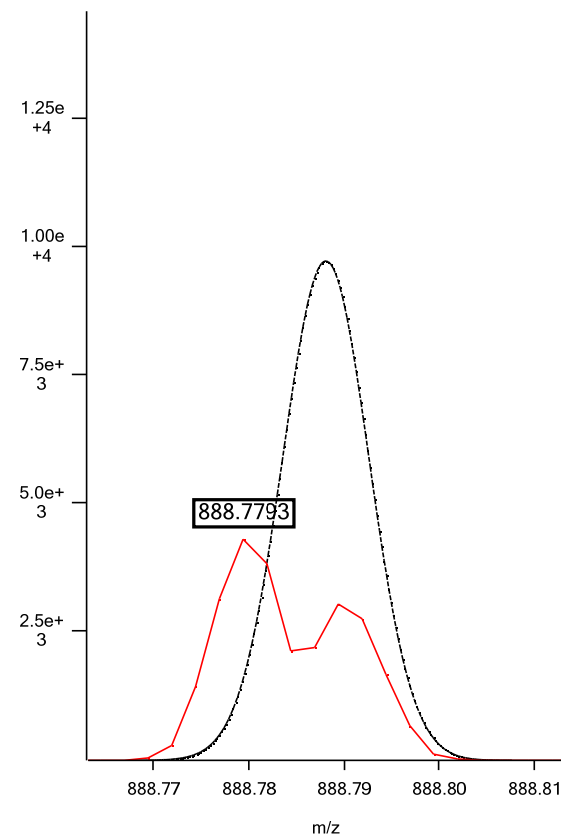
Isotope 1



Isotope 2

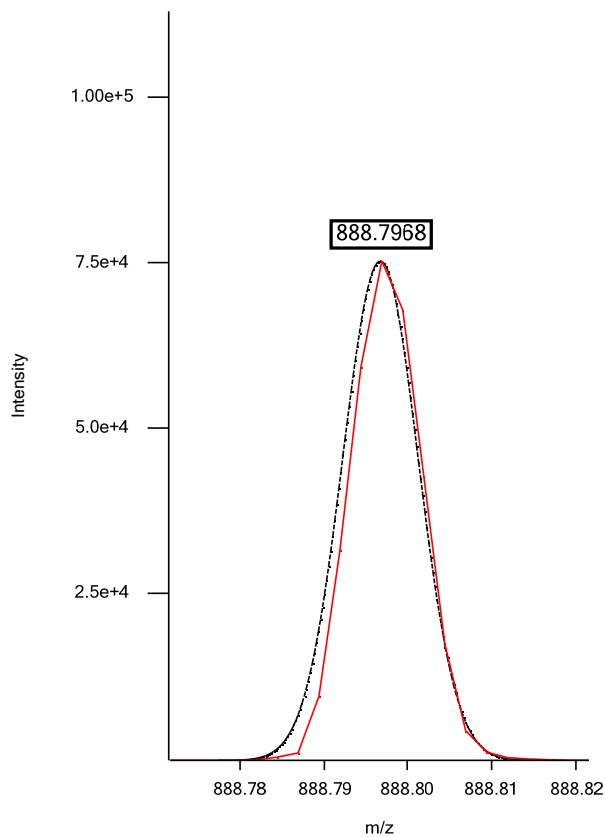


Isotope 3

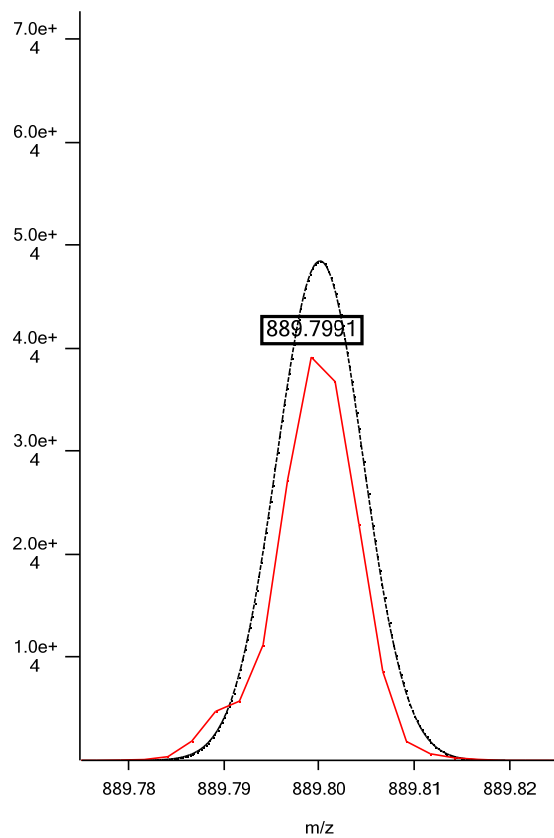


Positive ESI: TAG 53:3; C₅₆H₁₀₆NO₆; theoretical *m/z* 888.8020, (M+NH₄)⁺; isotopic fit 0.0215

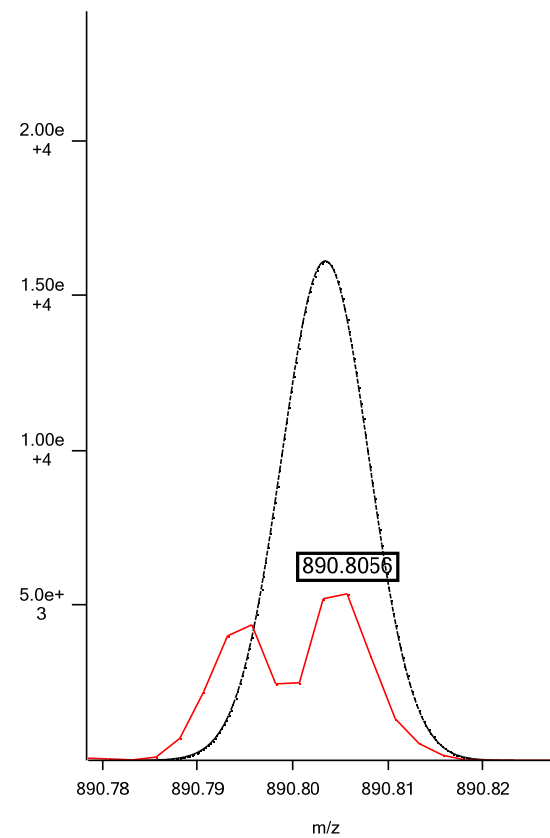
Isotope 1



Isotope 2

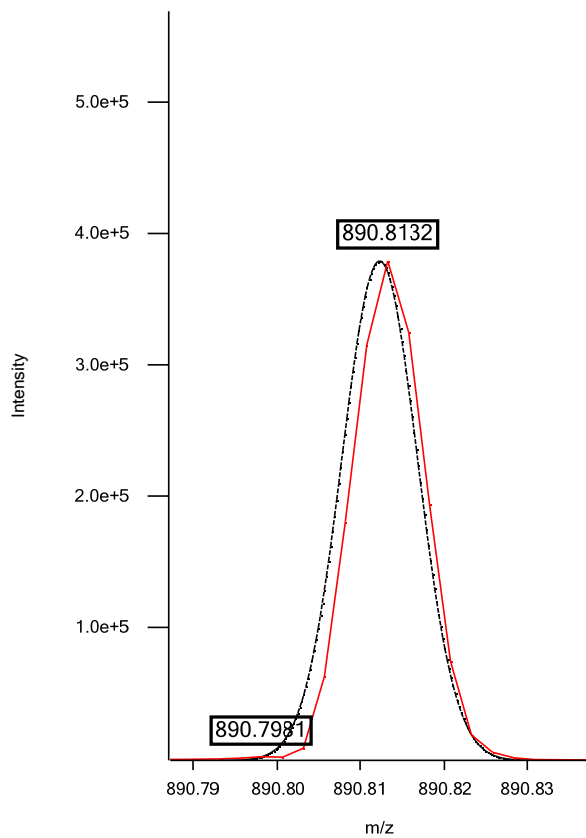


Isotope 3

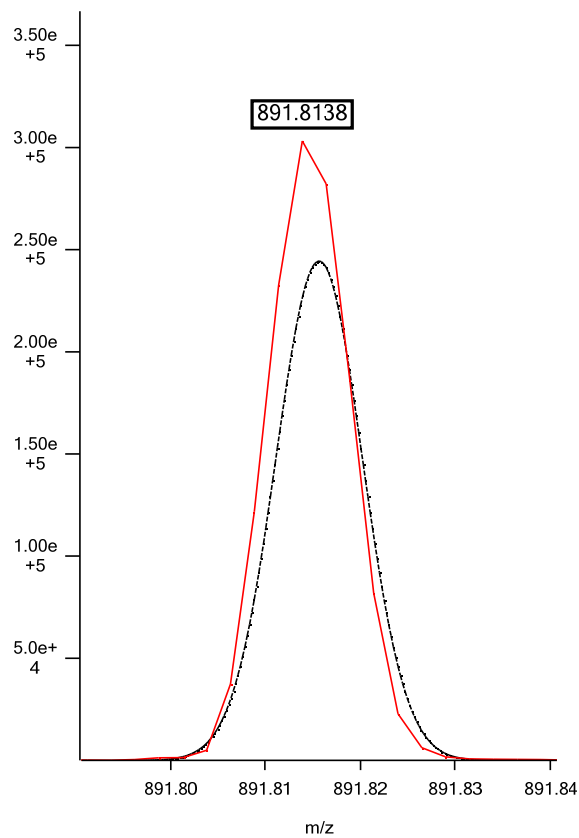


Positive ESI: TAG 53:2; $C_{56}H_{108}NO_6$; theoretical m/z 890.8176, $(M+NH_4)^+$; isotopic fit 0.0328

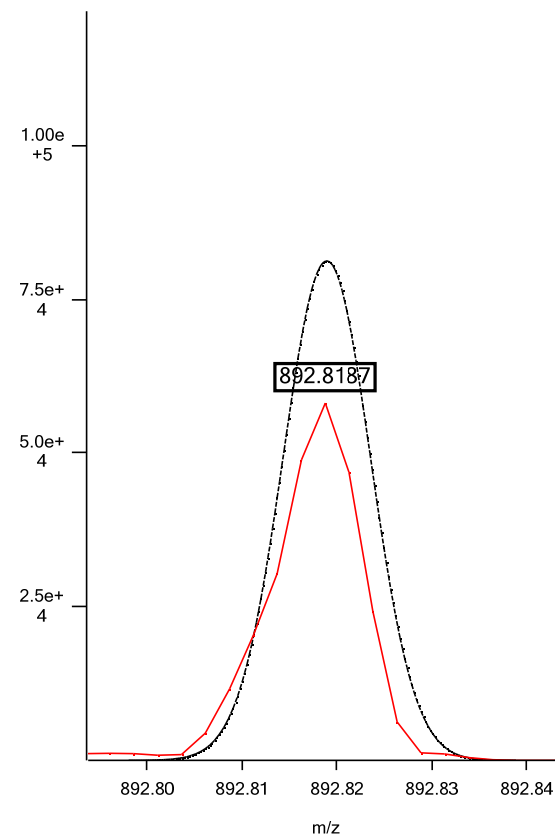
Isotope 1



Isotope 2

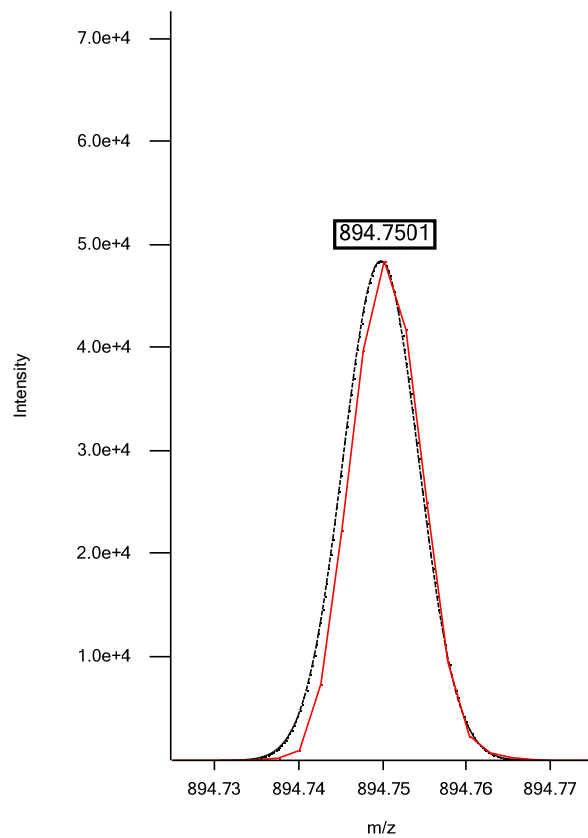


Isotope 3

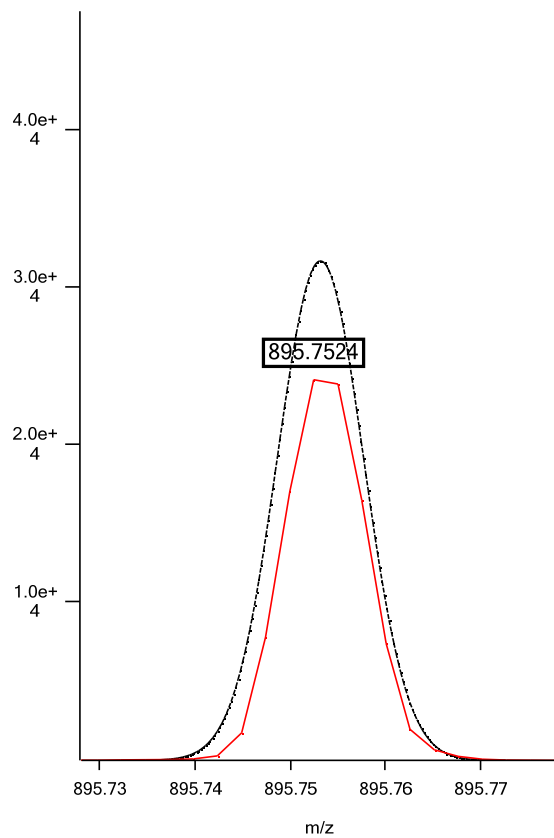


Positive ESI: TAG 54:7; C₅₇H₁₀₀NO₆; theoretical *m/z* 894.7551, (M+NH₄)⁺; isotopic fit 0.0224

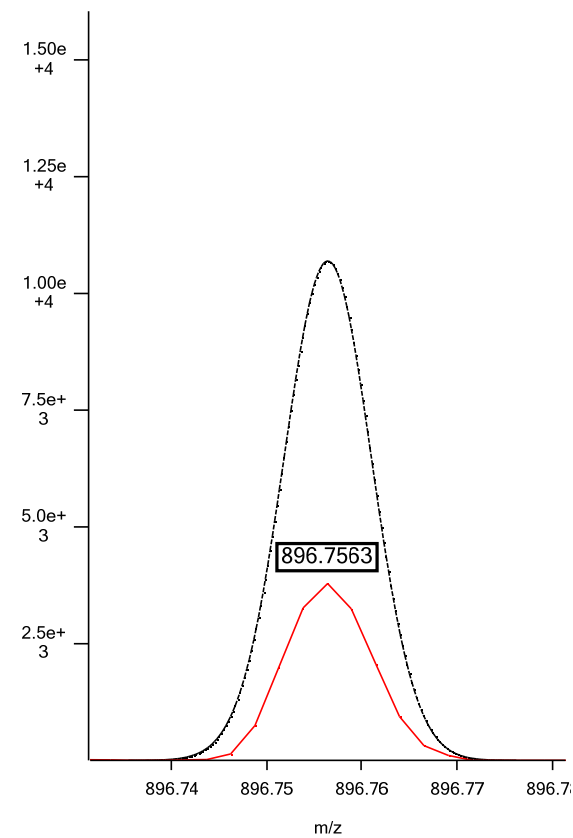
Isotope 1



Isotope 2

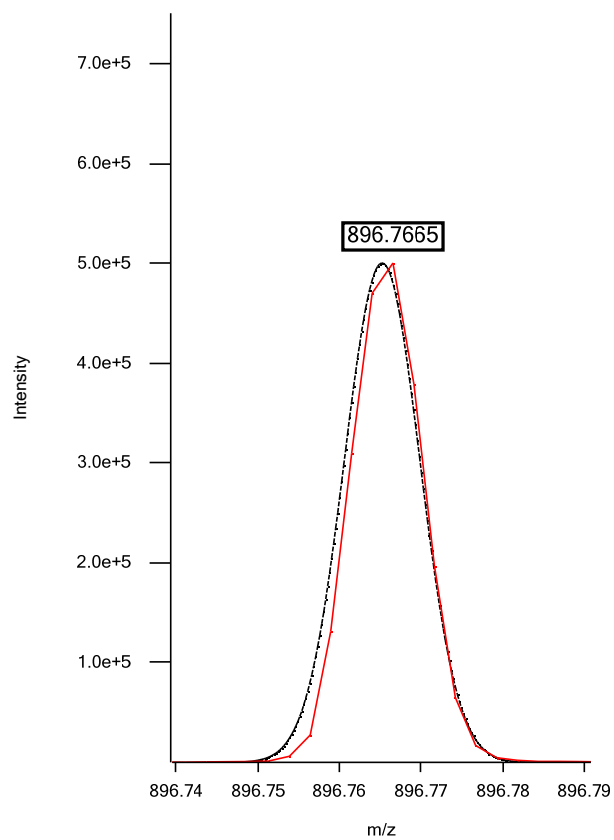


Isotope 3

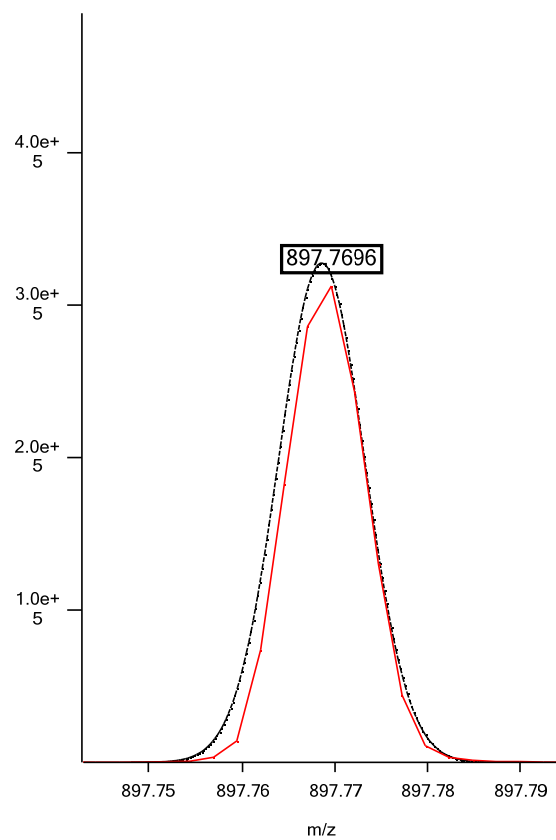


Positive ESI: TAG 54:6; $C_{57}H_{102}NO_6$; theoretical m/z 896.7707, $(M+NH_4)^+$; isotopic fit 0.0058

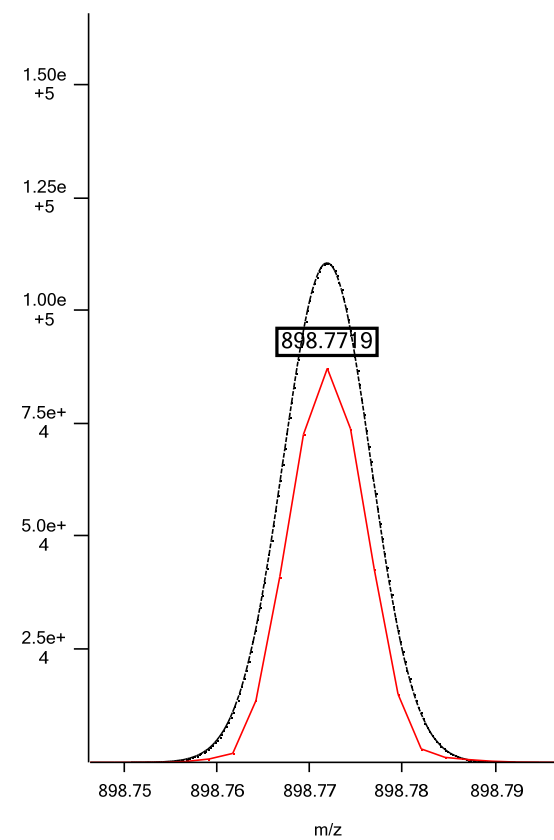
Isotope 1



Isotope 2

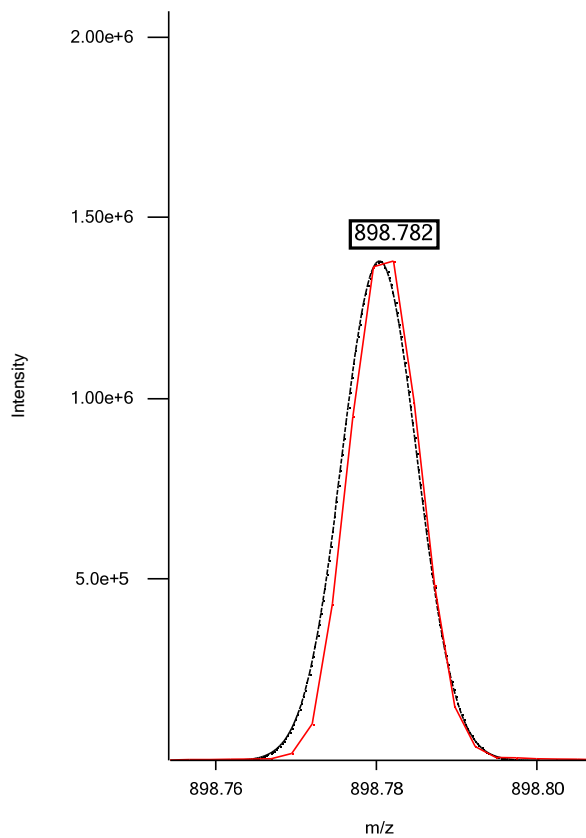


Isotope 3

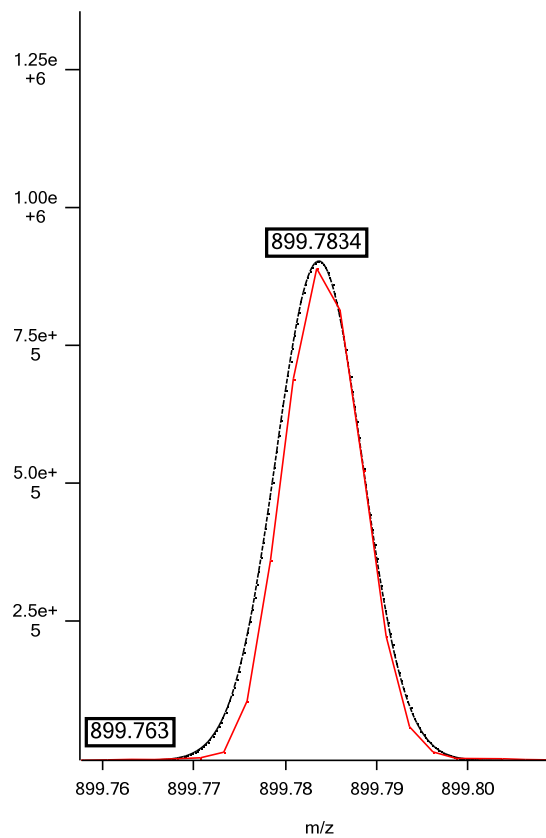


Positive ESI: TAG 54:5; C₅₇H₁₀₄NO₆; theoretical *m/z* 898.7864, (M+NH₄)⁺; isotopic fit 0.0038

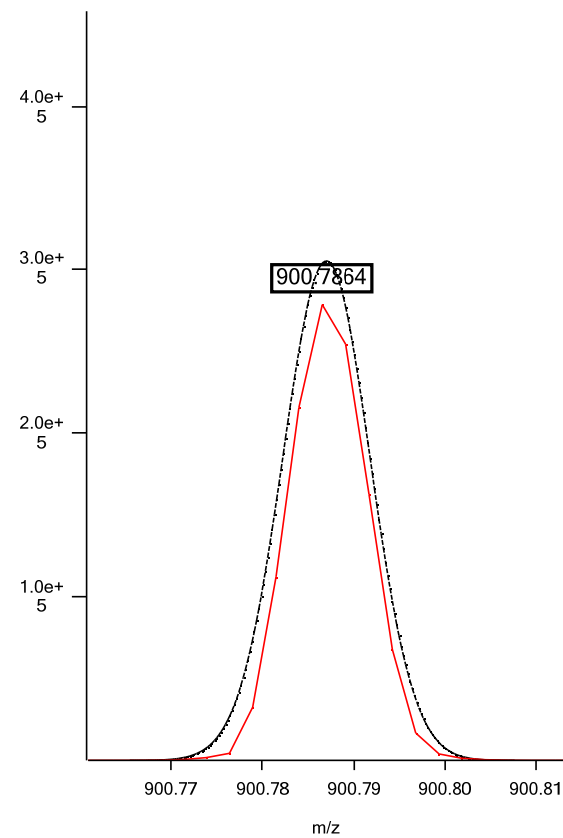
Isotope 1



Isotope 2

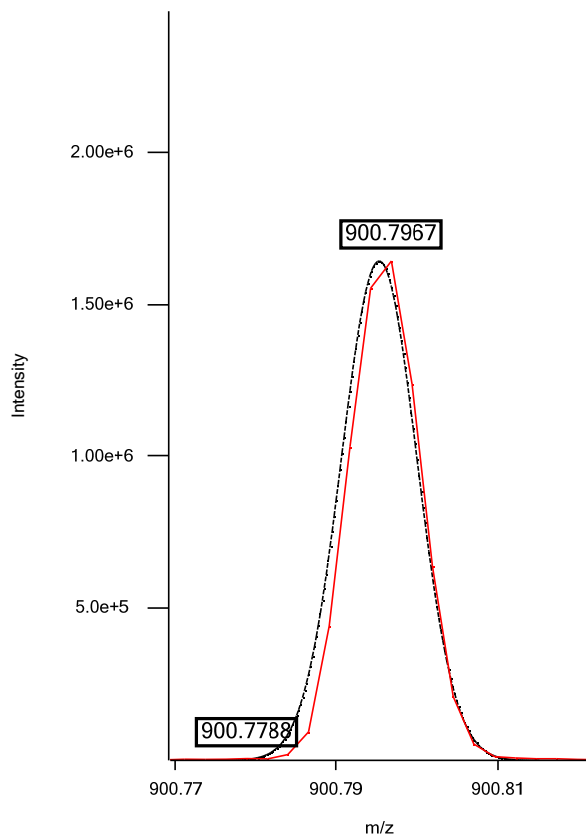


Isotope 3

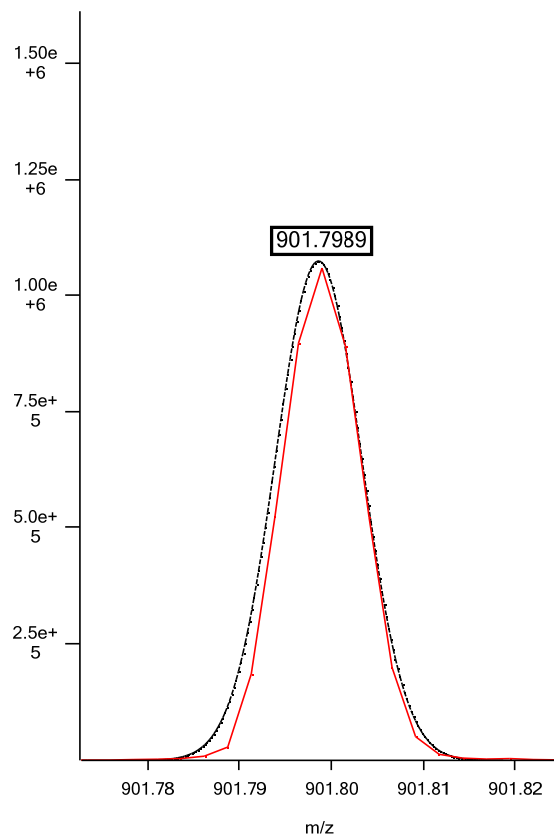


Positive ESI: TAG 54:4; C₅₇H₁₀₆NO₆; theoretical *m/z* 900.8020, (M+NH₄)⁺; isotopic fit 0.0035

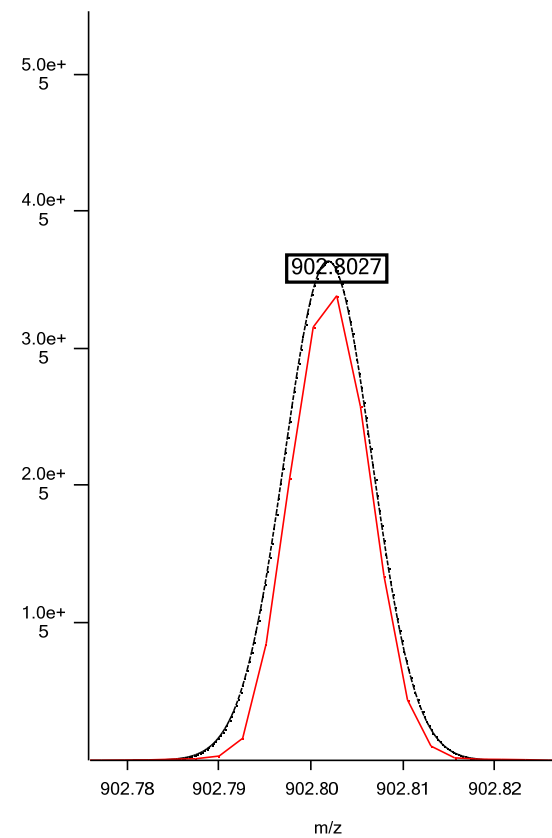
Isotope 1



Isotope 2

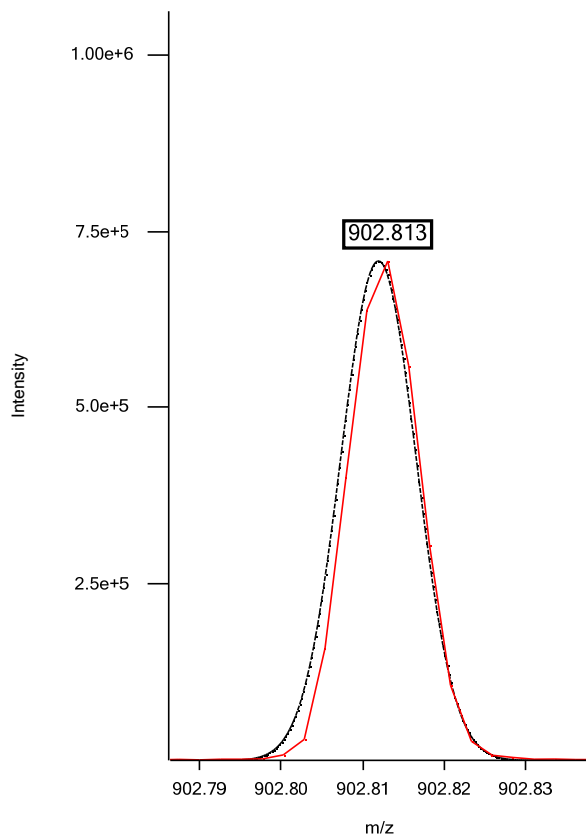


Isotope 3

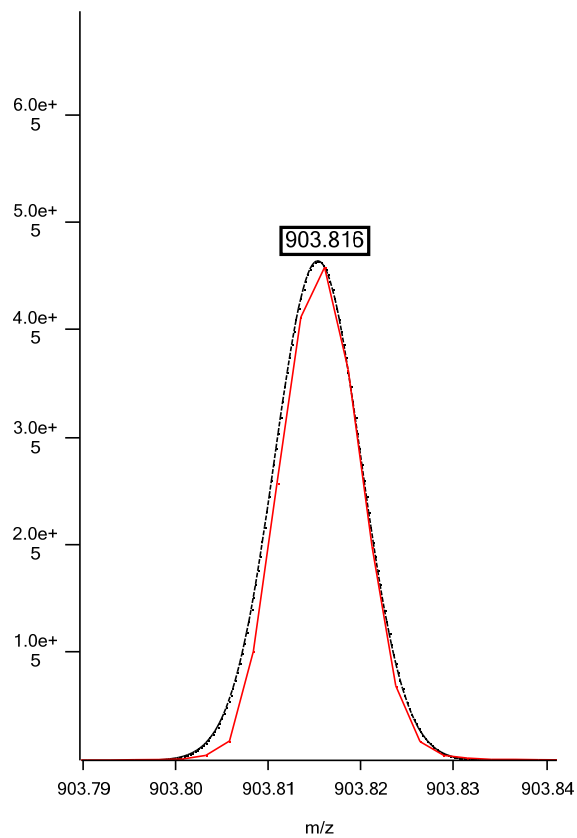


Positive ESI: TAG 54:3; C₅₇H₁₀₈NO₆; theoretical *m/z* 902.8177, (M+NH₄)⁺; isotopic fit 0.0025

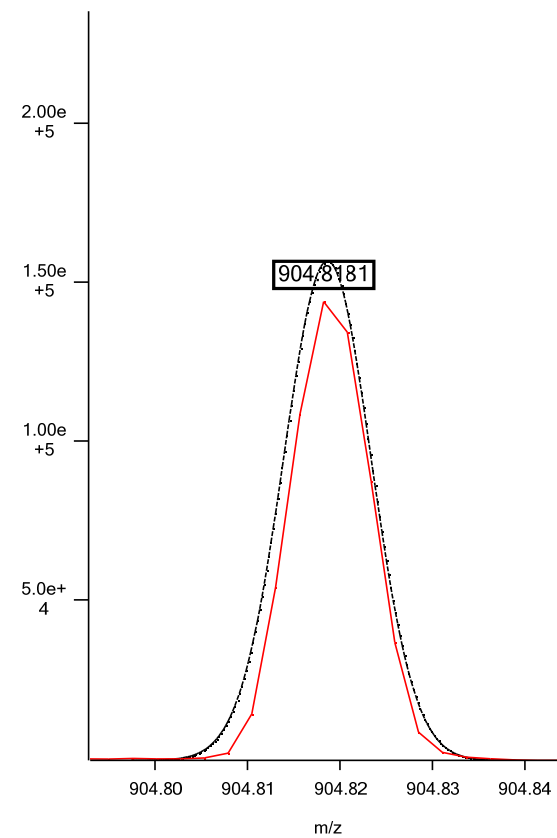
Isotope 1



Isotope 2

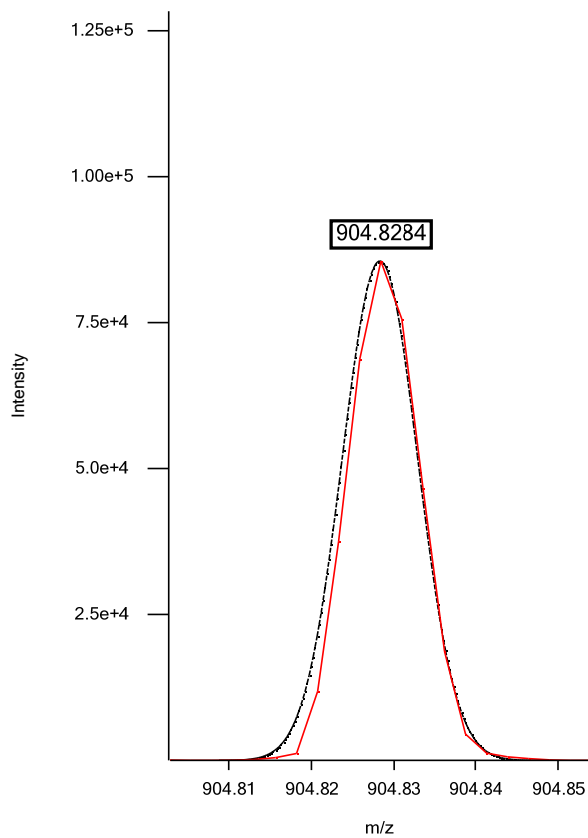


Isotope 3

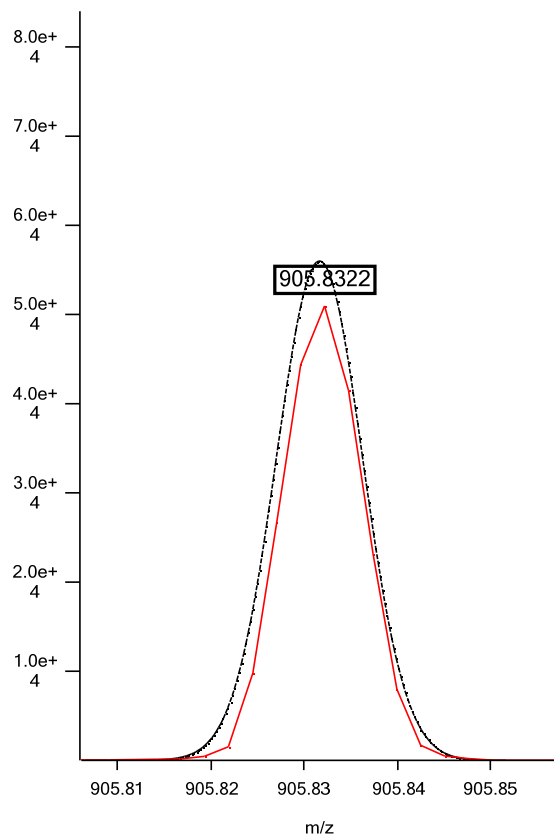


Positive ESI: TAG 54:2; C₅₇H₁₁₀NO₆; theoretical m/z 904.8333, (M+NH₄)⁺; isotopic fit 0.0075

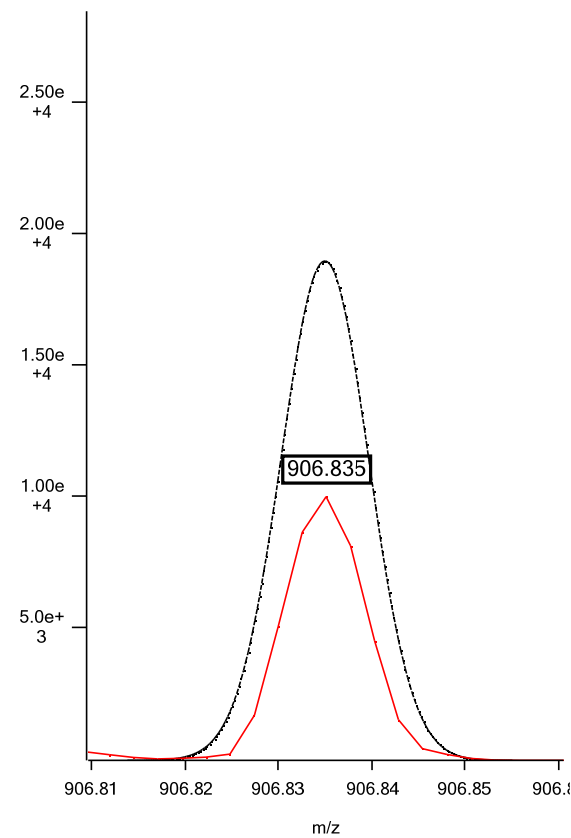
Isotope 1



Isotope 2

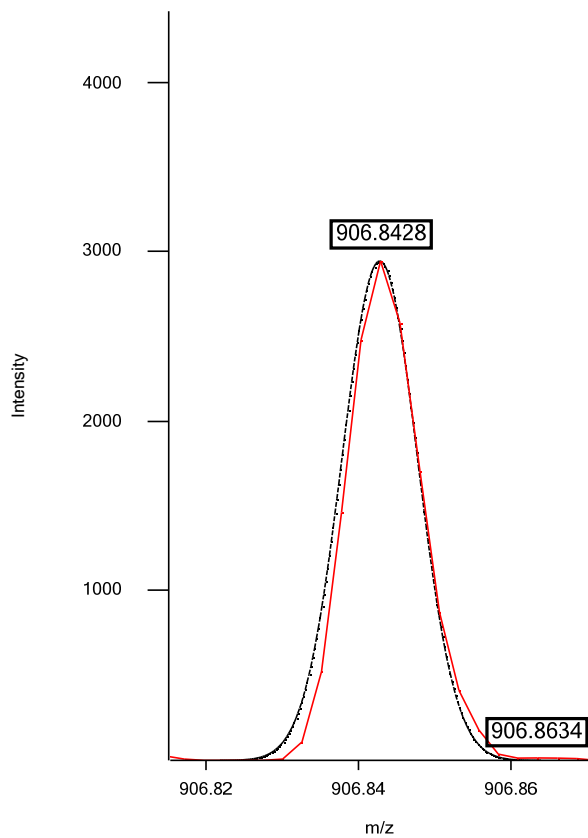


Isotope 3

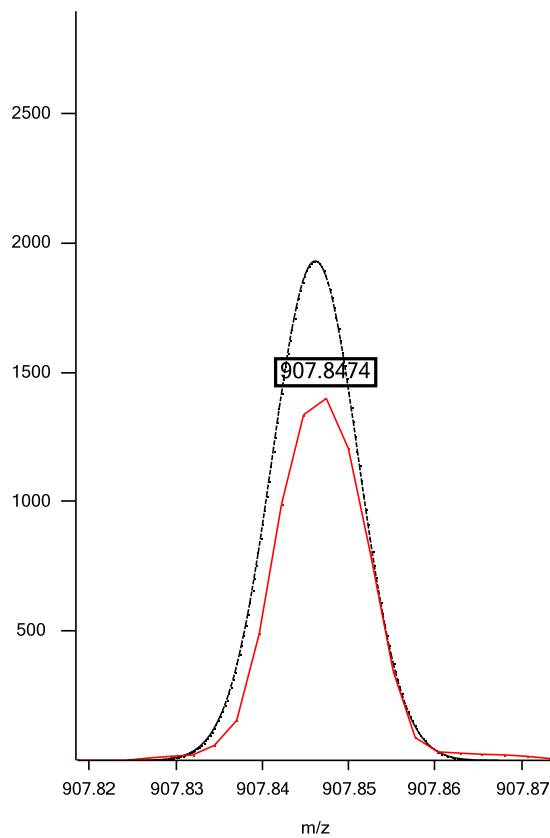


Positive ESI: TAG 54:1; C₅₇H₁₁₂NO₆; theoretical *m/z* 906.8489, (M+NH₄)⁺; isotopic fit 0.0238

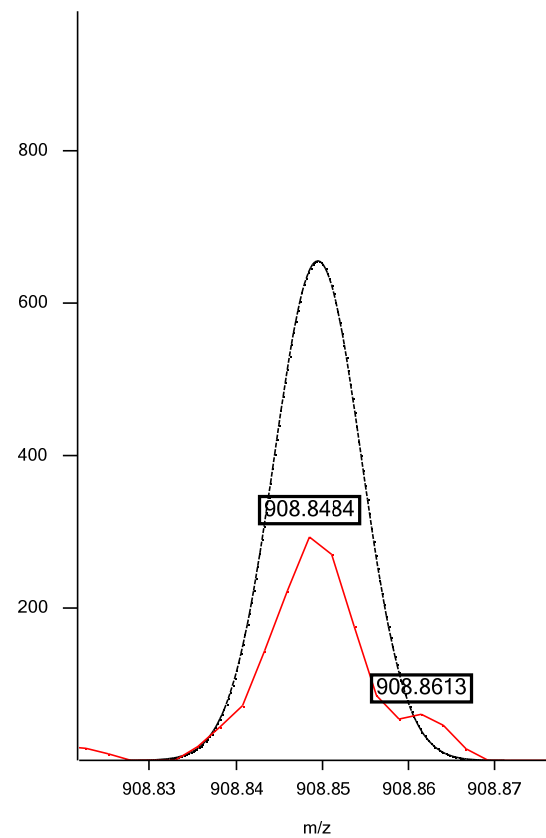
Isotope 1



Isotope 2

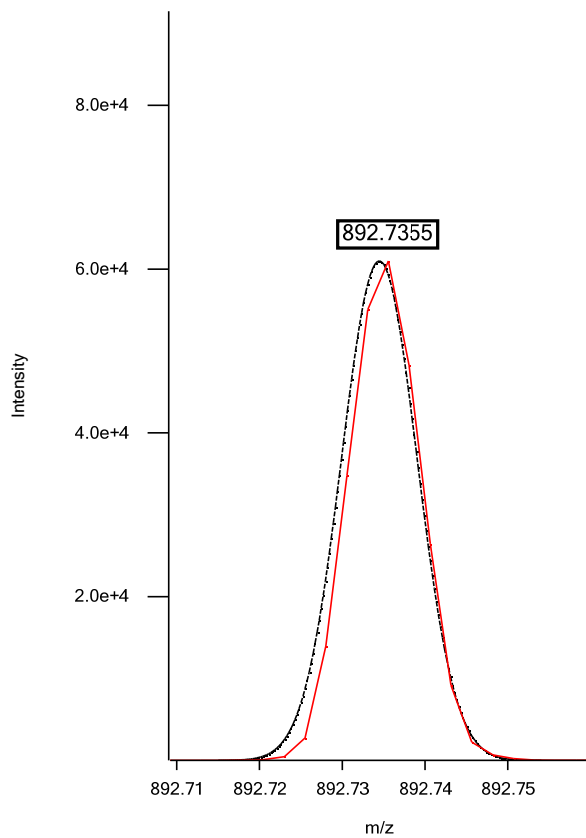


Isotope 3

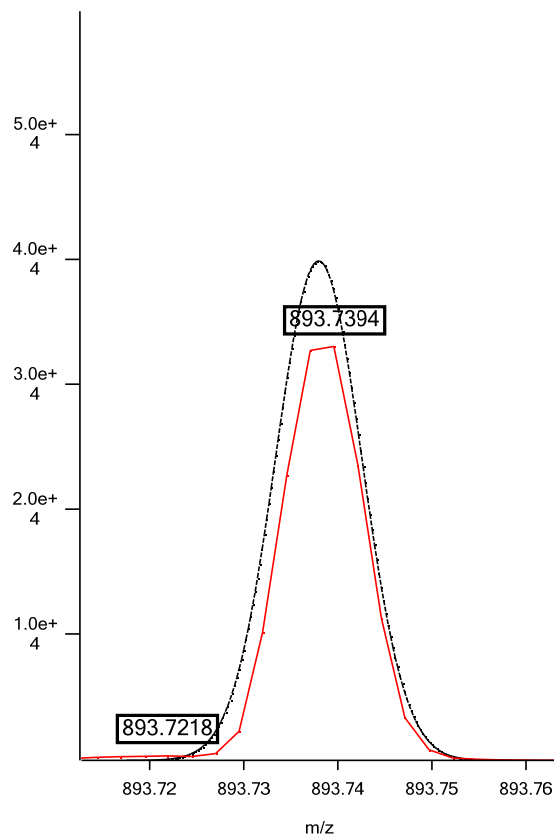


Positive ESI: TAG 54:8; C₅₇H₉₈NO₆; theoretical m/z 892.7394, (M+NH₄)⁺; isotopic fit 0.0121

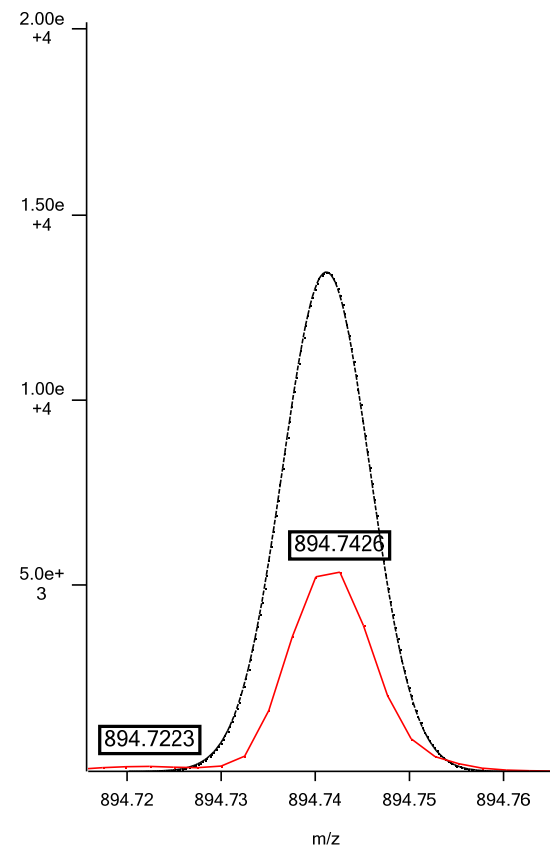
Isotope 1



Isotope 2

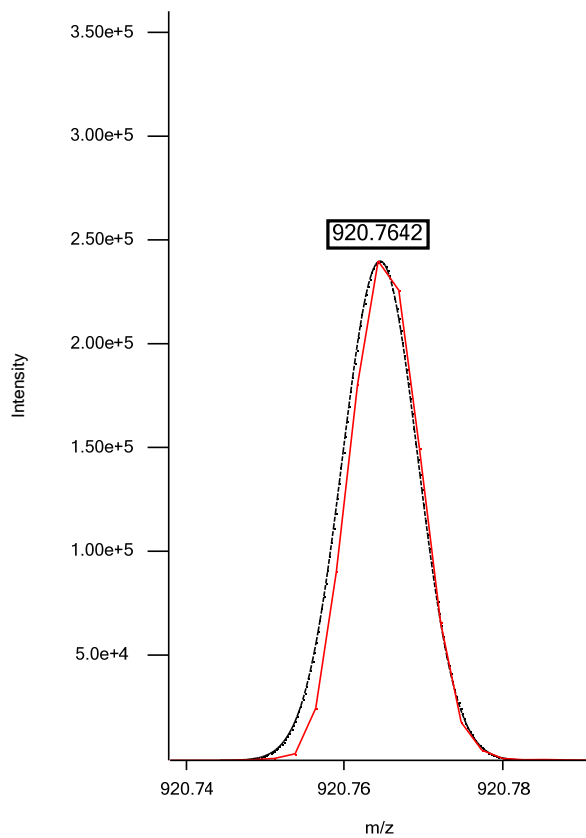


Isotope 3

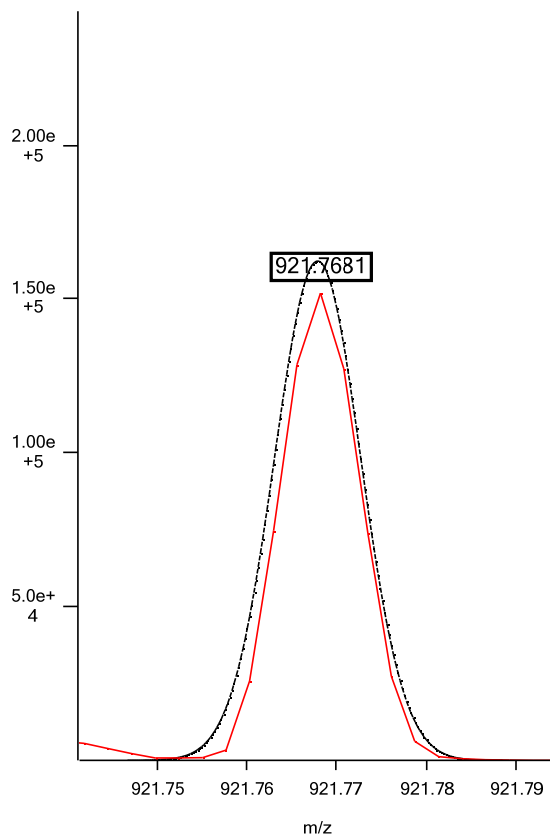


Positive ESI: TAG 56:8; C₅₉H₁₀₂NO₆; theoretical m/z 920.7707, (M+NH₄)⁺; isotopic fit 0.0066

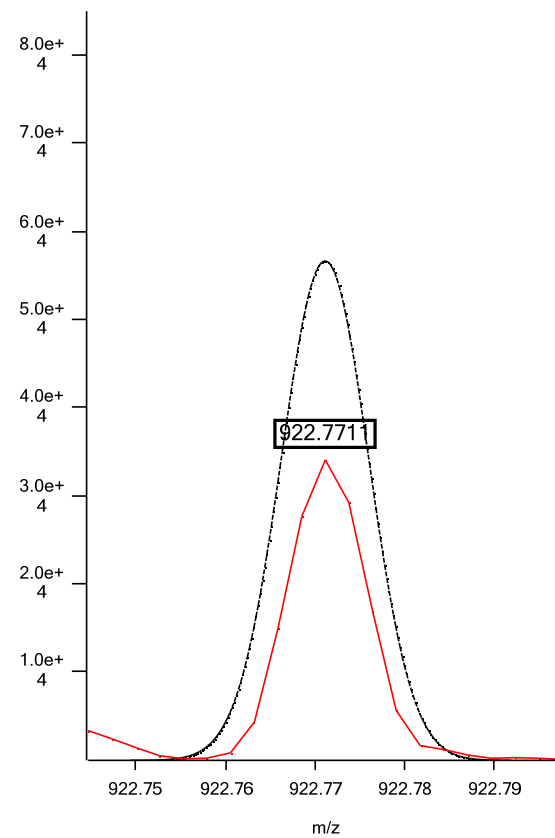
Isotope 1



Isotope 2

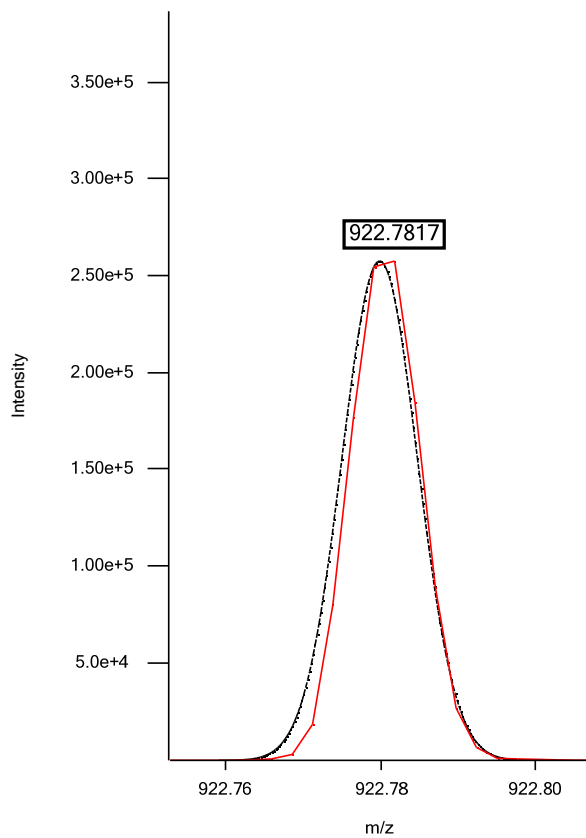


Isotope 3

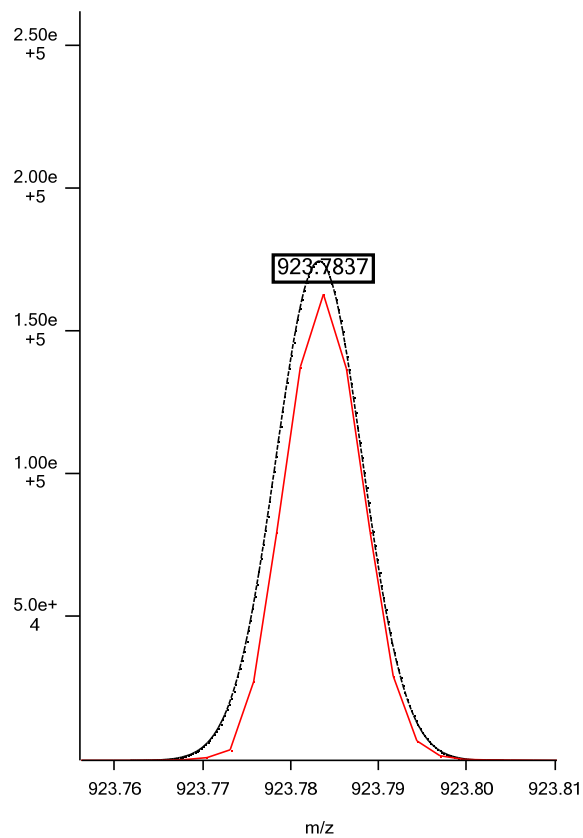


Positive ESI: TAG 56:7; C₅₉H₁₀₄NO₆; theoretical *m/z* 922.7864, (M+NH₄)⁺; isotopic fit 0.0068

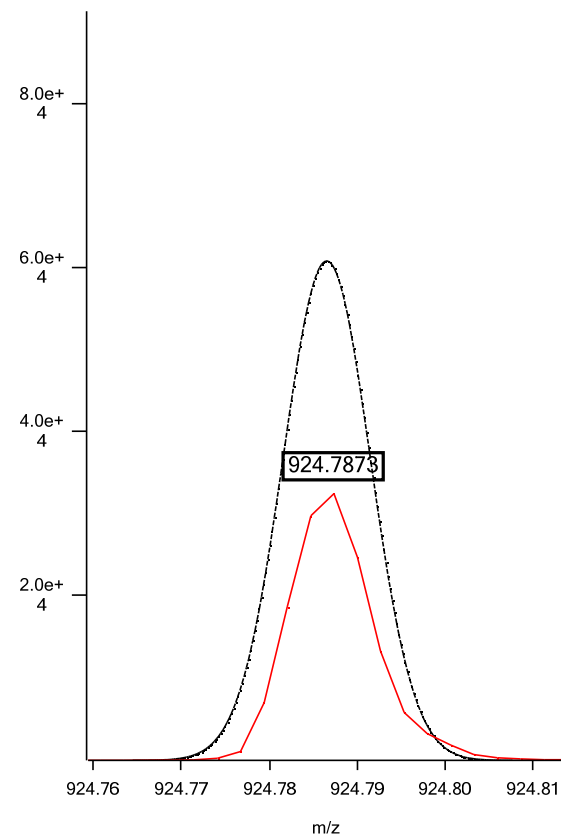
Isotope 1



Isotope 2

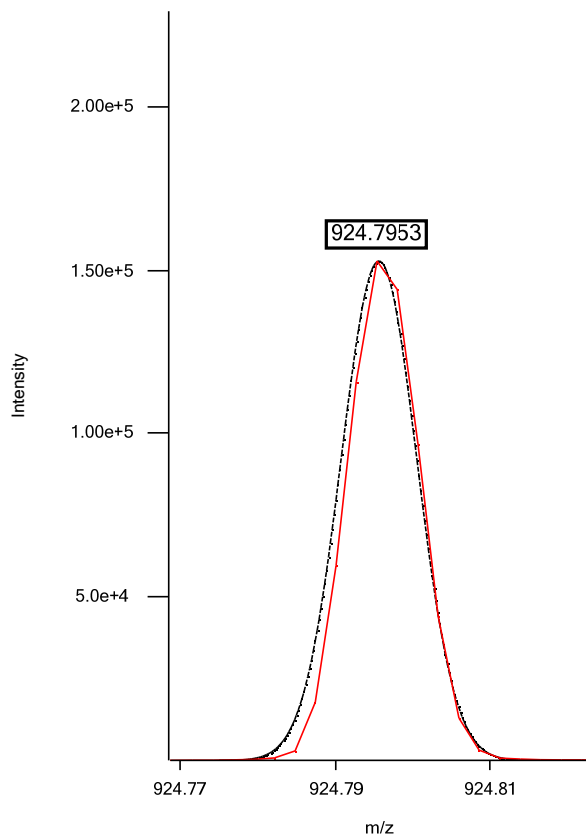


Isotope 3

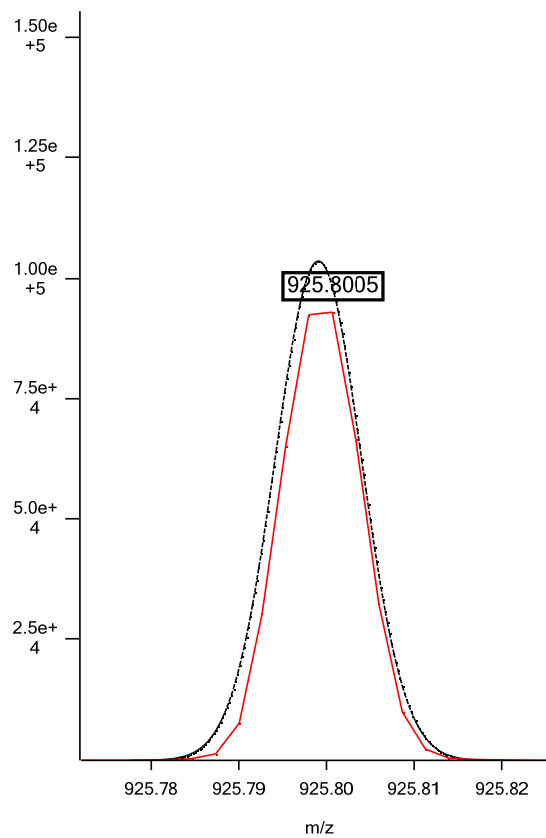


Positive ESI: TAG 56:6; C₅₉H₁₀₆NO₆; theoretical m/z 924.8020, (M+NH₄)⁺; isotopic fit 0.0068

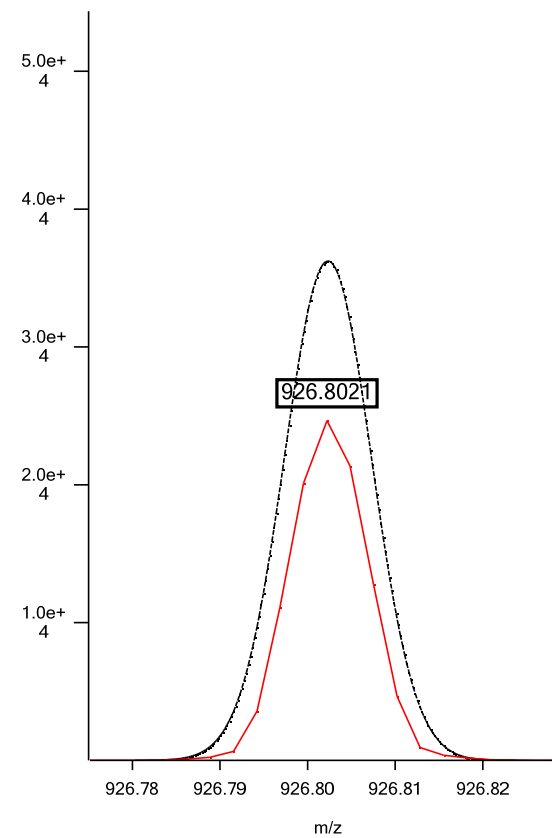
Isotope 1



Isotope 2

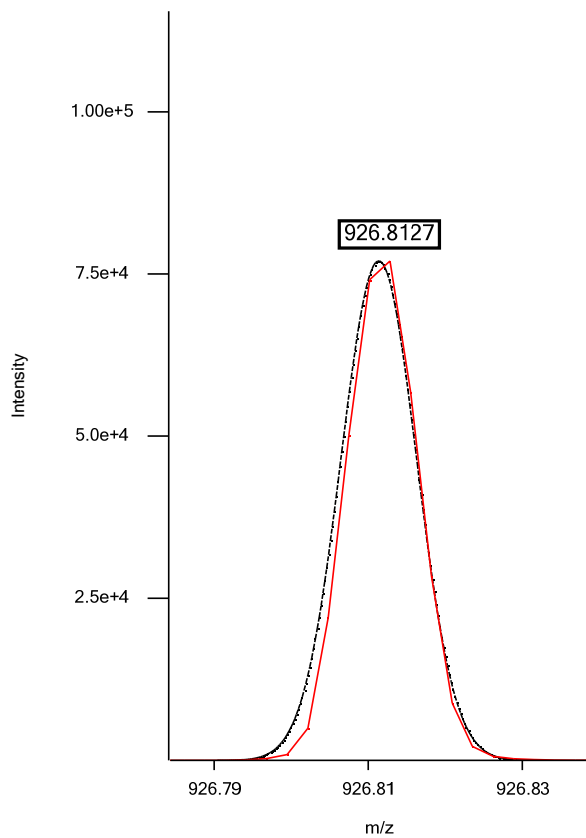


Isotope 3

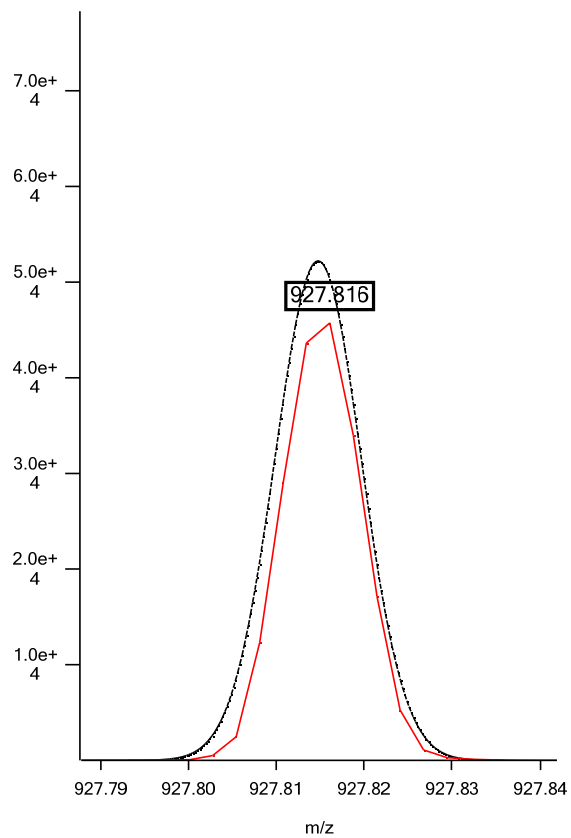


Positive ESI: TAG 56:5; C₅₉H₁₀₈NO₆; theoretical *m/z* 926.8176, (M+NH₄)⁺; isotopic fit 0.0109

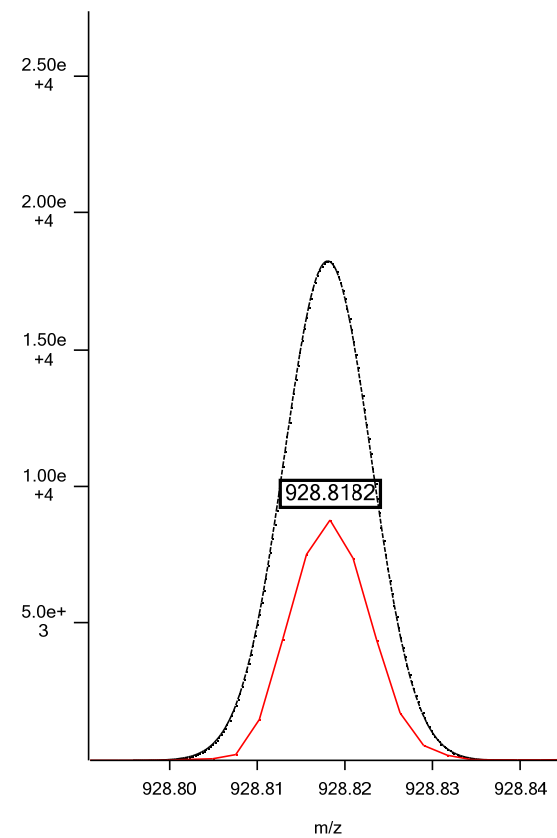
Isotope 1



Isotope 2

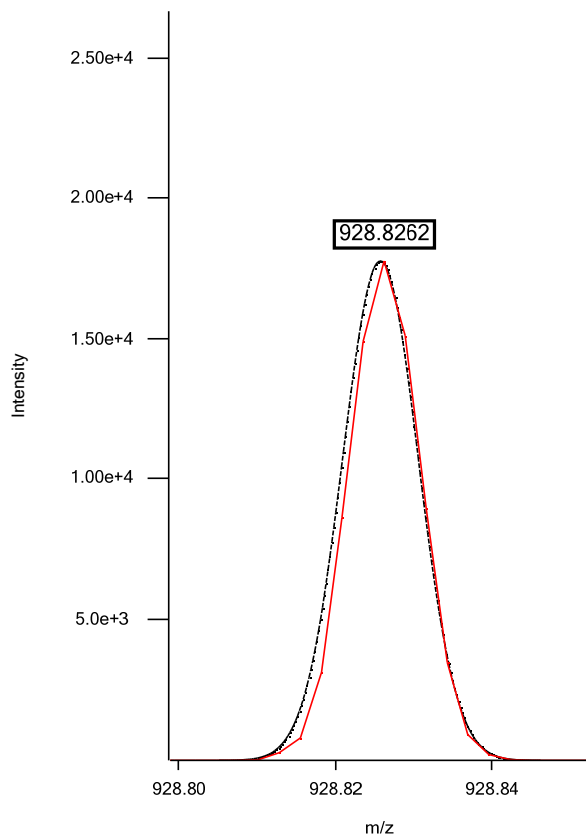


Isotope 3

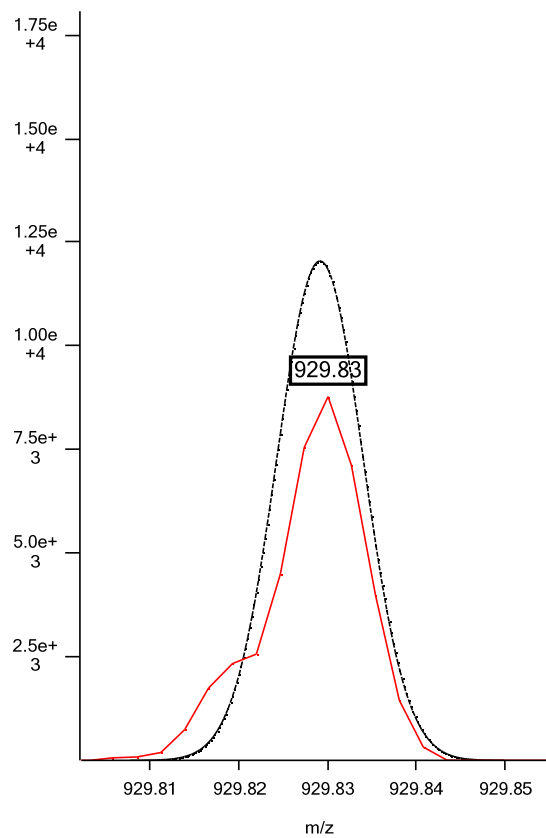


Positive ESI: TAG 56:4; C₅₉H₁₁₀NO₆; theoretical m/z 928.8333, (M+NH₄)⁺; isotopic fit 0.0335

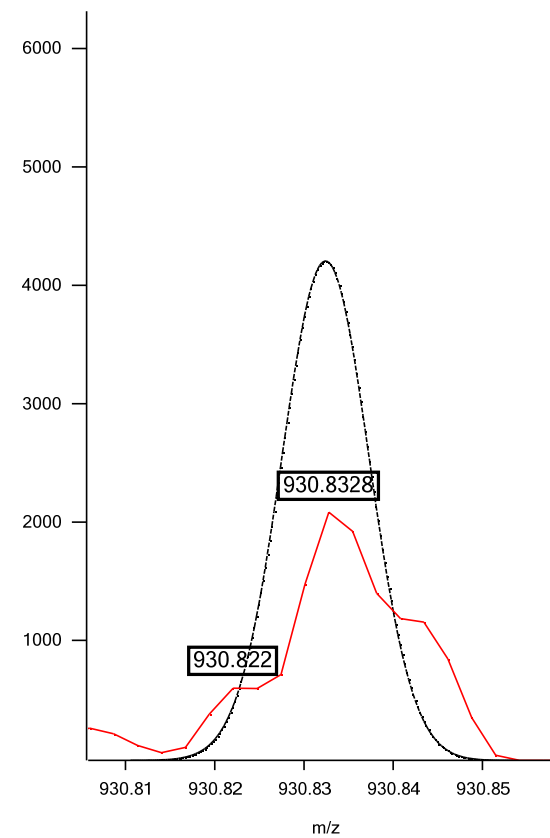
Isotope 1



Isotope 2

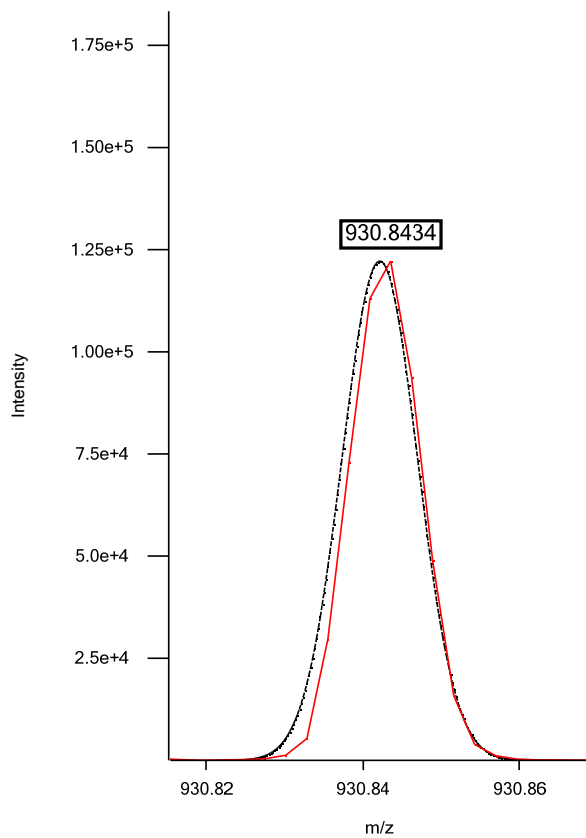


Isotope 3

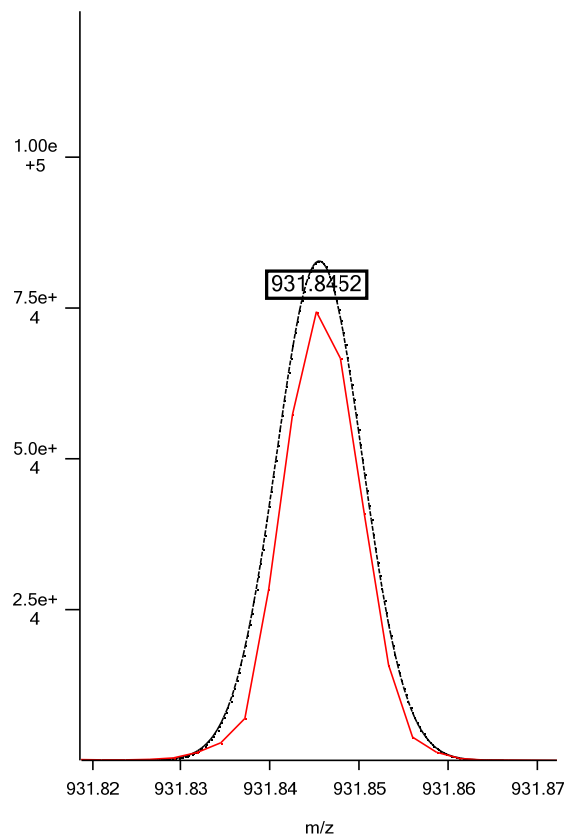


Positive ESI: TAG 56:3; C₅₉H₁₁₂NO₆; theoretical *m/z* 930.8489, (M+NH₄)⁺; isotopic fit 0.0101

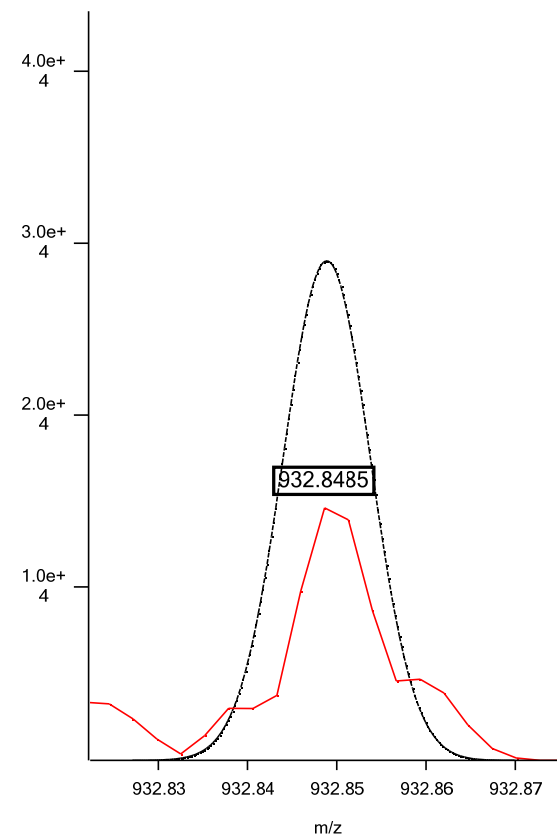
Isotope 1



Isotope 2

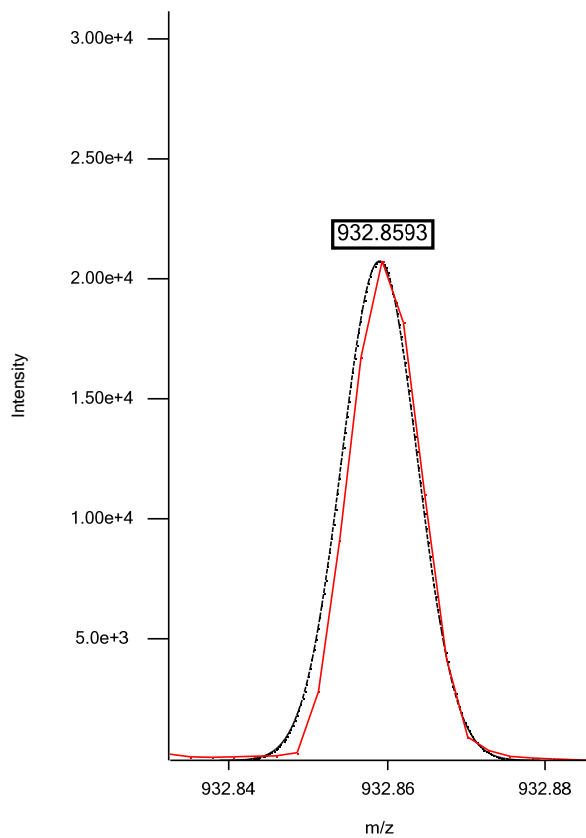


Isotope 3

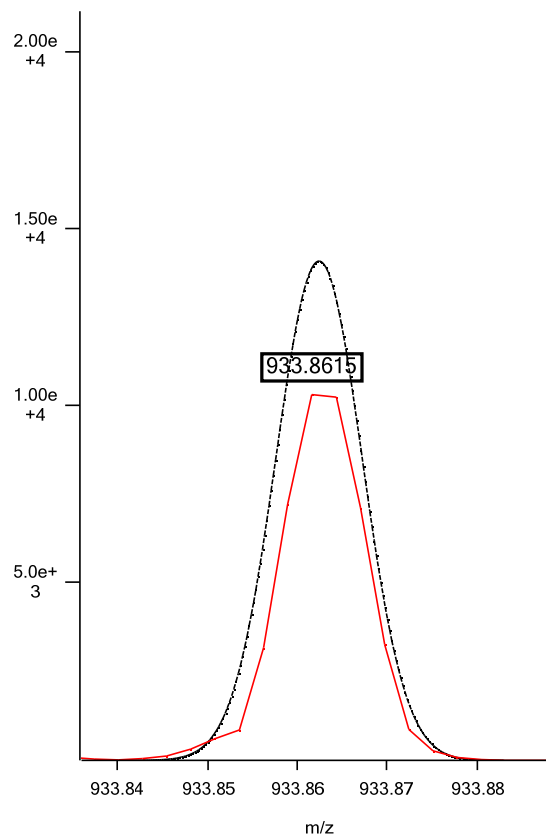


Positive ESI: TAG 56:2; C₅₉H₁₁₄NO₆; theoretical *m/z* 932.8646, (M+NH₄)⁺; isotopic fit 0.0250

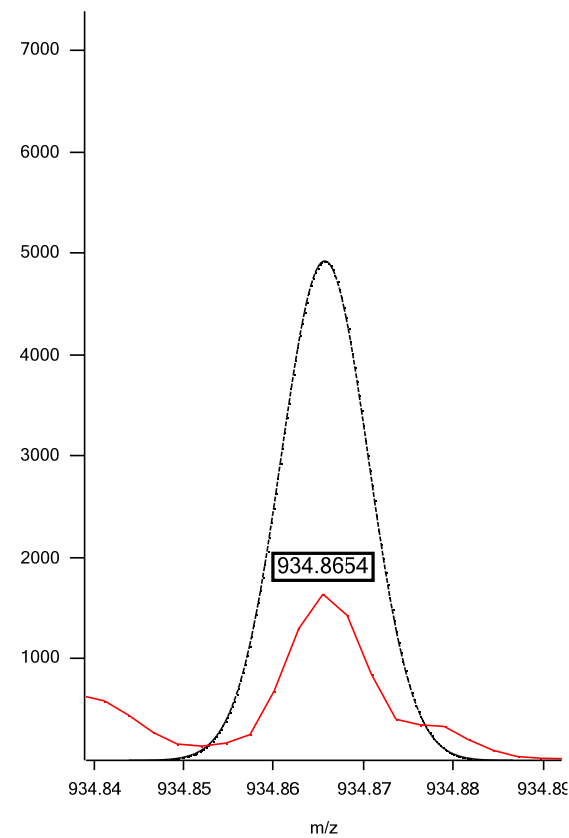
Isotope 1



Isotope 2

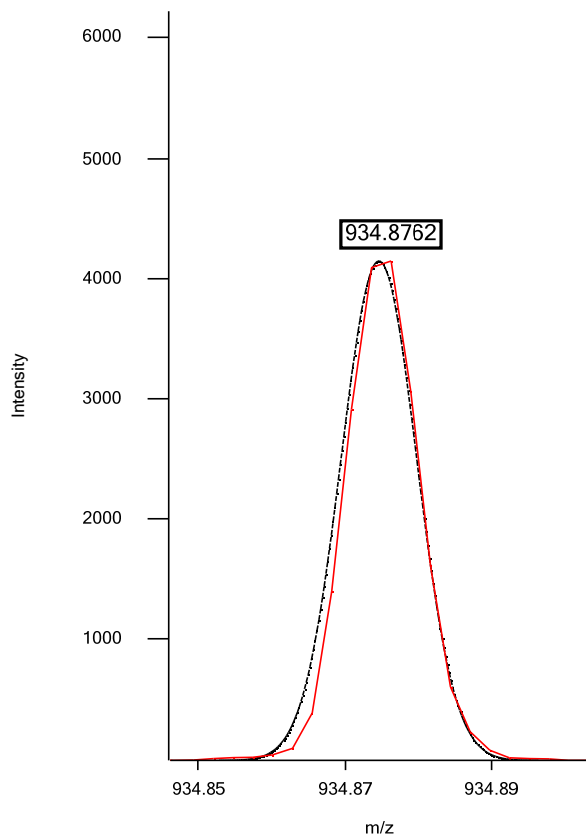


Isotope 3

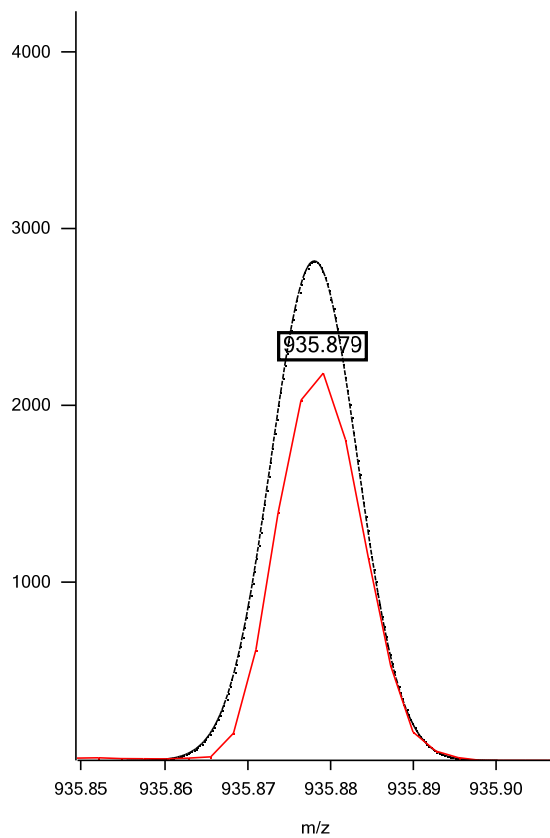


Positive ESI: TAG 56:1; $C_{59}H_{116}NO_6$; theoretical m/z 934.8802, $(M+NH_4)^+$; isotopic fit 0.0185

Isotope 1



Isotope 2



Isotope 3

