

Representative MS/MS spectra of identified lipids

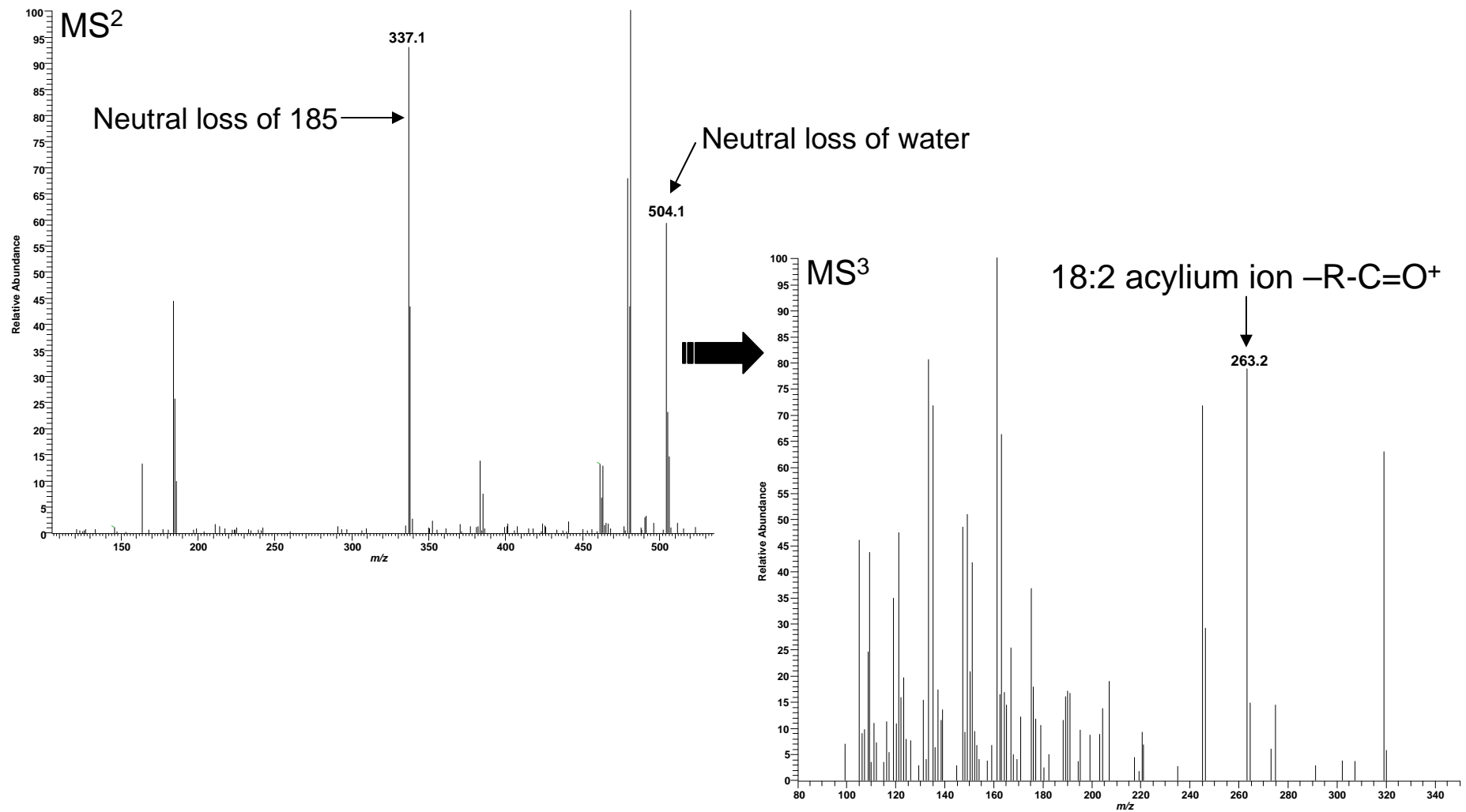
Glycerophosphoserines

(Neutral loss-triggered MS³ – 185 Da)

Low mass measurement accuracy MS/MS utilizing LTQ

Positive ESI: LPS 18:2; $C_{24}H_{44}NO_9P$; theoretical m/z 522.3, $(M+H)^+$

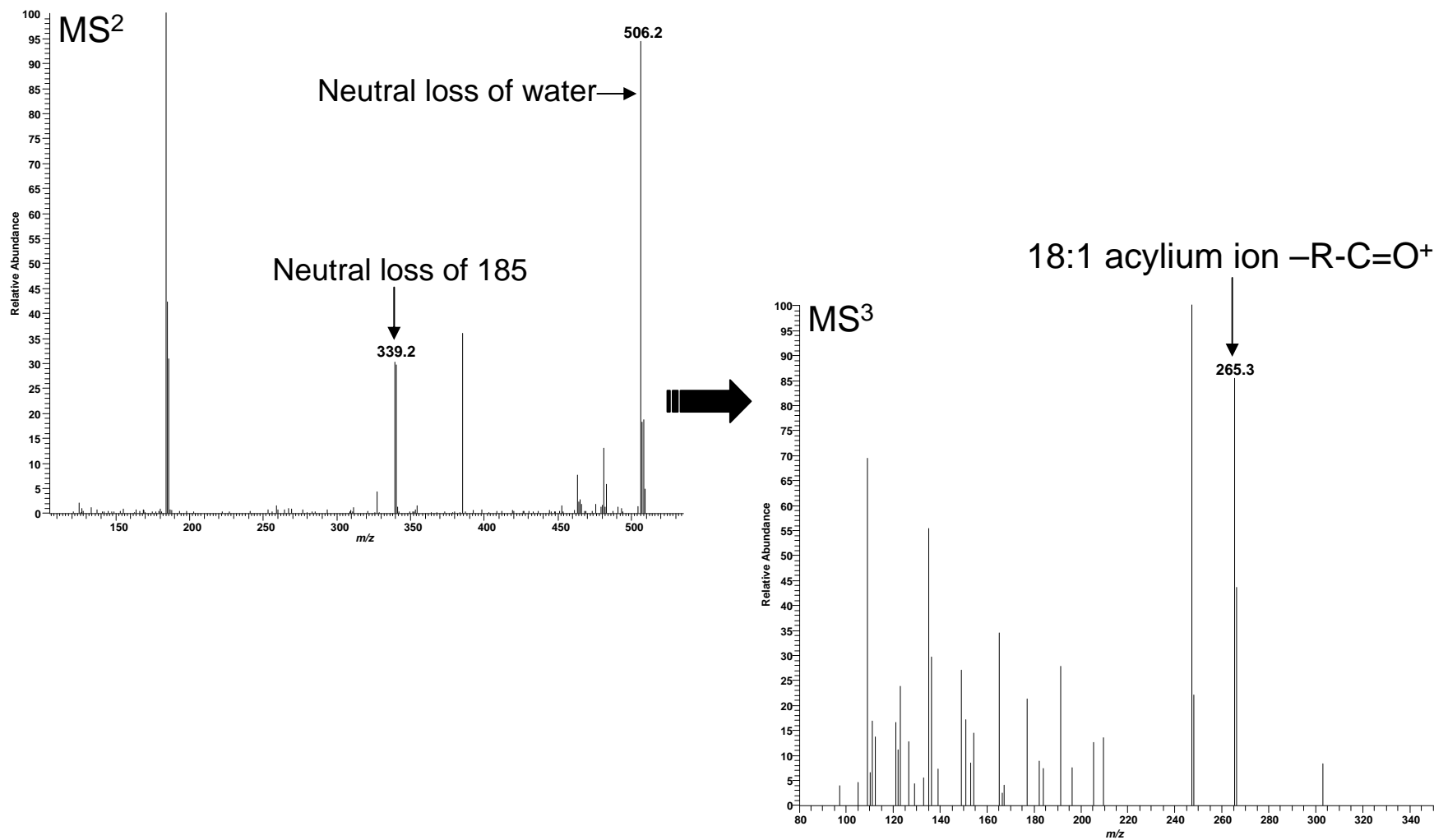
Neutral loss-triggered MS³



Low mass measurement accuracy MS/MS utilizing LTQ

Positive ESI: LPS 18:1; $C_{24}H_{46}NO_9P$; theoretical m/z 524.3, $(M+H)^+$

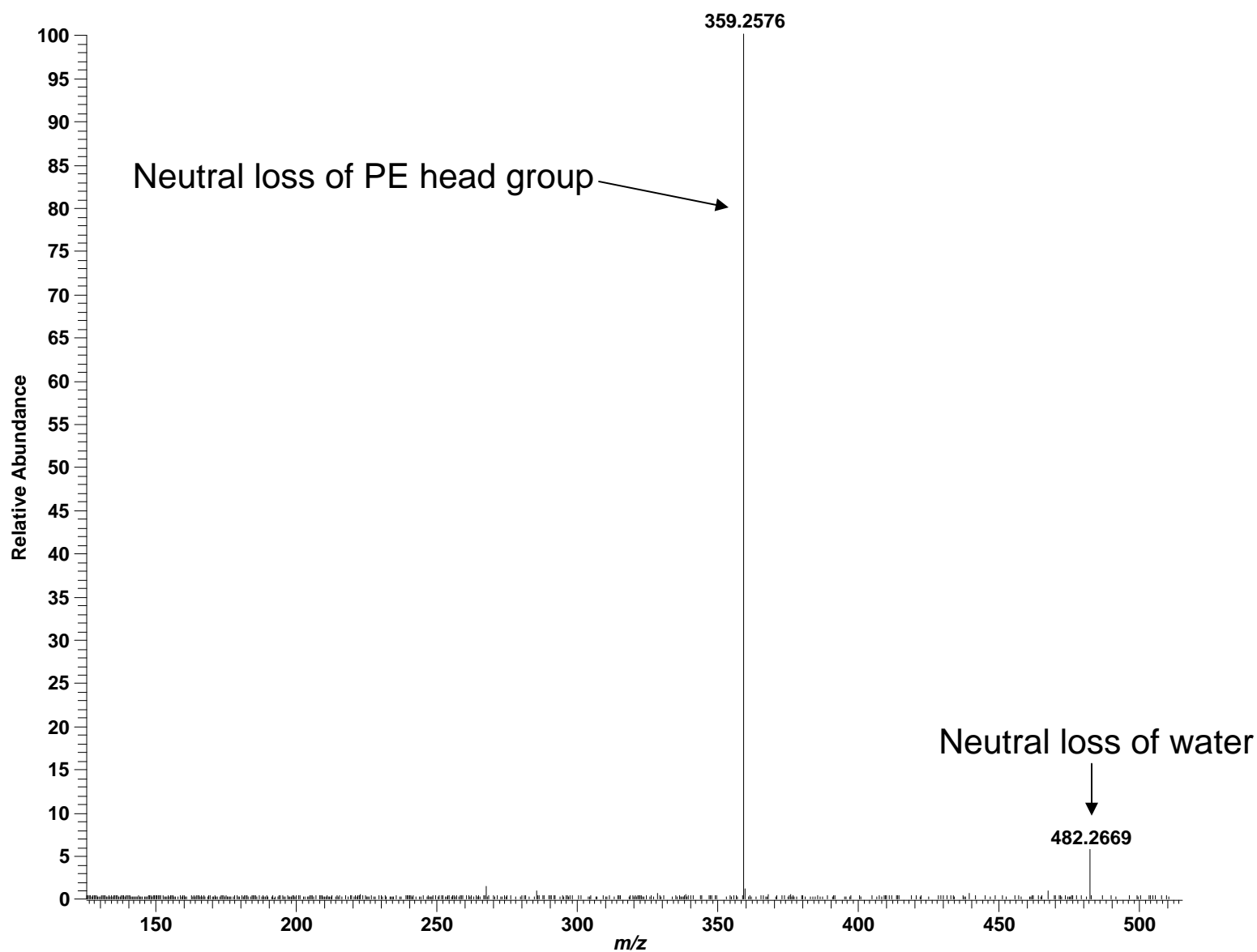
Neutral loss-triggered MS³



Glycerophosphoethanolamines

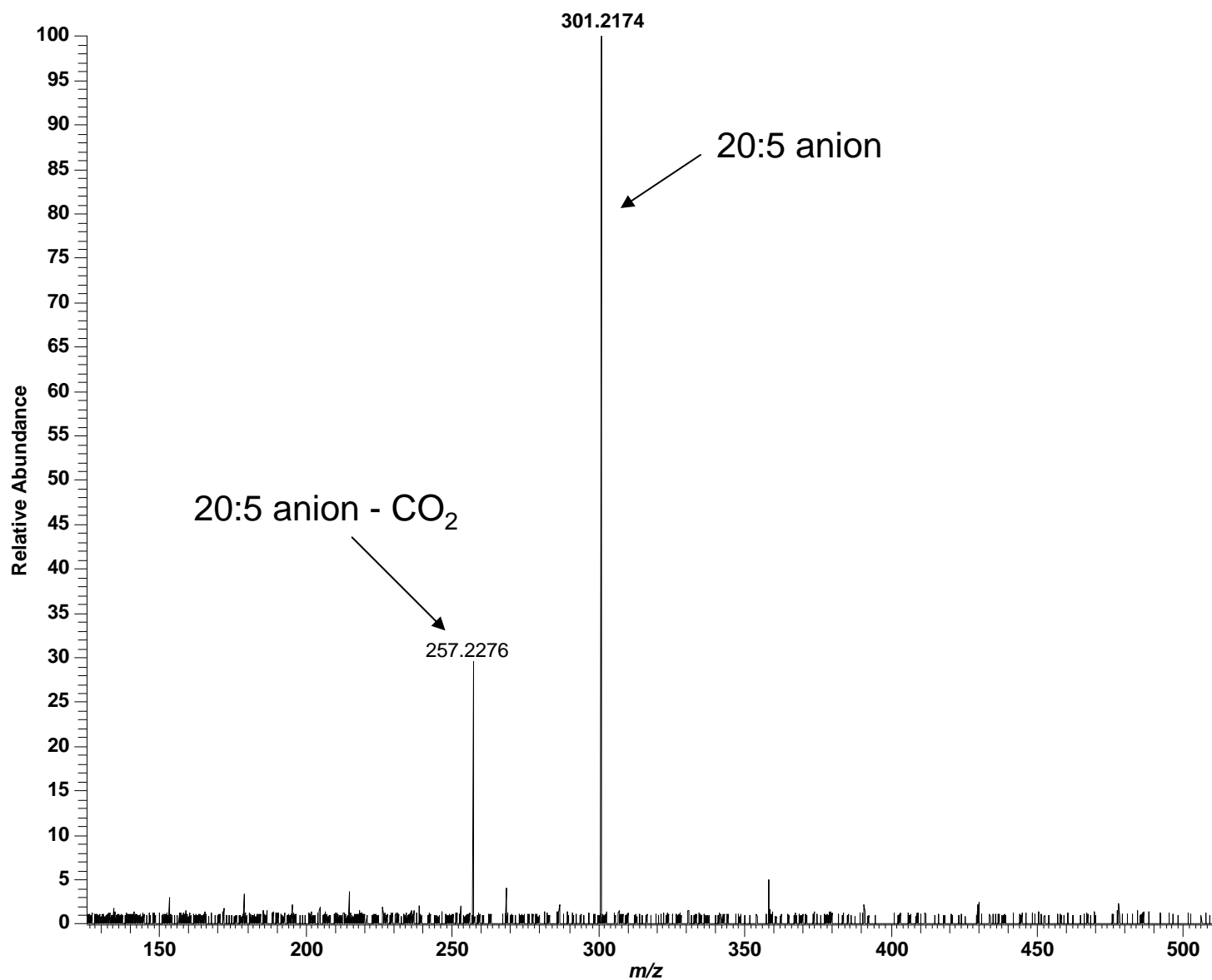
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 20:5; $C_{25}H_{42}NO_7P$; theoretical m/z 500.2777, $(M+H)^+$



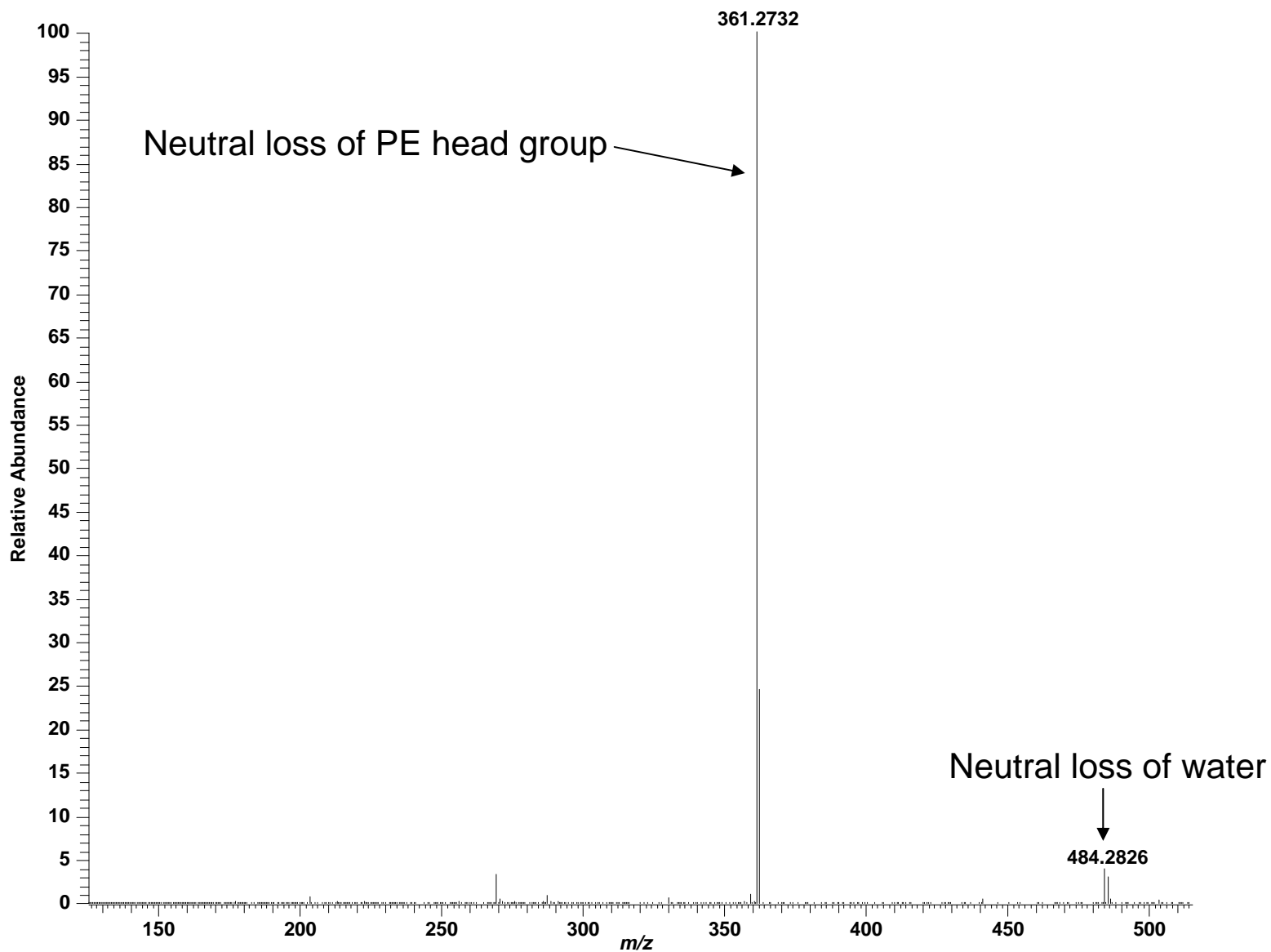
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 20:5; $C_{25}H_{42}NO_7P$; theoretical m/z 498.2621, (M-H)⁻



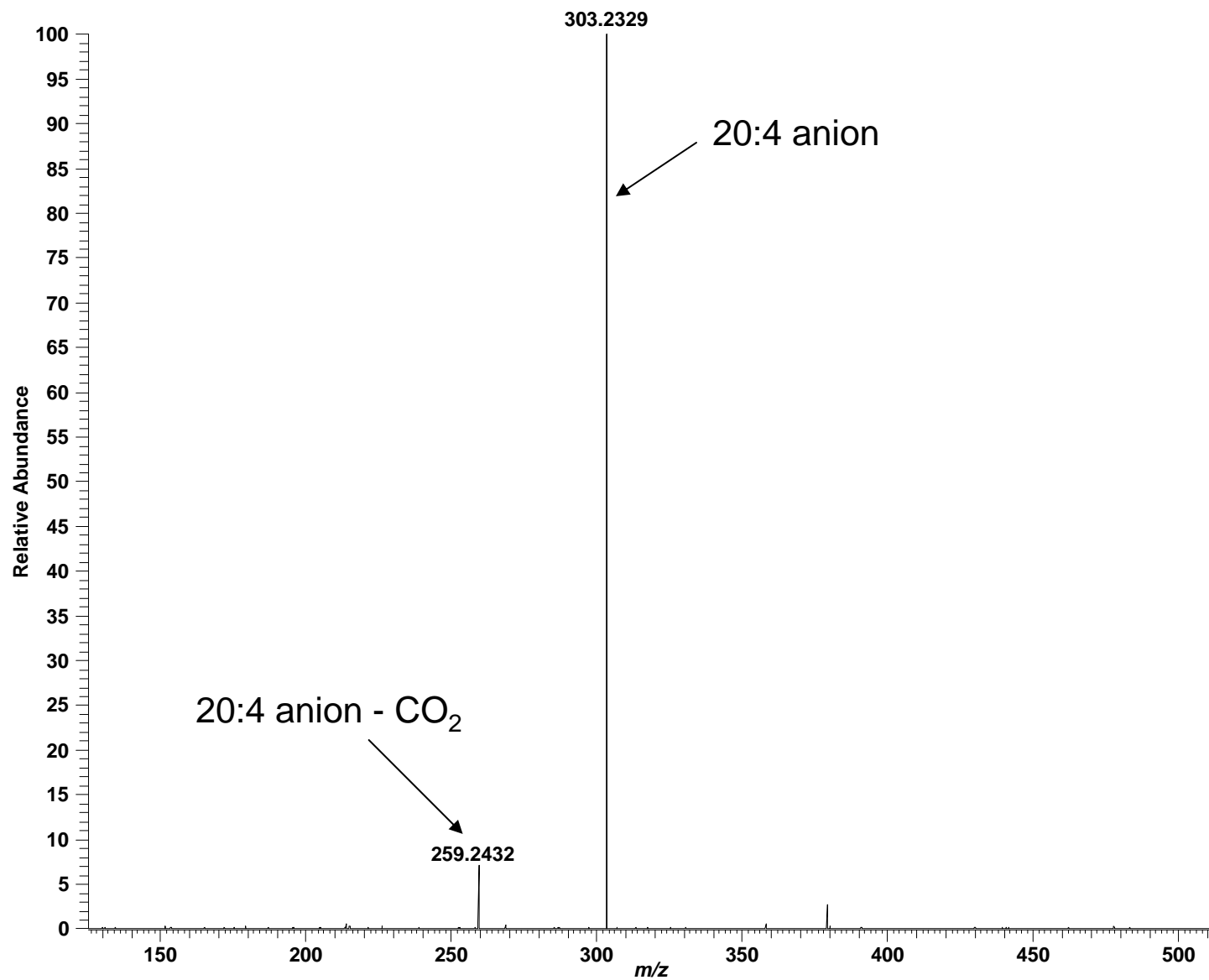
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 20:4; $C_{25}H_{44}NO_7P$; theoretical m/z 502.2933, $(M+H)^+$



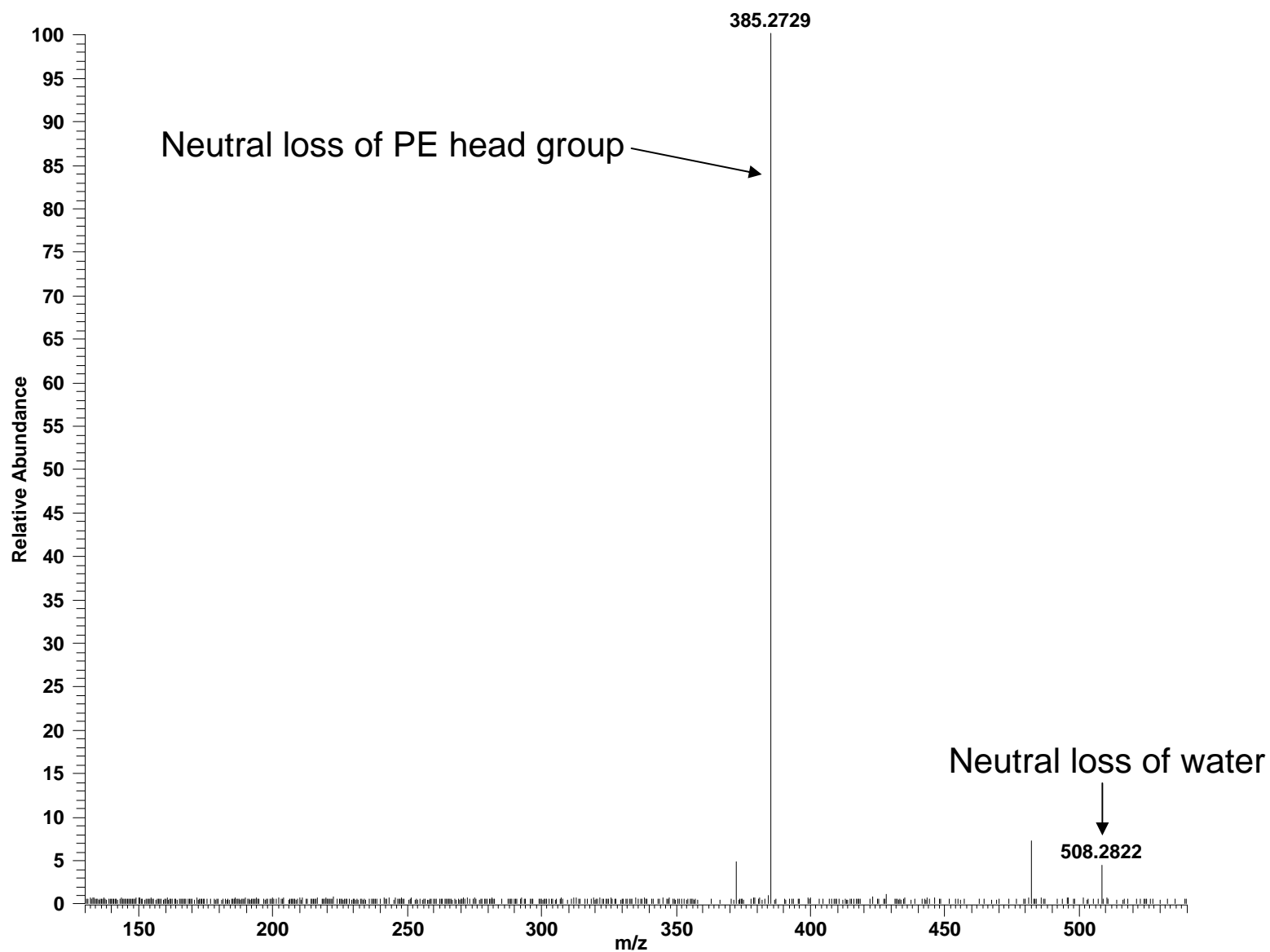
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 20:4; $C_{25}H_{44}NO_7P$; theoretical m/z 500.2777, $(M-H)^-$



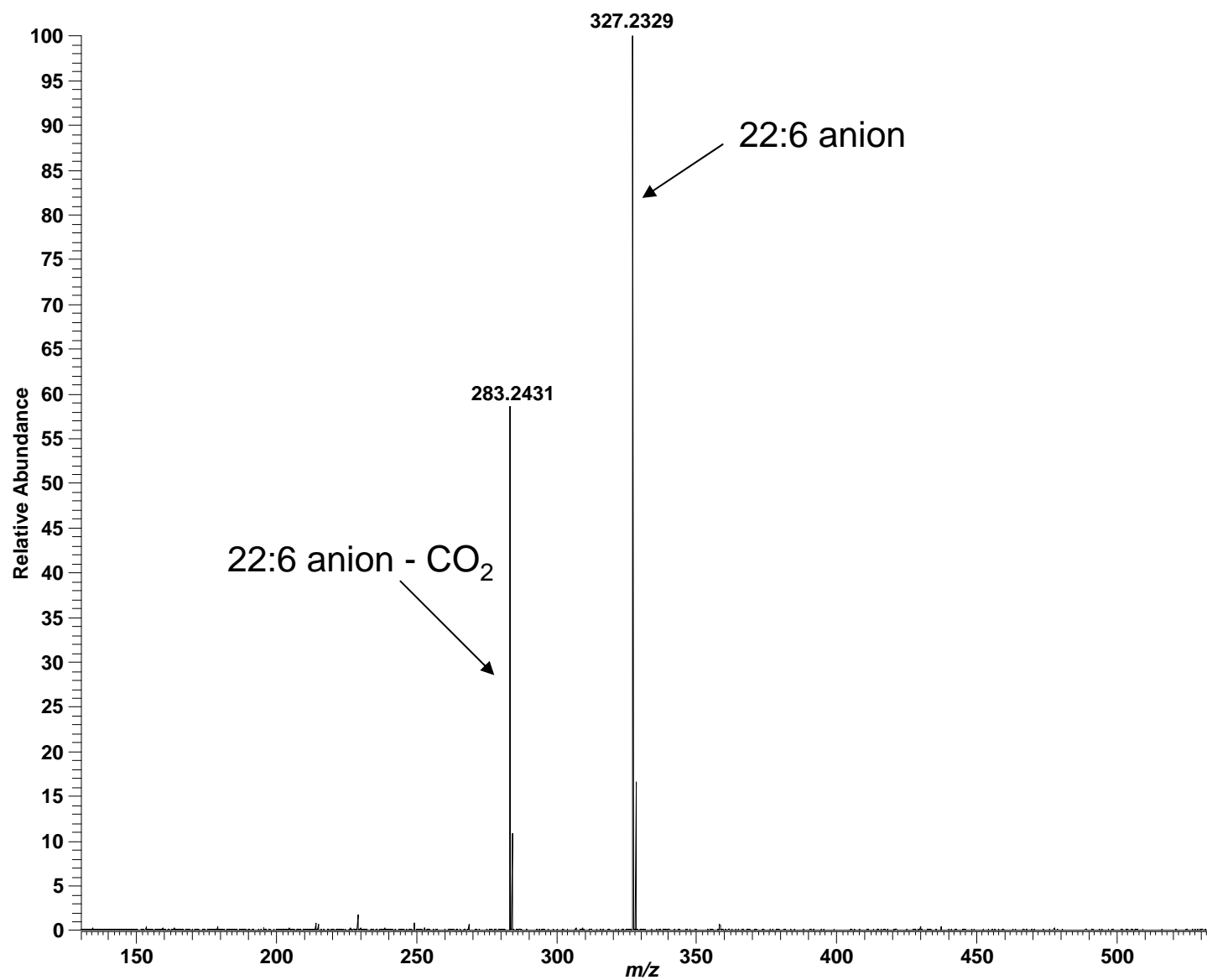
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 22:6; $C_{27}H_{44}NO_7P$; theoretical m/z 526.2933, $(M+H)^+$



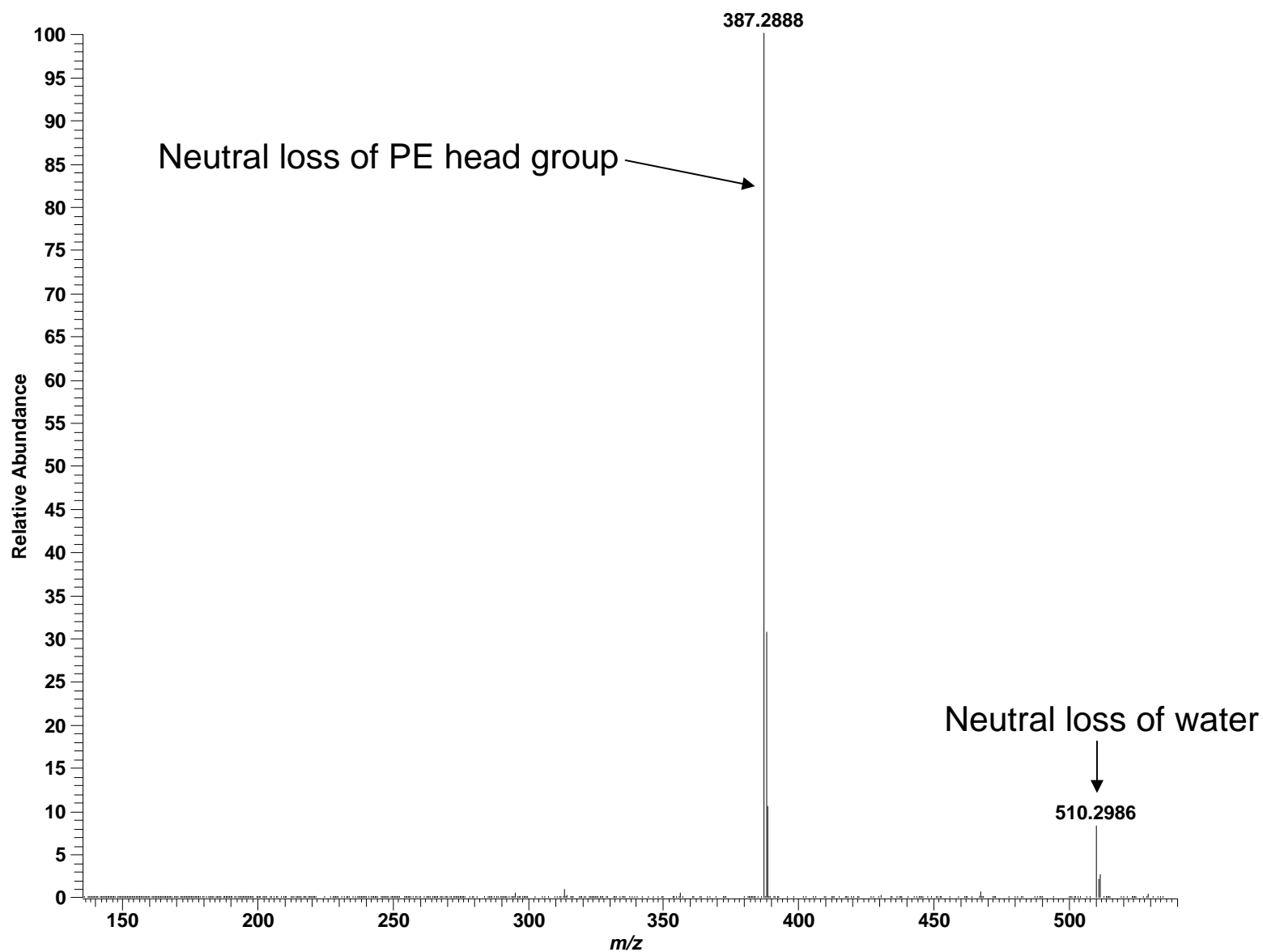
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 22:6; $C_{27}H_{44}NO_7P$; theoretical m/z 524.2777, $(M-H)^-$



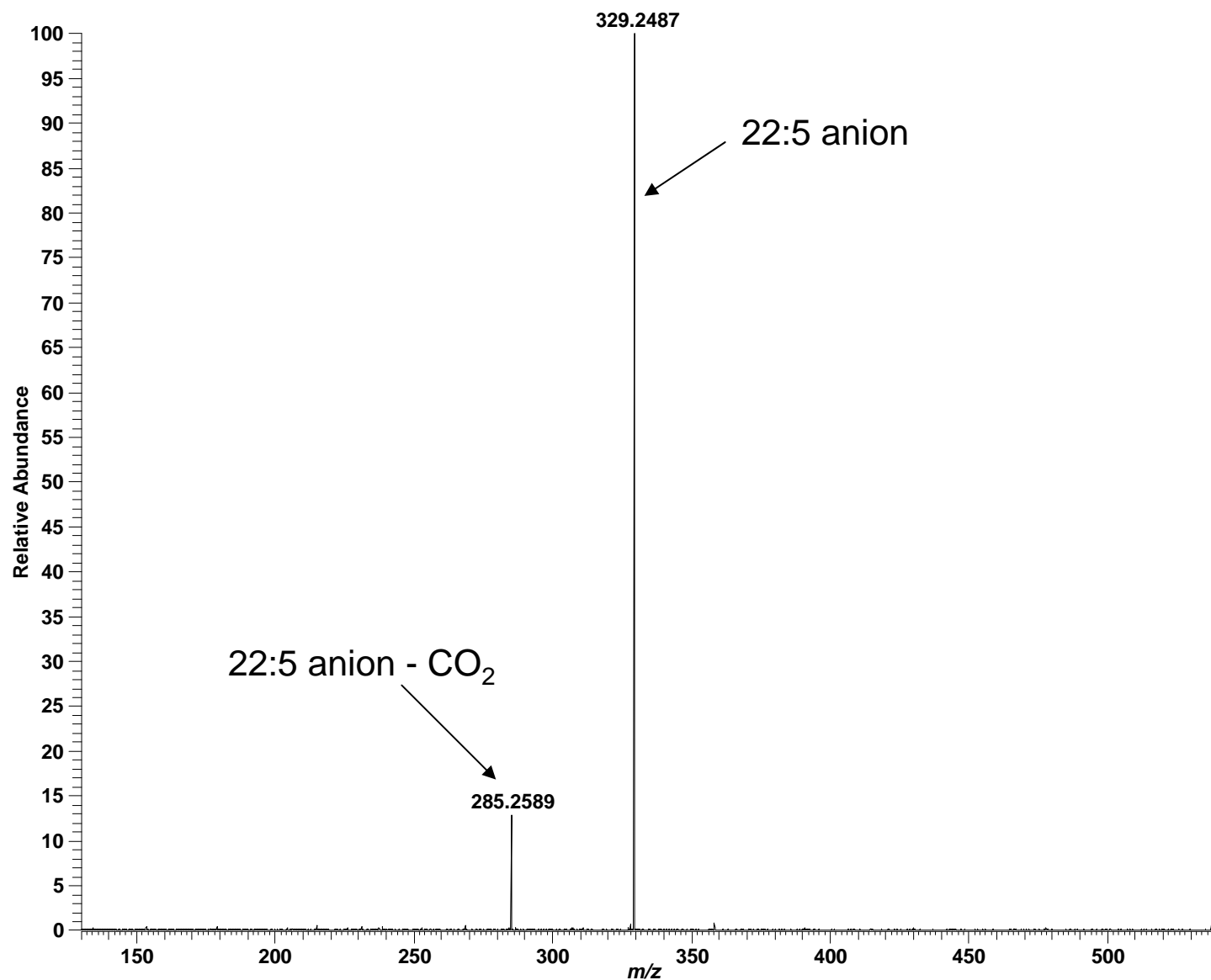
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 22:5; $C_{27}H_{46}NO_7P$; theoretical m/z 528.3090, $(M+H)^+$



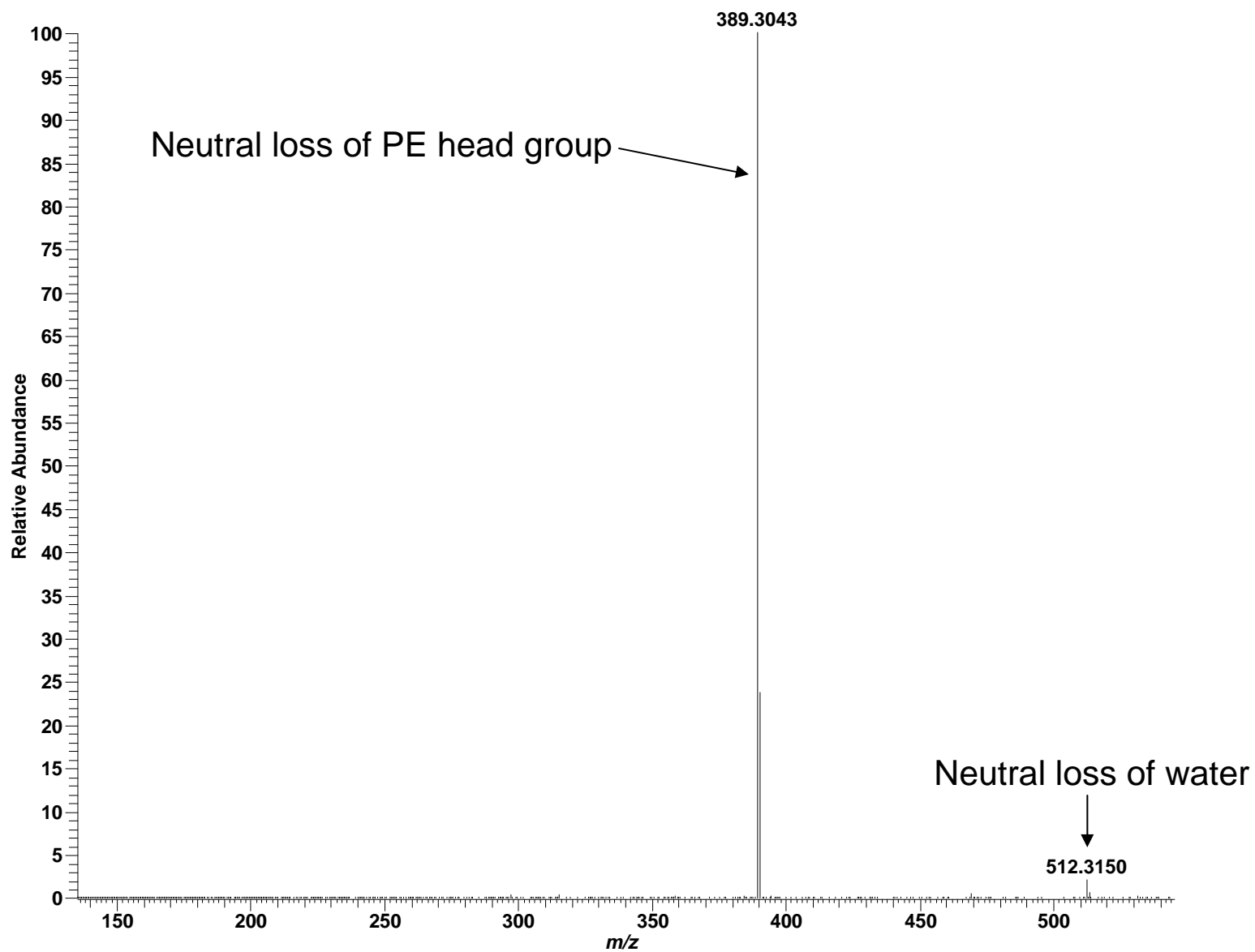
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 22:5; $C_{27}H_{46}NO_7P$; theoretical m/z 526.2933, (M-H)⁻



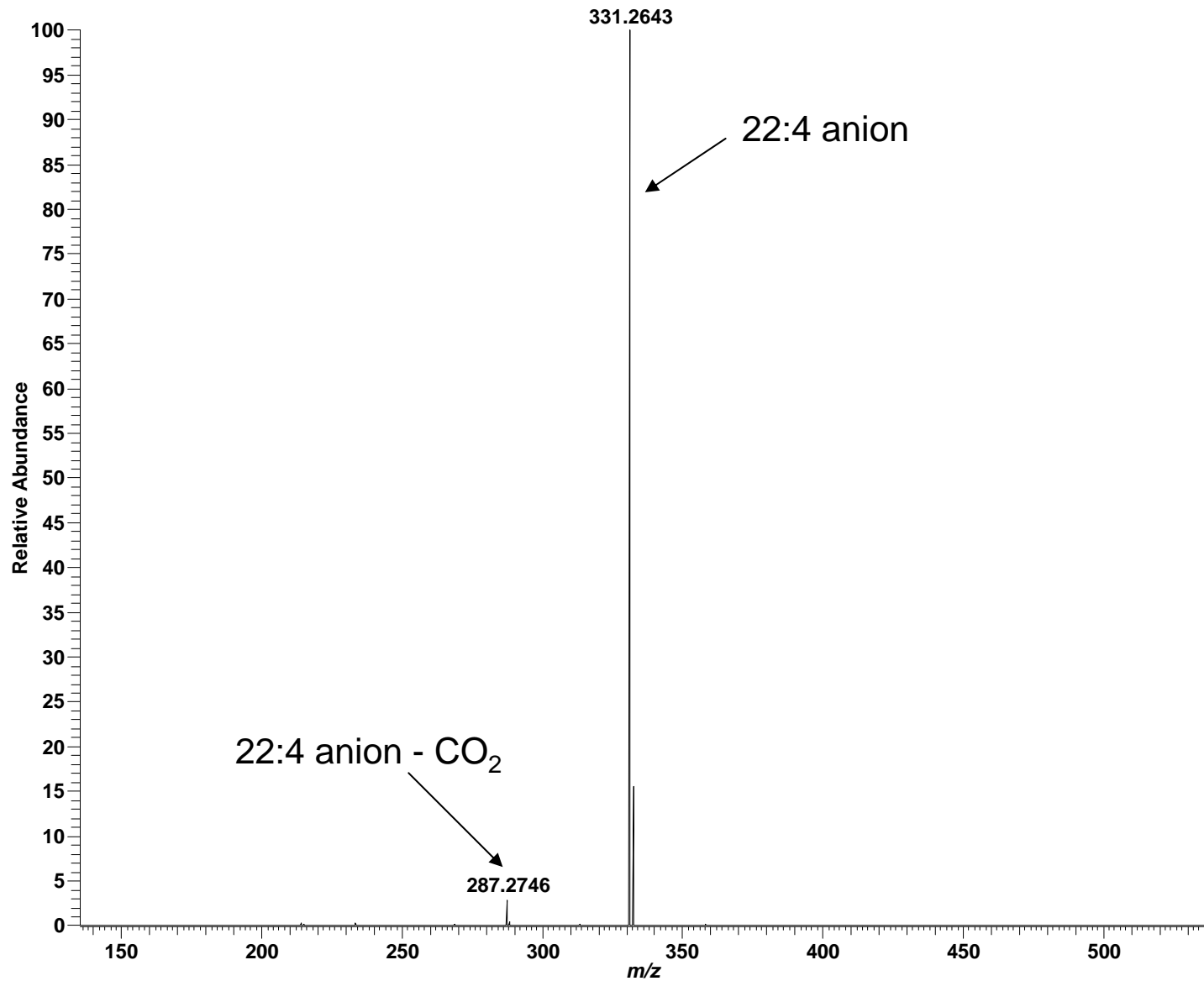
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 22:4; $C_{27}H_{48}NO_7P$; theoretical m/z 530.3246, (M+H)⁺



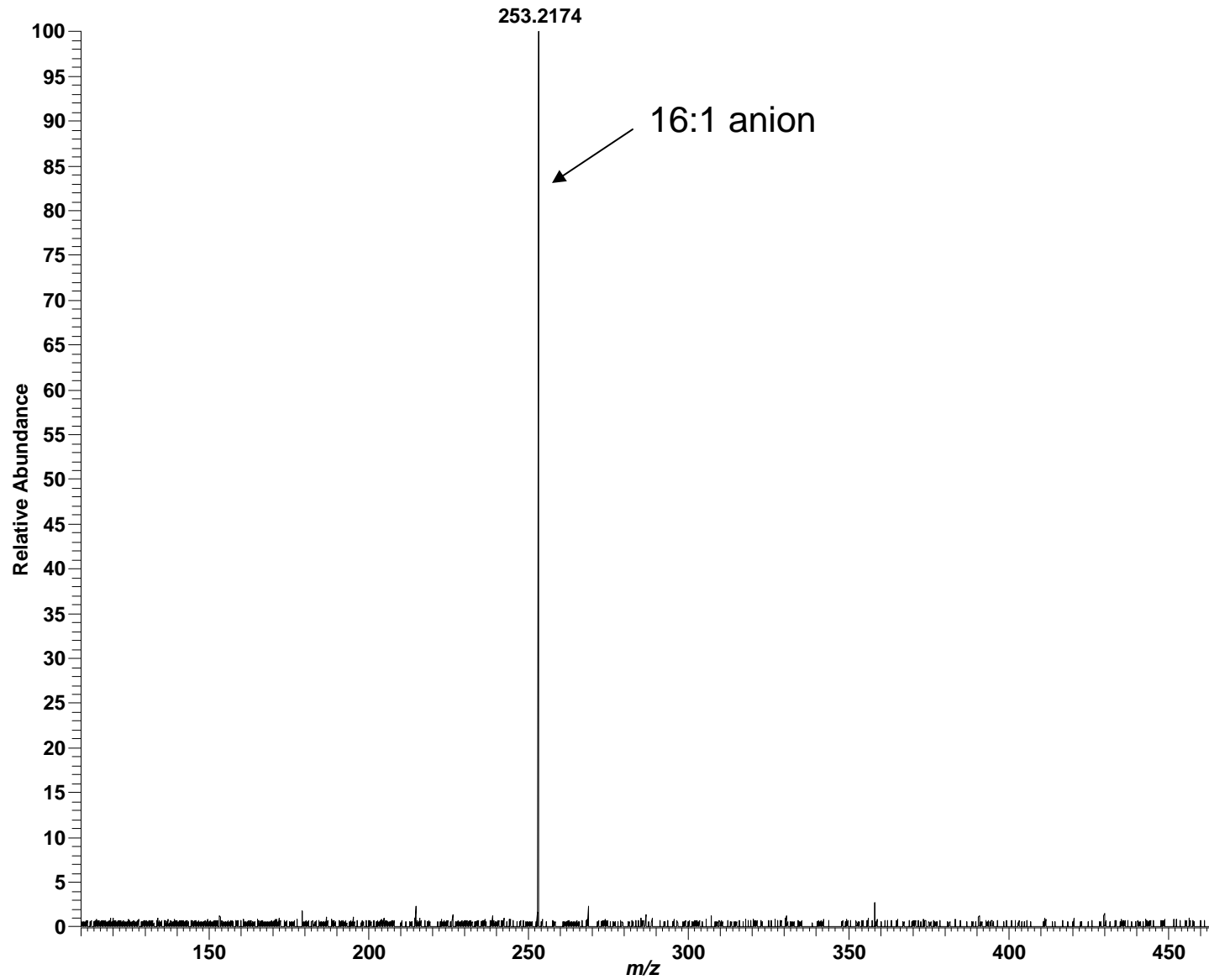
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 22:4; $C_{27}H_{48}NO_7P$; theoretical m/z 528.3090, (M-H)⁻



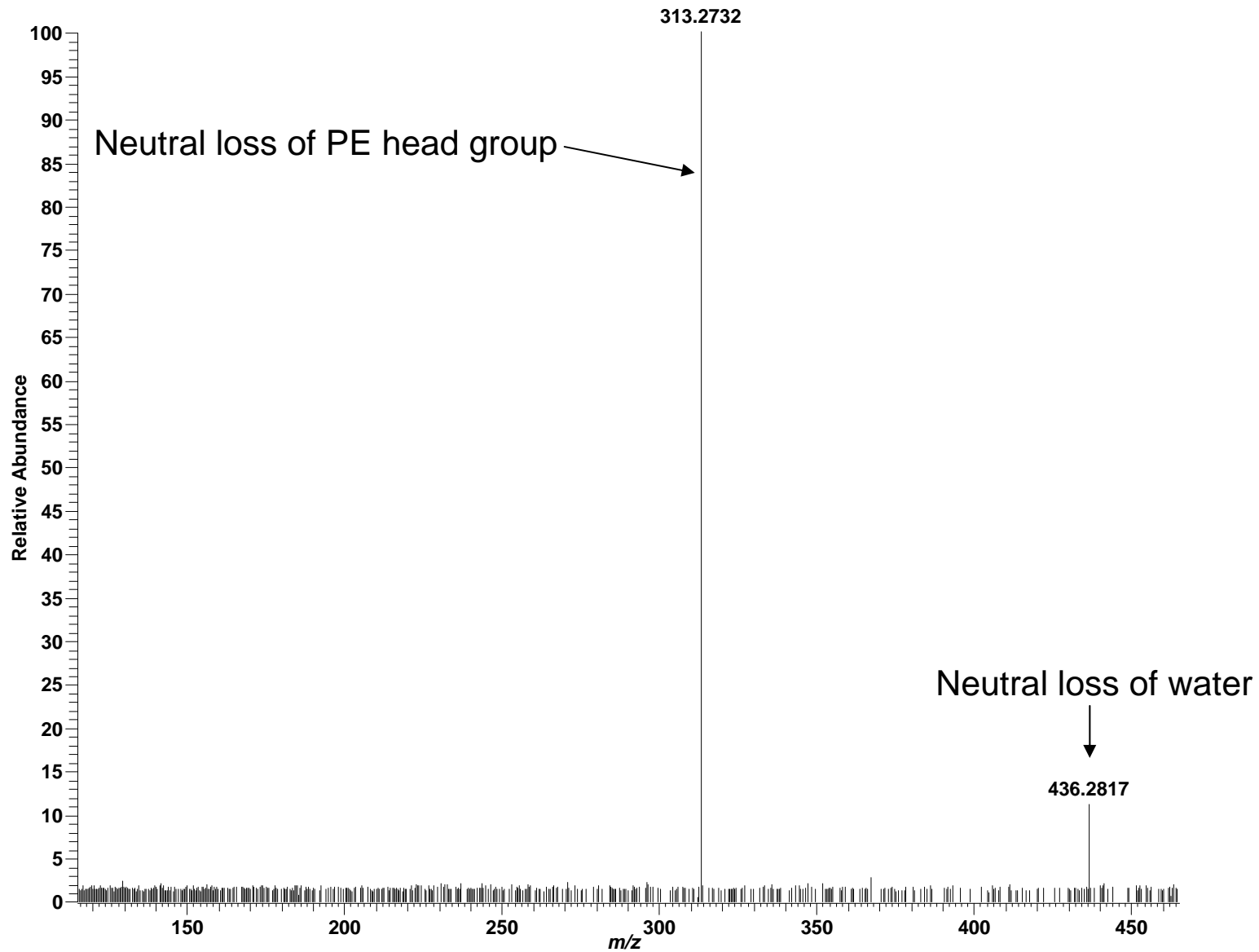
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 16:1; $C_{21}H_{42}NO_7P$; theoretical m/z 450.2621, (M-H)⁻



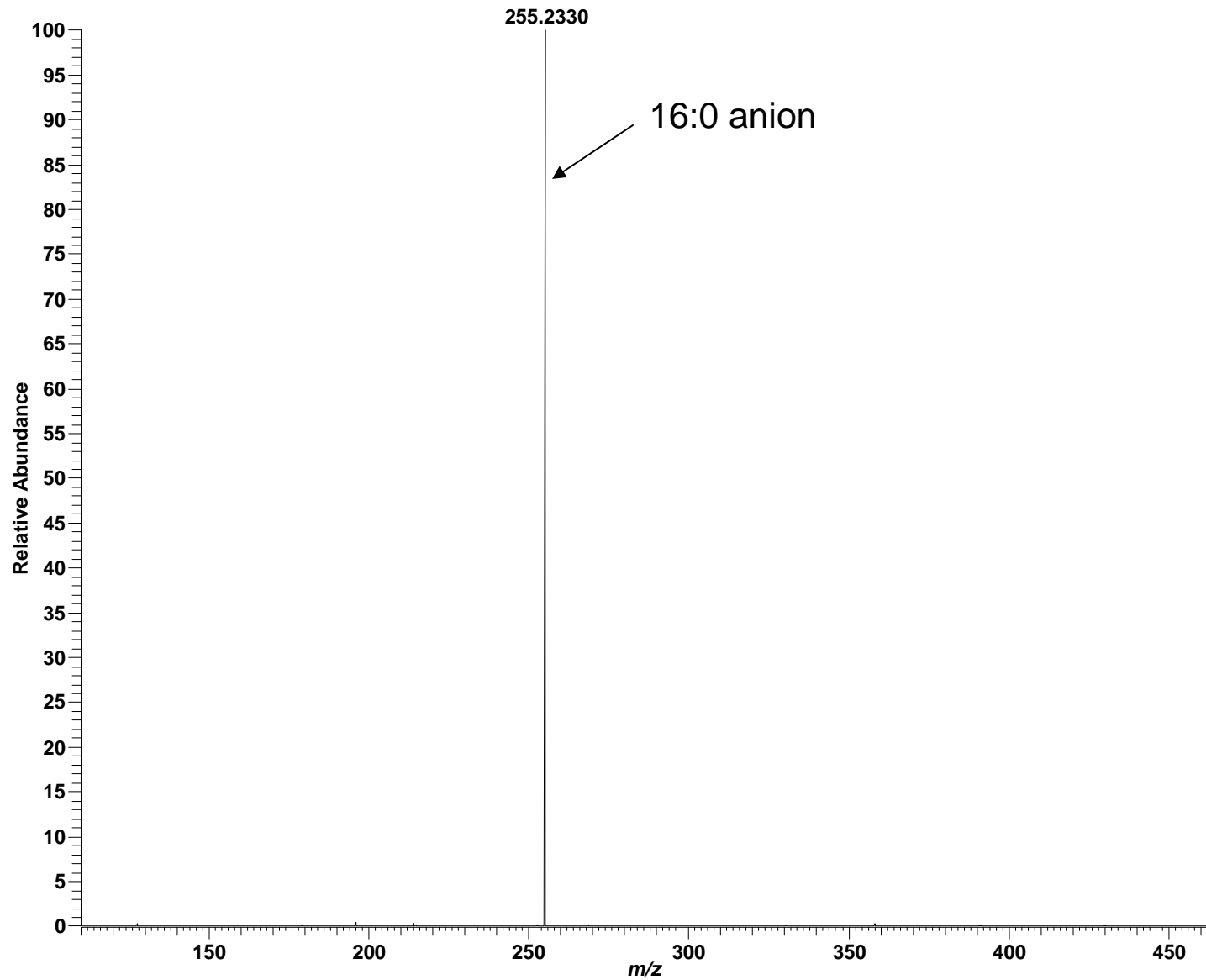
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 16:0; $C_{21}H_{44}NO_7P$; theoretical m/z 454.2934, $(M+H)^+$



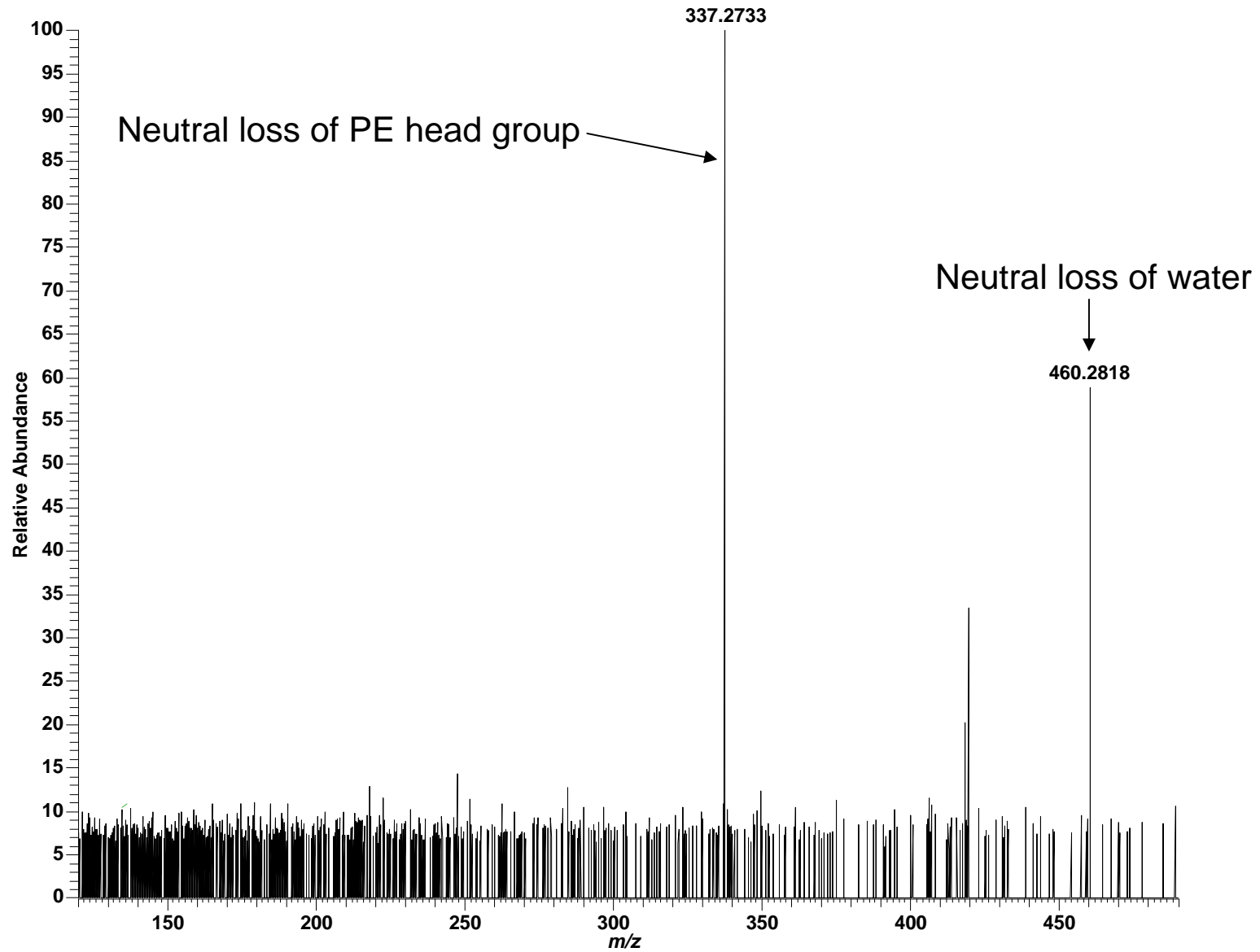
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 16:0; $C_{21}H_{44}NO_7P$; theoretical m/z 452.2777, (M-H)⁻



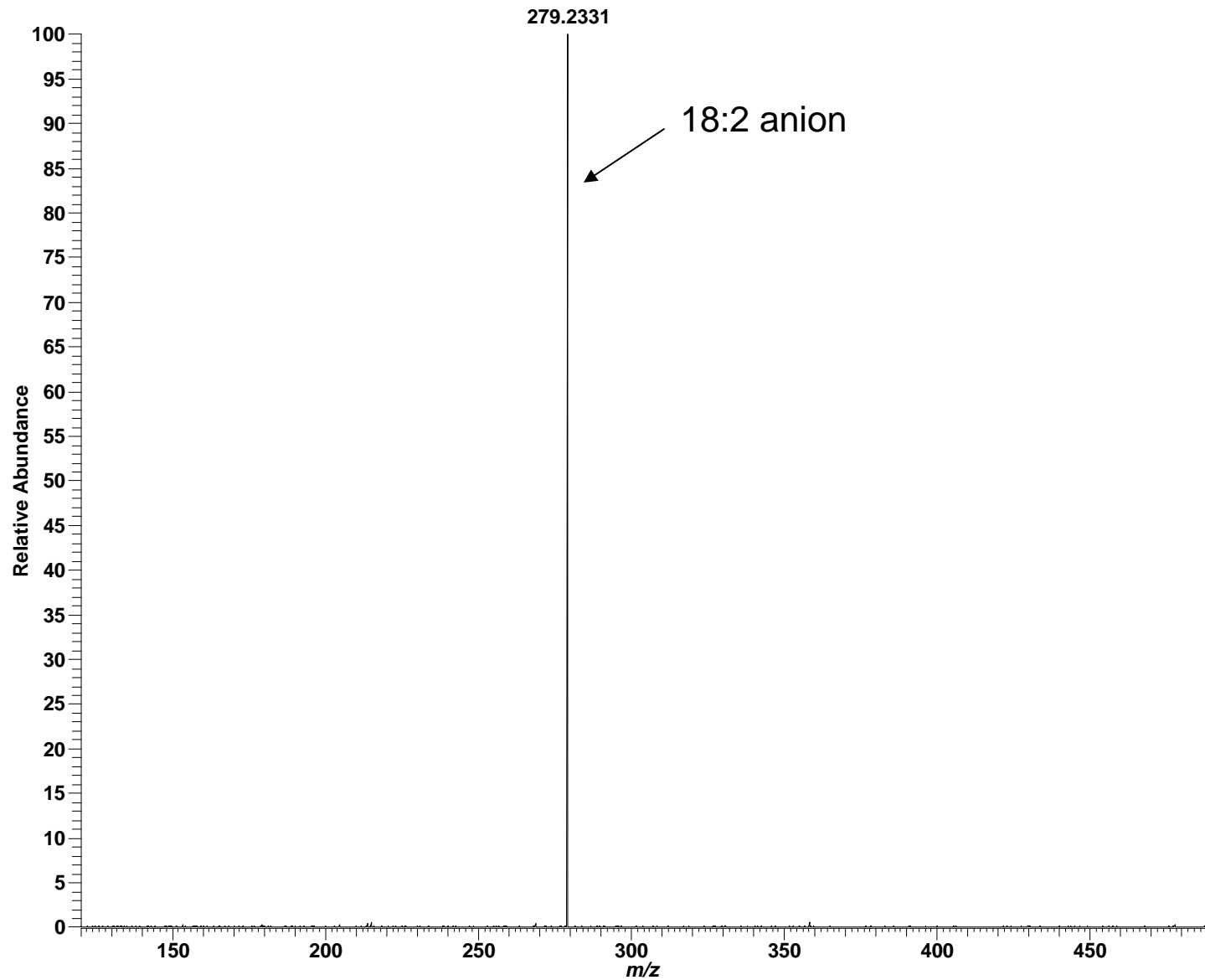
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 18:2; $C_{23}H_{44}NO_7P$; theoretical m/z 478.2933, $(M+H)^+$



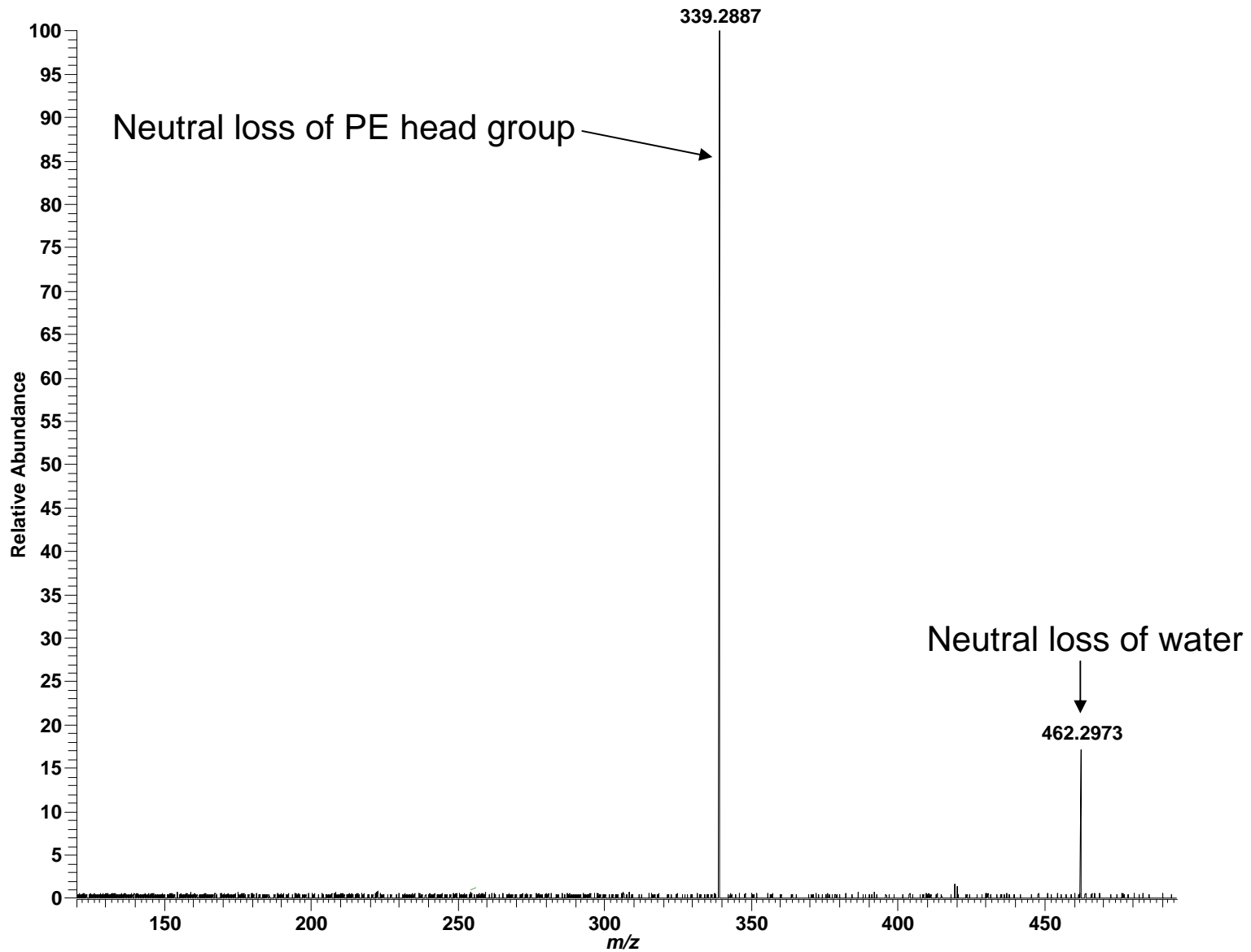
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 18:2; $C_{23}H_{44}NO_7P$; theoretical m/z 476.2777, (M-H)⁻



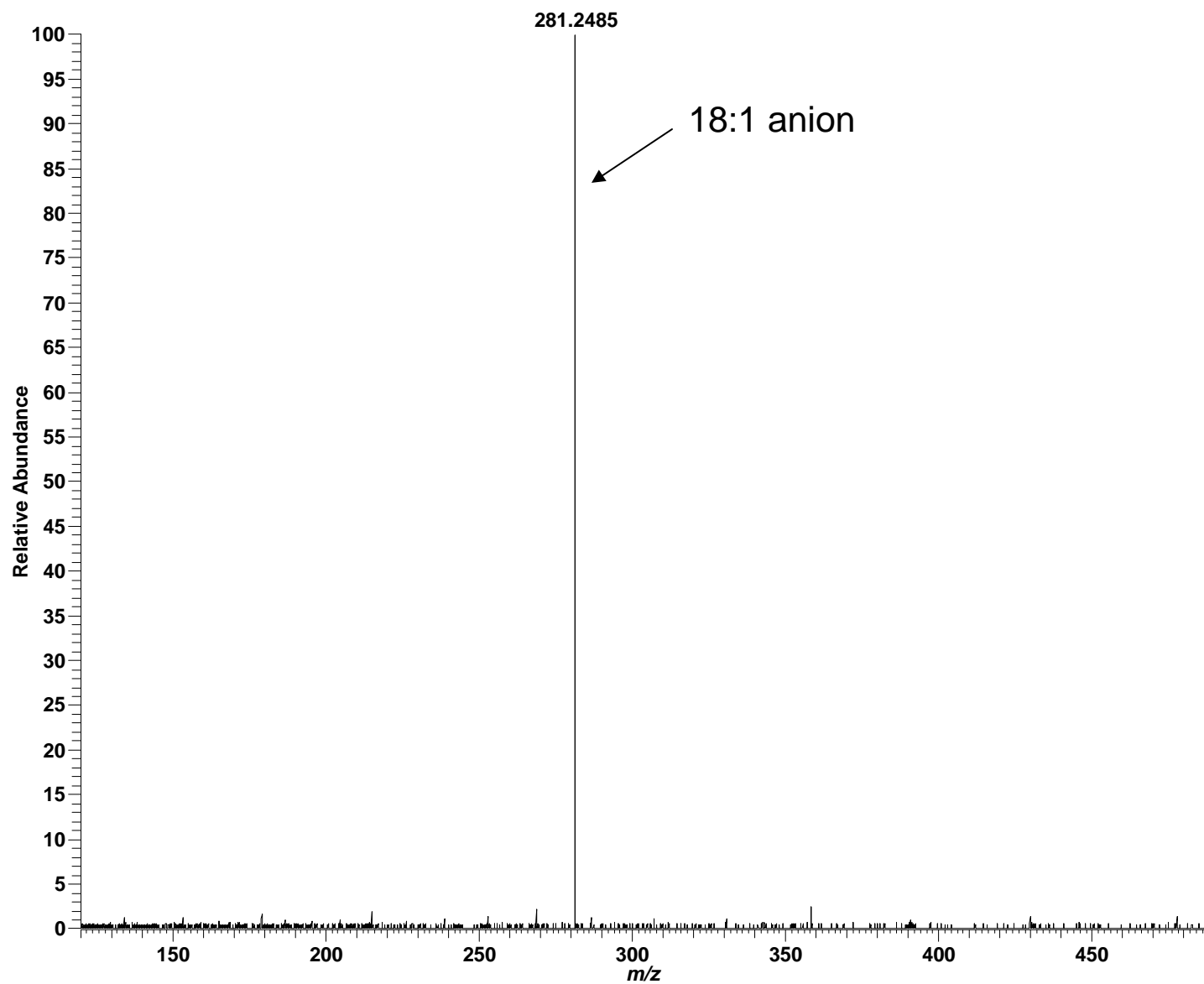
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 18:1; $C_{23}H_{46}NO_7P$; theoretical m/z 480.3090, $(M+H)^+$



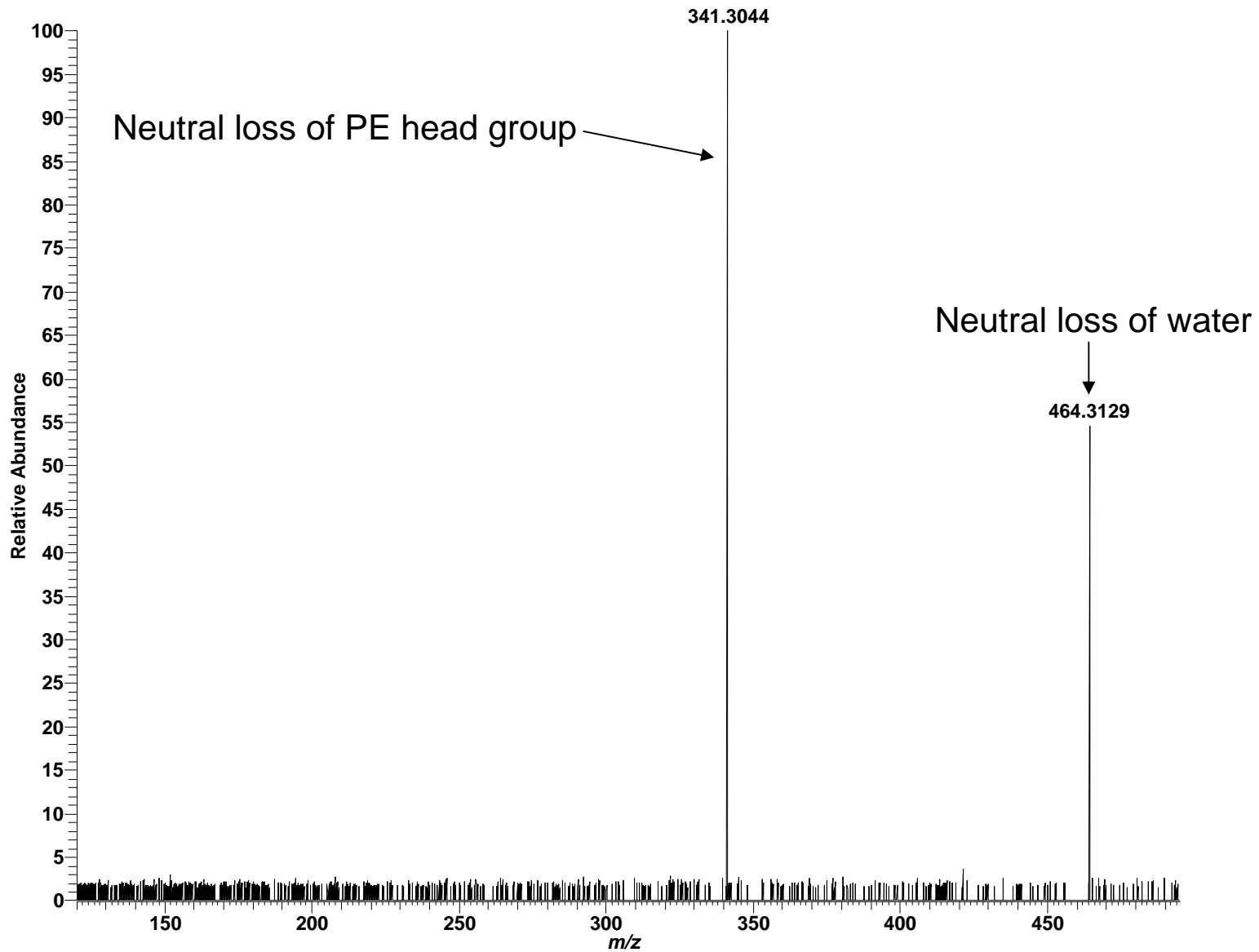
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 18:1; $C_{23}H_{46}NO_7P$; theoretical m/z 478.2933, $(M-H)^-$



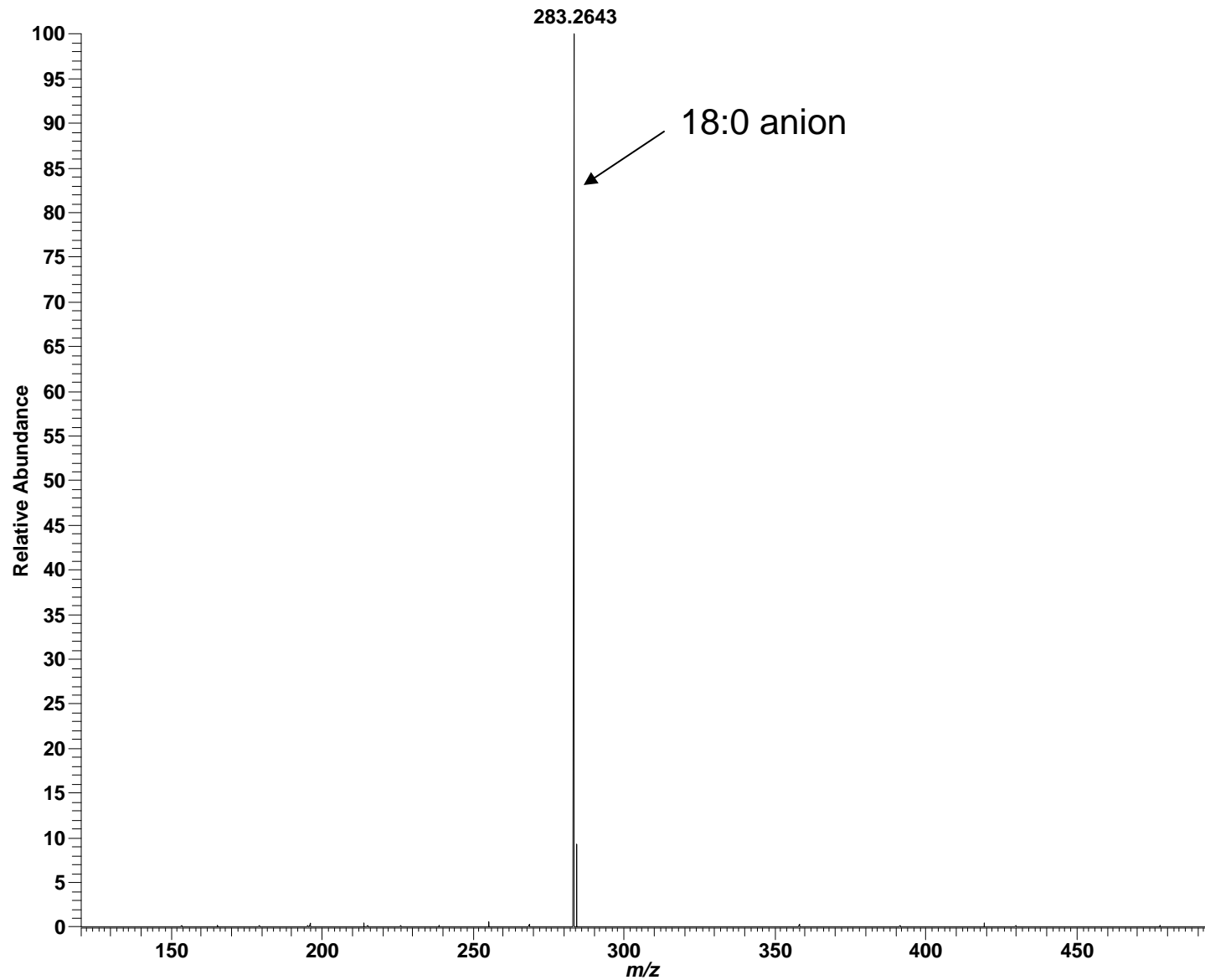
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 18:0; $C_{23}H_{48}NO_7P$; theoretical m/z 482.3246, $(M+H)^+$



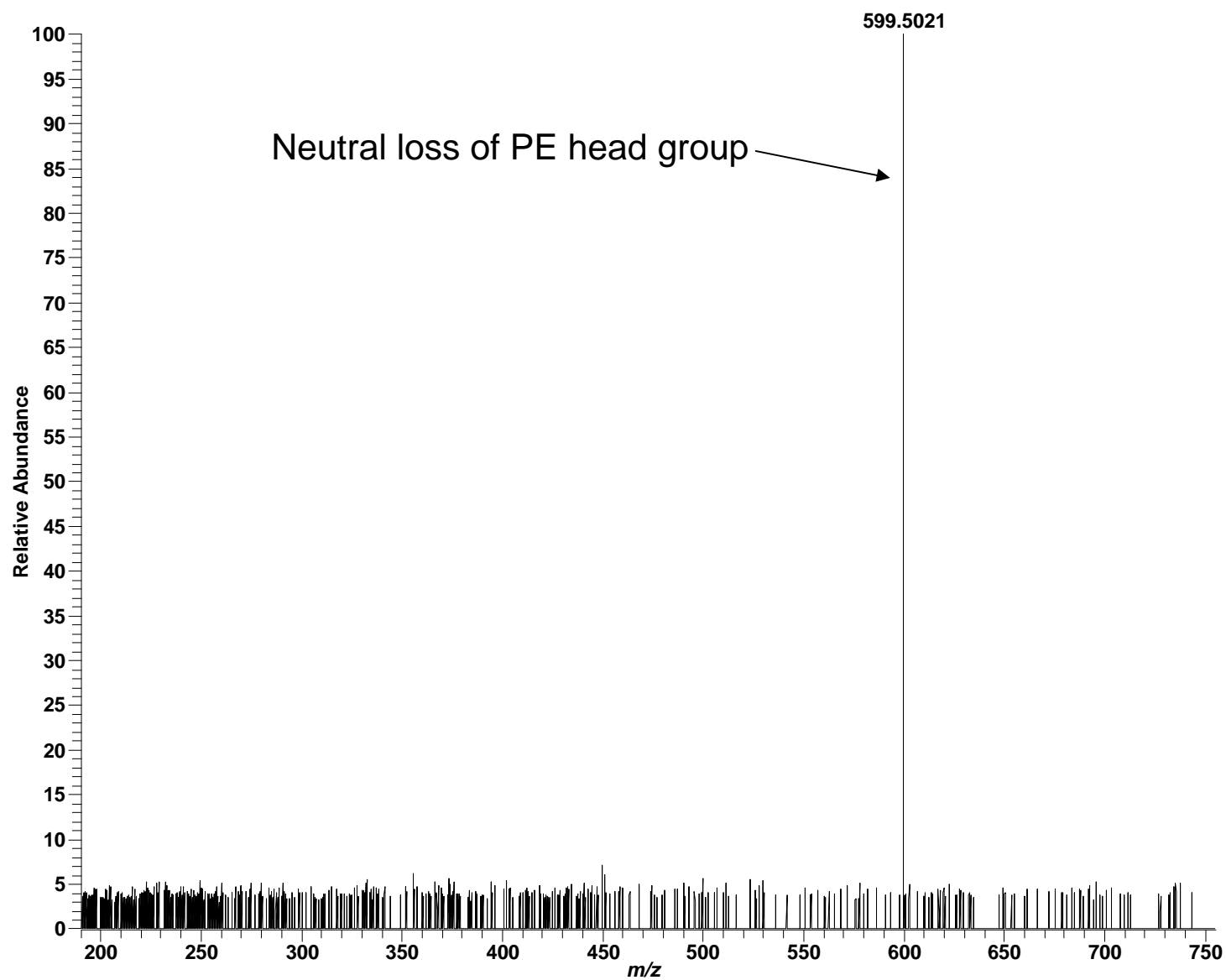
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPE 18:0; $C_{23}H_{48}NO_7P$; theoretical m/z 480.3090, (M-H)⁻



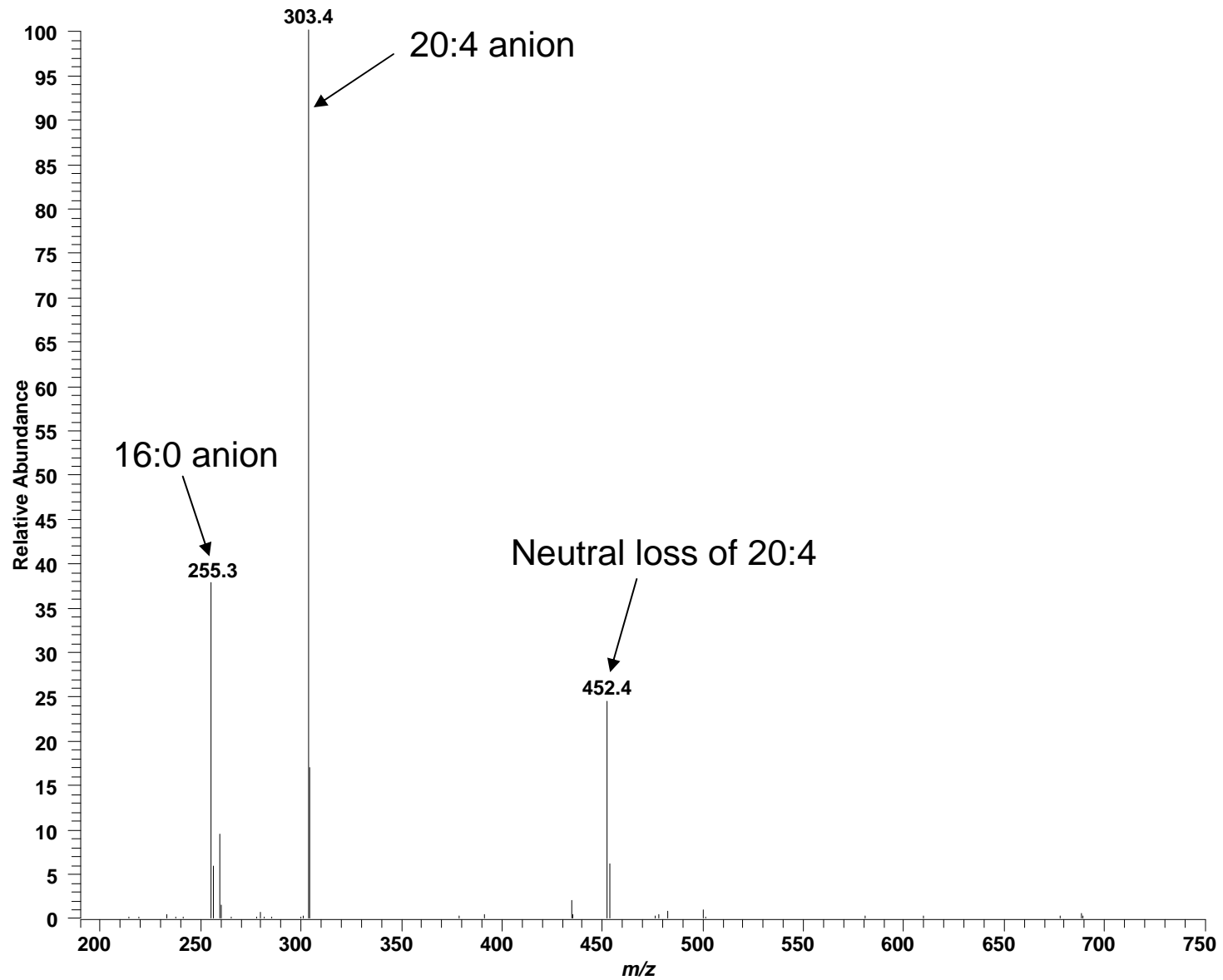
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PE 16:0/20:4; $C_{41}H_{74}NO_8P$; theoretical m/z 740.5230, $(M+H)^+$



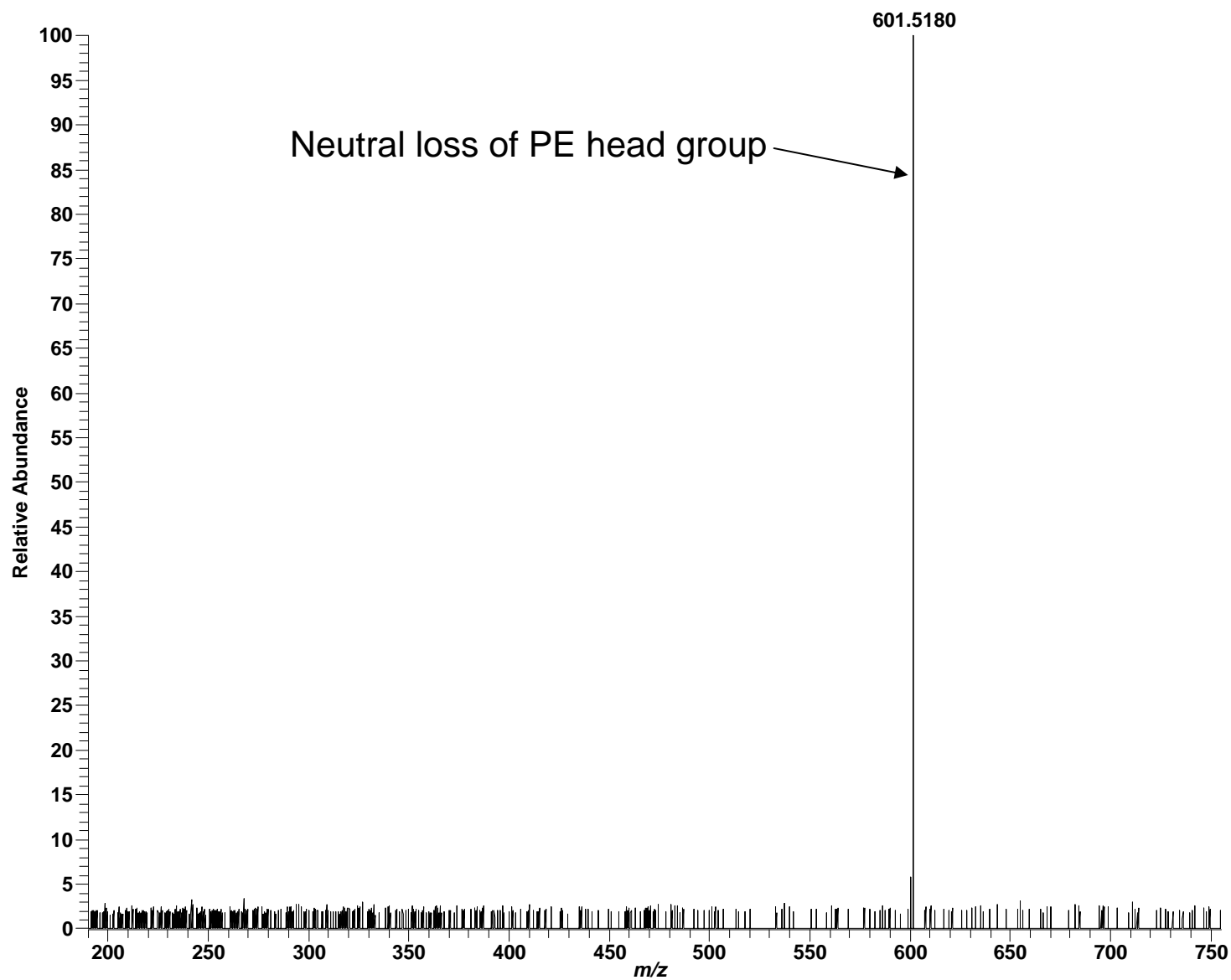
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 16:0/20:4; $C_{41}H_{74}NO_8P$; theoretical m/z 738.5, (M-H)⁻



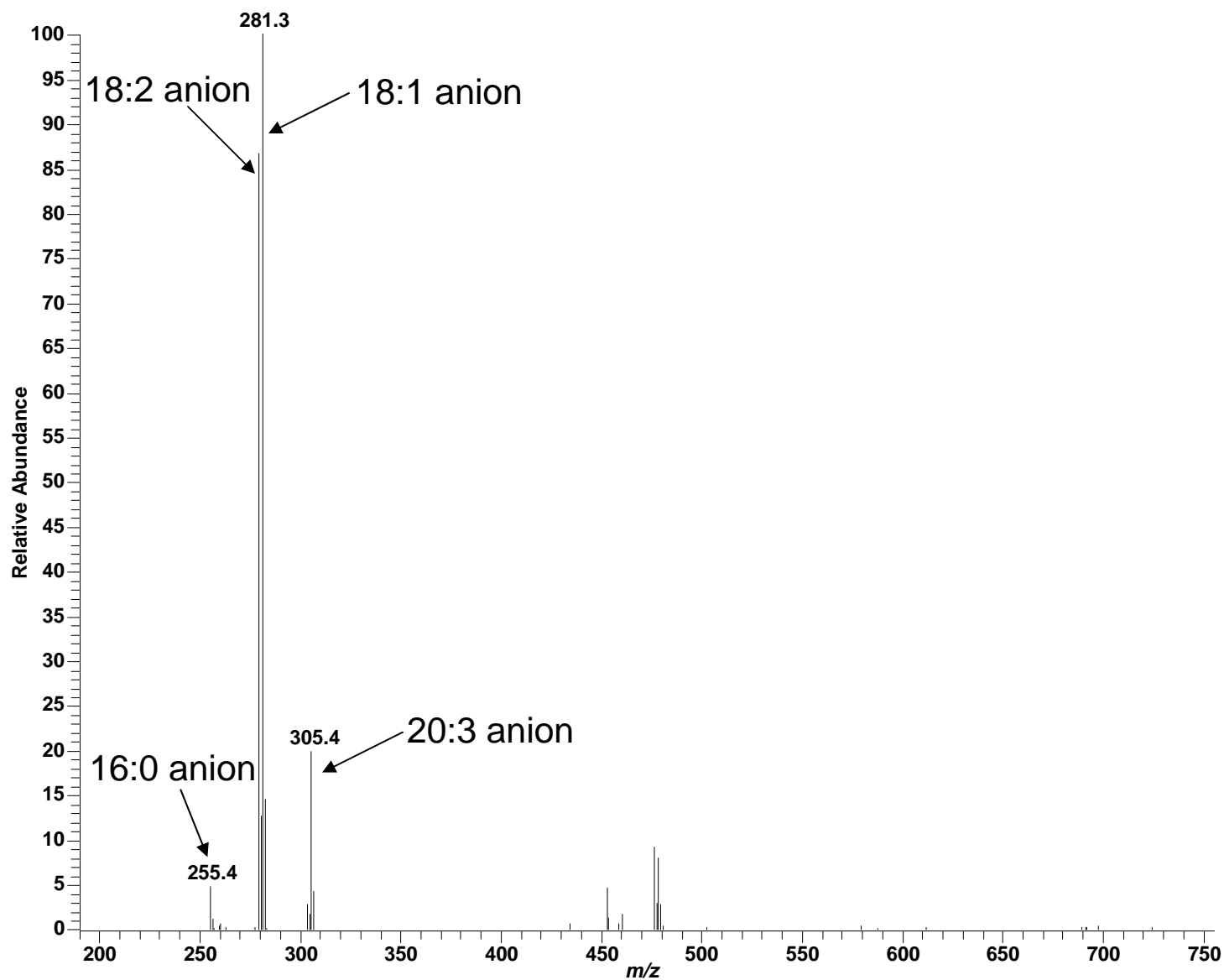
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PE 16:0/20:3 or 18:2/18:1; $C_{41}H_{76}NO_8P$; theoretical m/z 742.5387, $(M+H)^+$



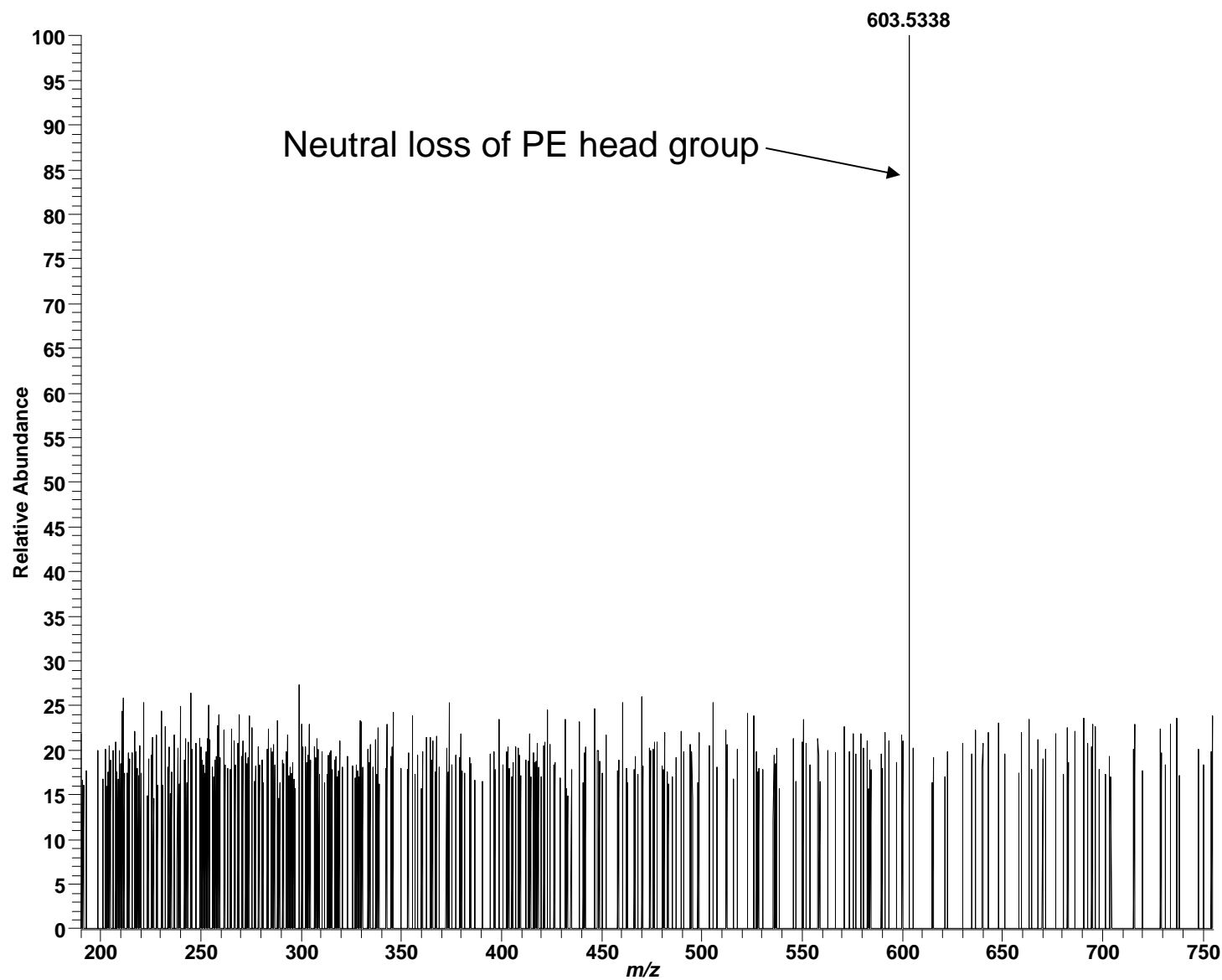
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 16:0/20:3 or 18:2/18:1; $C_{41}H_{76}NO_8P$; theoretical m/z 740.5, (M-H)⁻



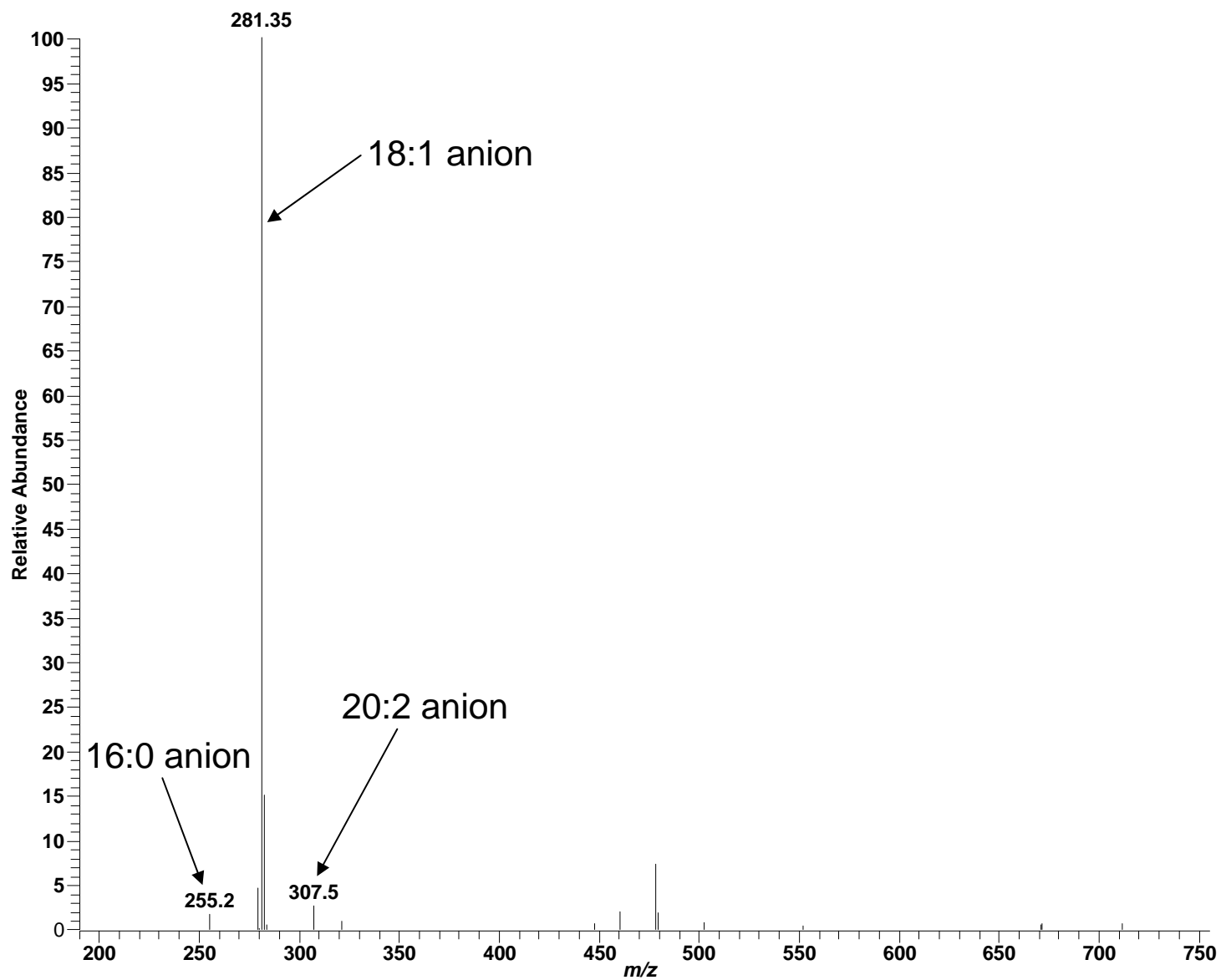
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPE 16:0/20:2 or 18:1/18:1; $C_{41}H_{78}NO_8P$; theoretical m/z 744.5543, $(M+H)^+$



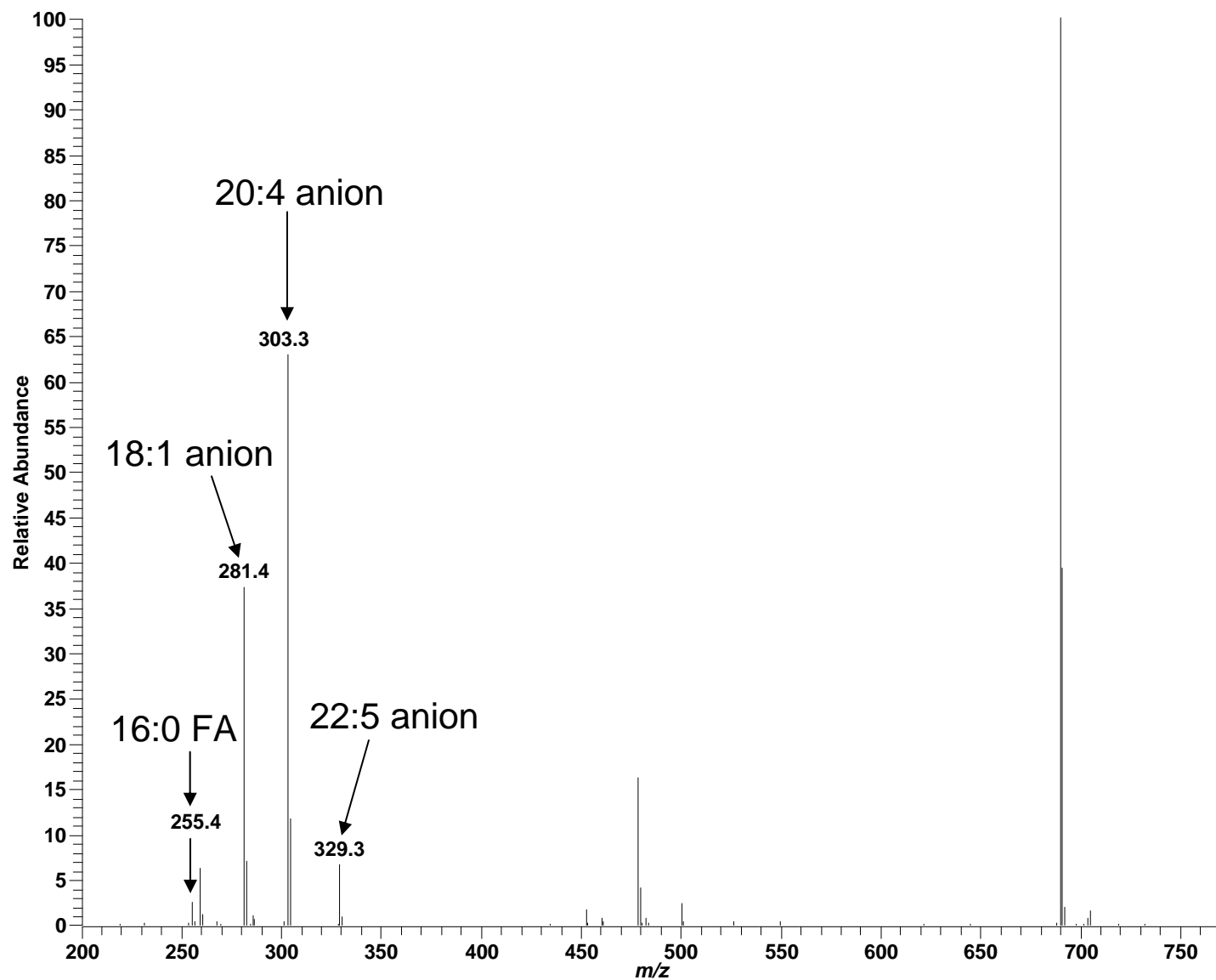
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 16:0/20:2 or 18:1/18:1; $C_{41}H_{78}NO_8P$; theoretical m/z 742.5, (M-H)⁻



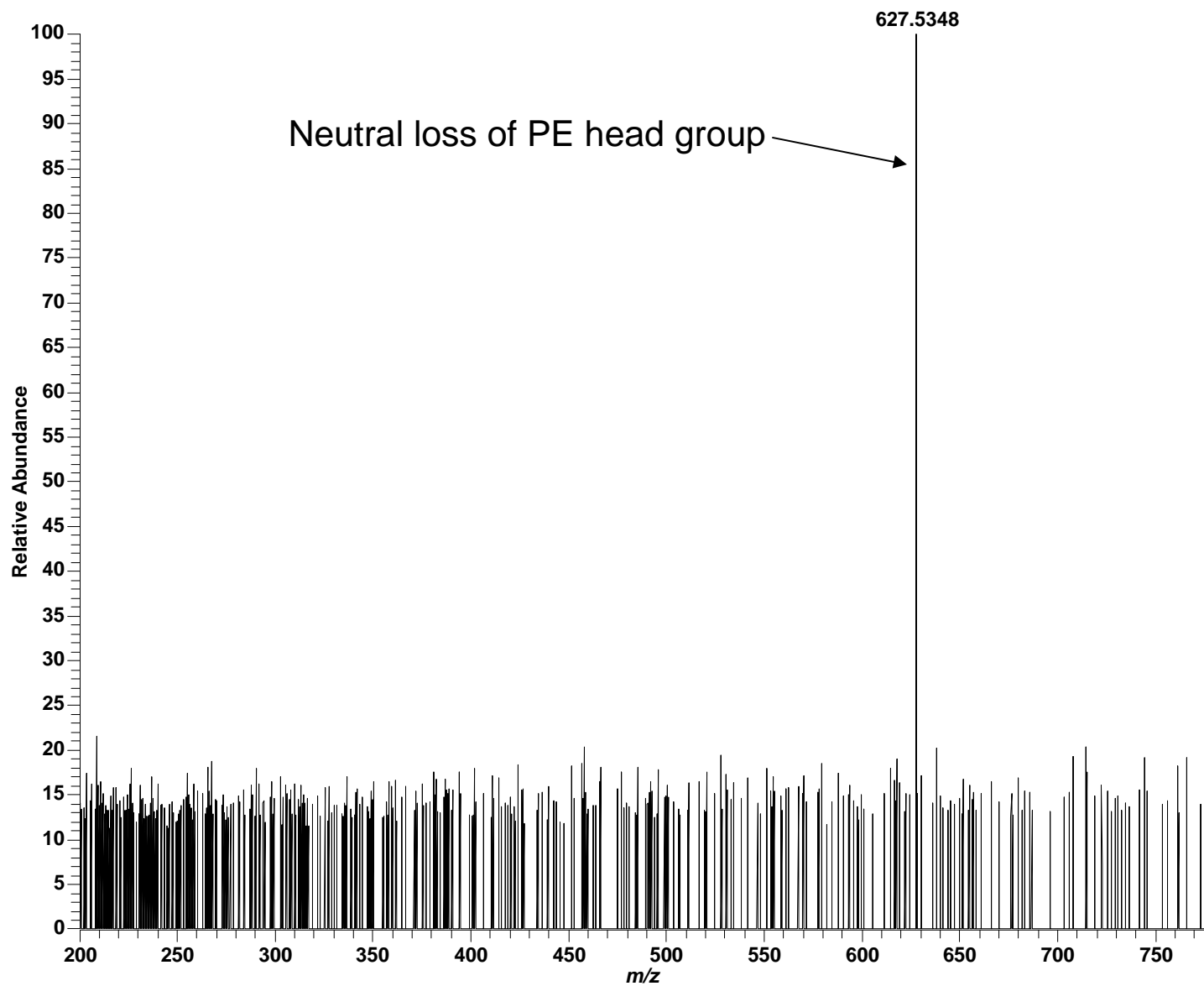
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 18:1/20:4 or 16:0/22:5; $C_{43}H_{76}NO_8P$; theoretical m/z 764.5, (M-H)⁻



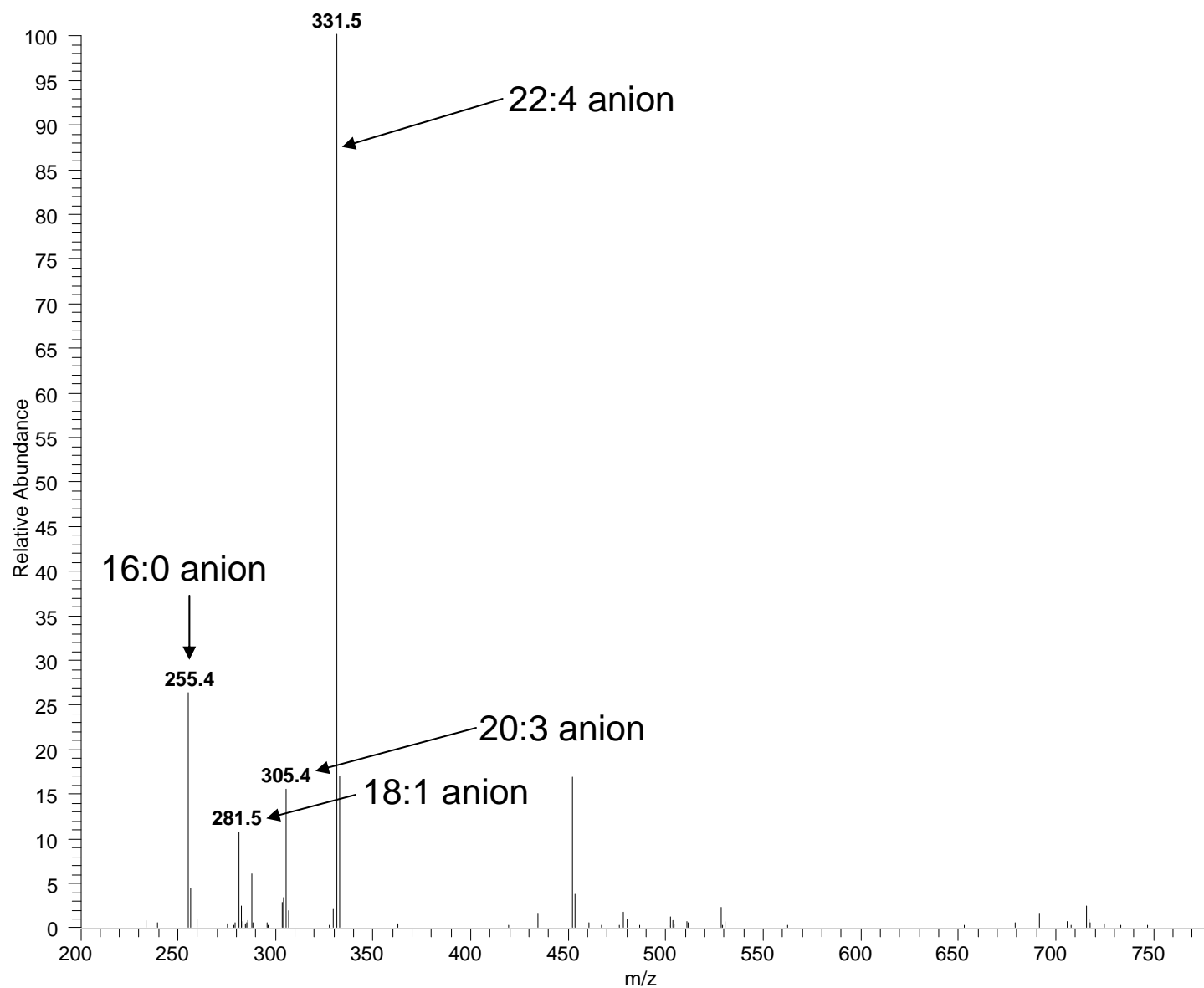
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PE 18:1/20:3 or 16:0/22:4; $C_{43}H_{78}NO_8P$; theoretical m/z 768.5543, $(M+H)^+$



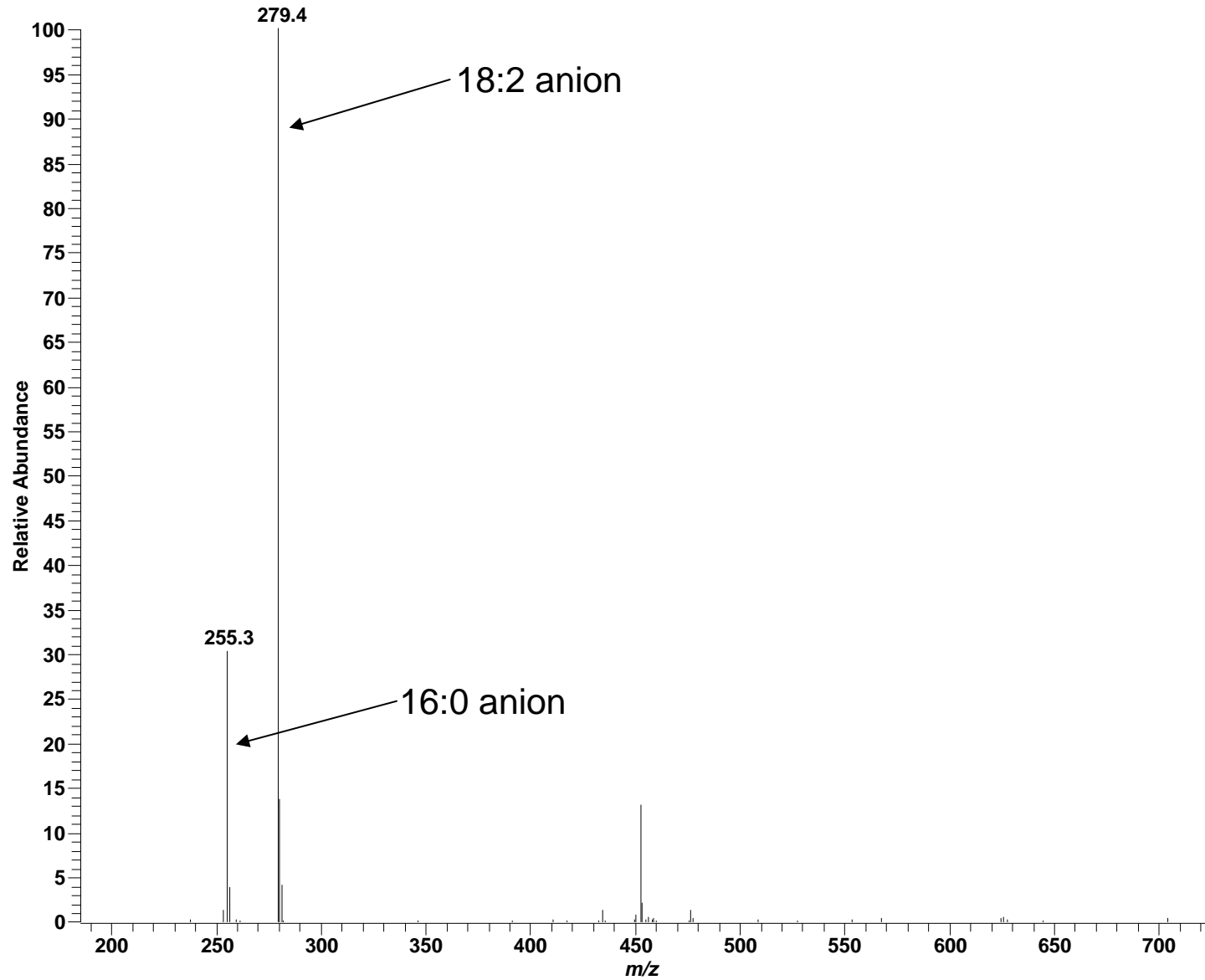
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 18:1/20:3 or 16:0/22:4; $C_{43}H_{78}NO_8P$; theoretical m/z 766.5, (M-H)⁻



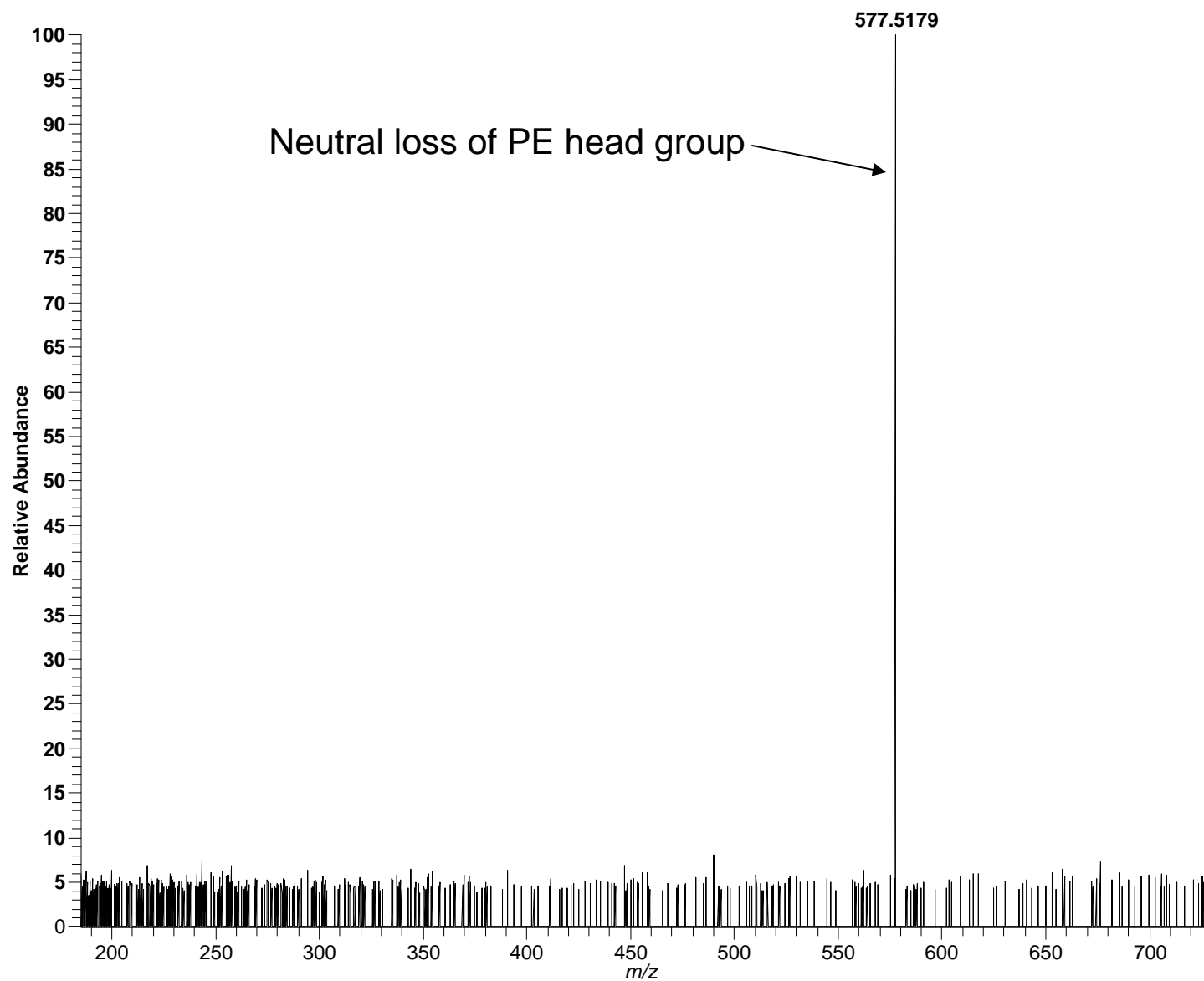
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 16:0/18:2; $C_{39}H_{74}NO_8P$; theoretical m/z 714.5, (M-H)⁻



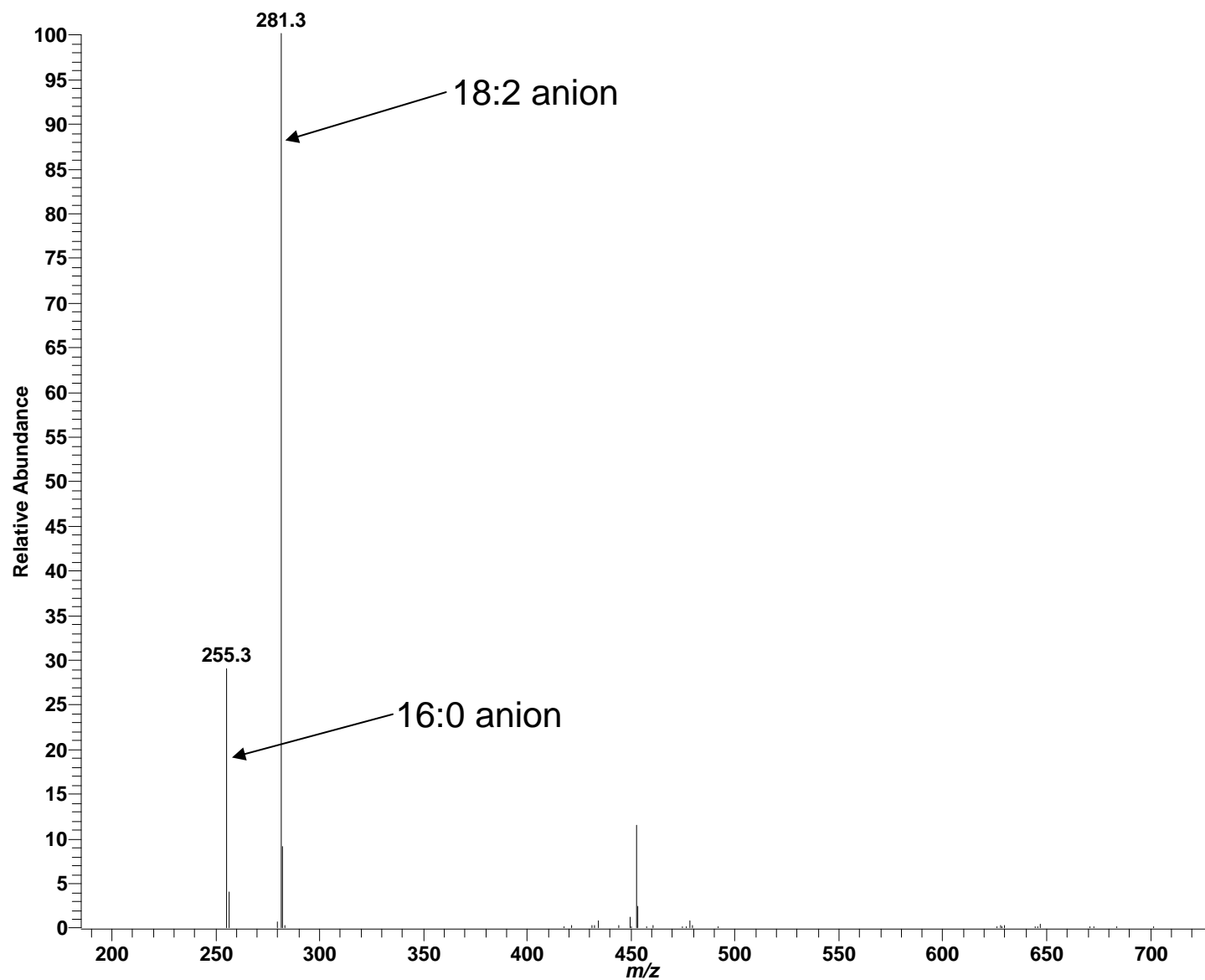
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PE 16:0/18:1; $C_{39}H_{76}NO_8P$; theoretical m/z 718.5387, $(M+H)^+$



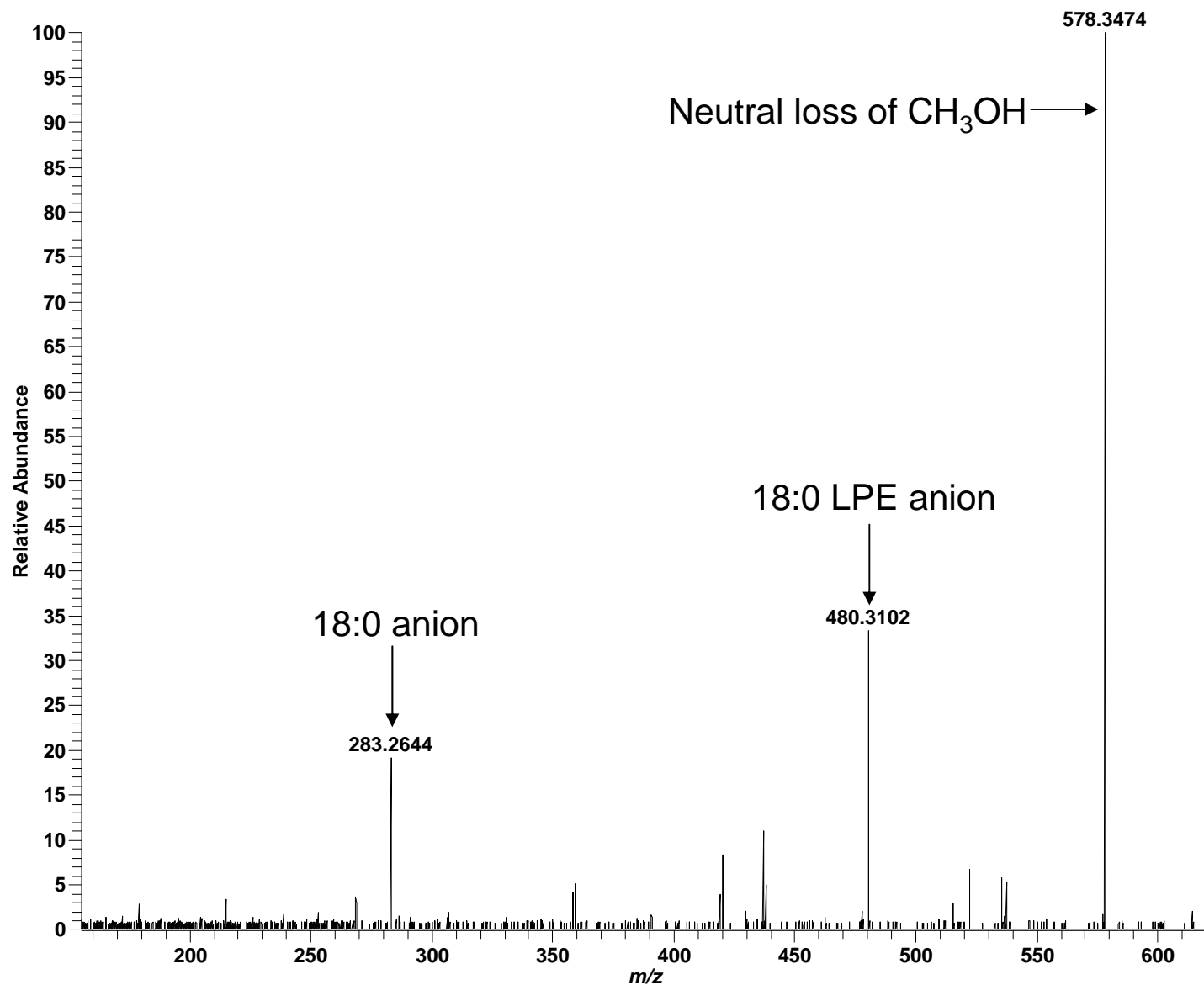
Low mass measurement accuracy MS/MS utilizing LTQ

Negative ESI: PE 16:0/18:1; $C_{39}H_{76}NO_8P$; theoretical m/z 716.5, (M-H)⁻



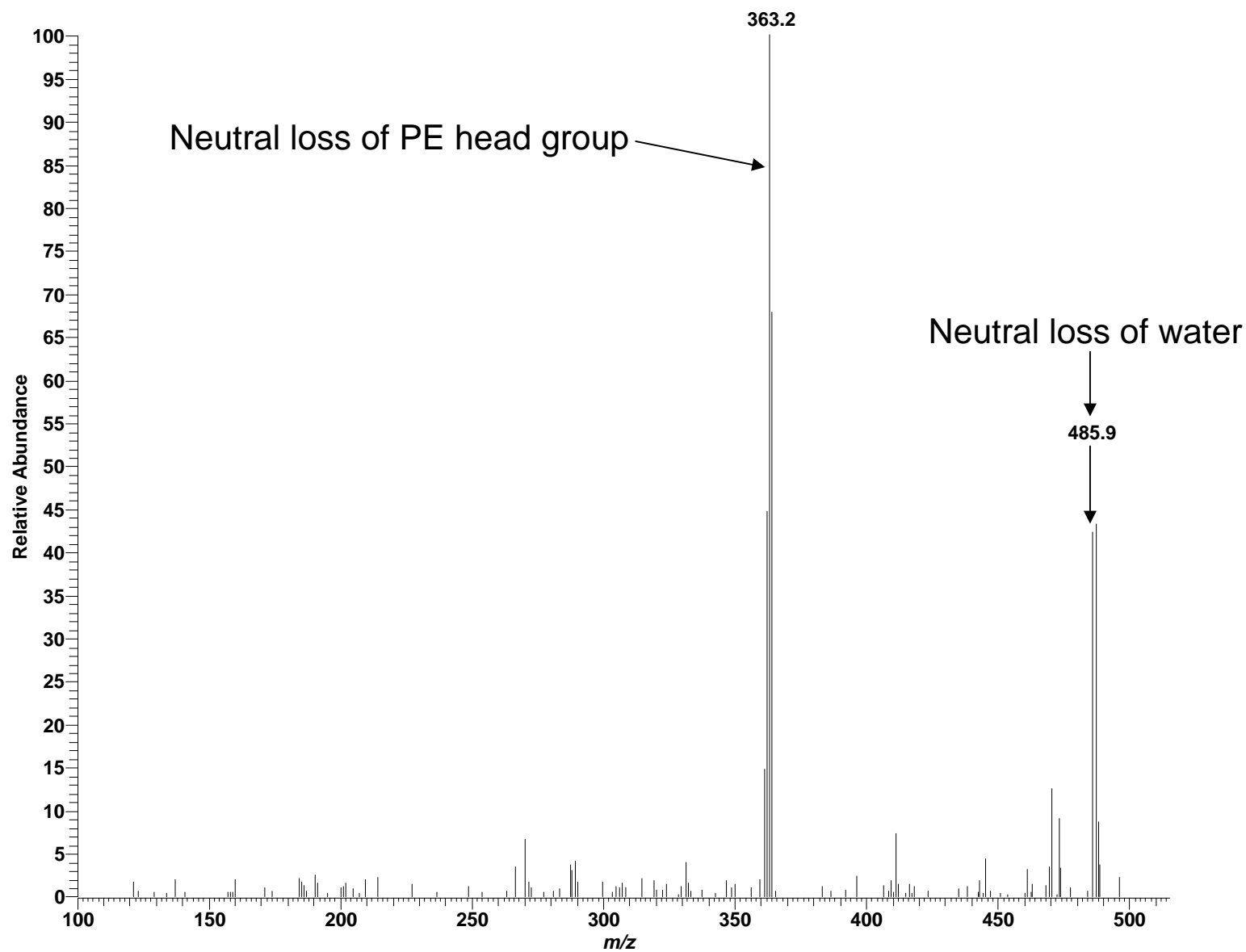
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: PE (18:0/6:0-dihydroxy); $C_{23}H_{44}NO_7P$; theoretical m/z 610.3720, $(M-H)^-$



Low mass measurement accuracy MS/MS utilizing LTQ

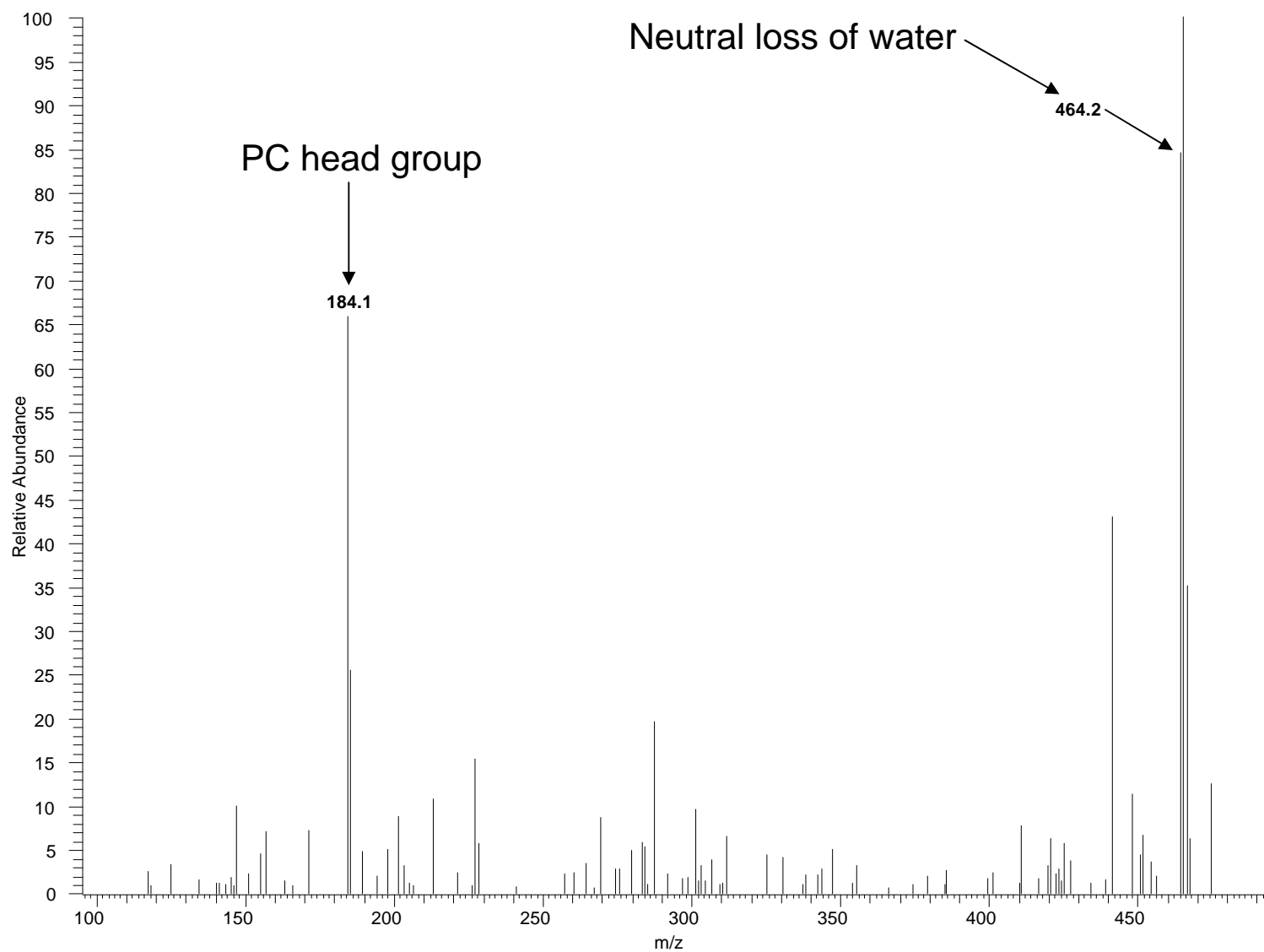
Positive ESI: LPE (20:3); $C_{25}H_{46}NO_7P$; theoretical m/z 504.3, $(M+H)^+$



Glycerophosphocholines

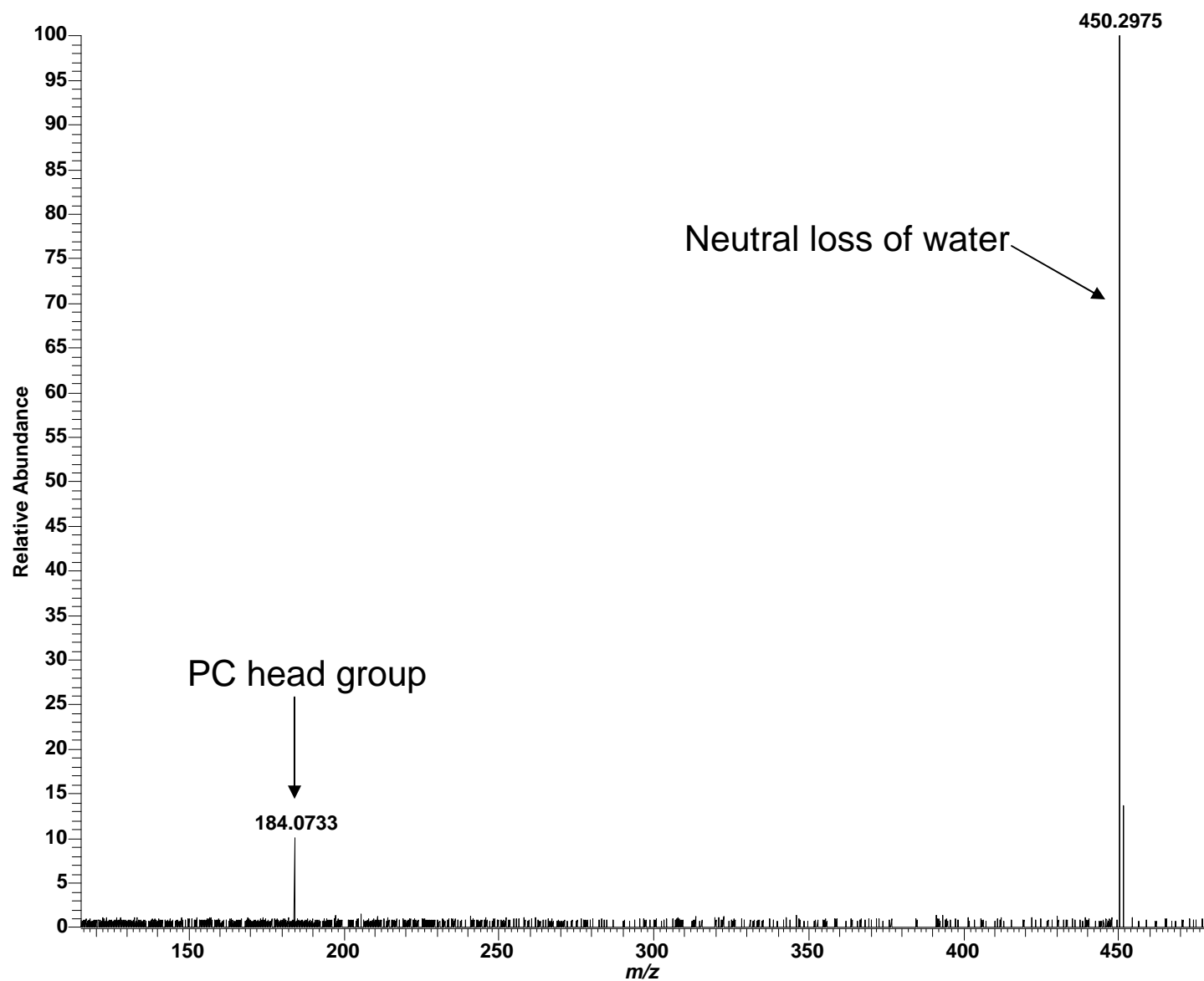
Low mass measurement accuracy MS/MS utilizing LTQ

Positive ESI: LPC (15:0); $C_{23}H_{48}NO_7P$; theoretical m/z 482.3, $(M+H)^+$



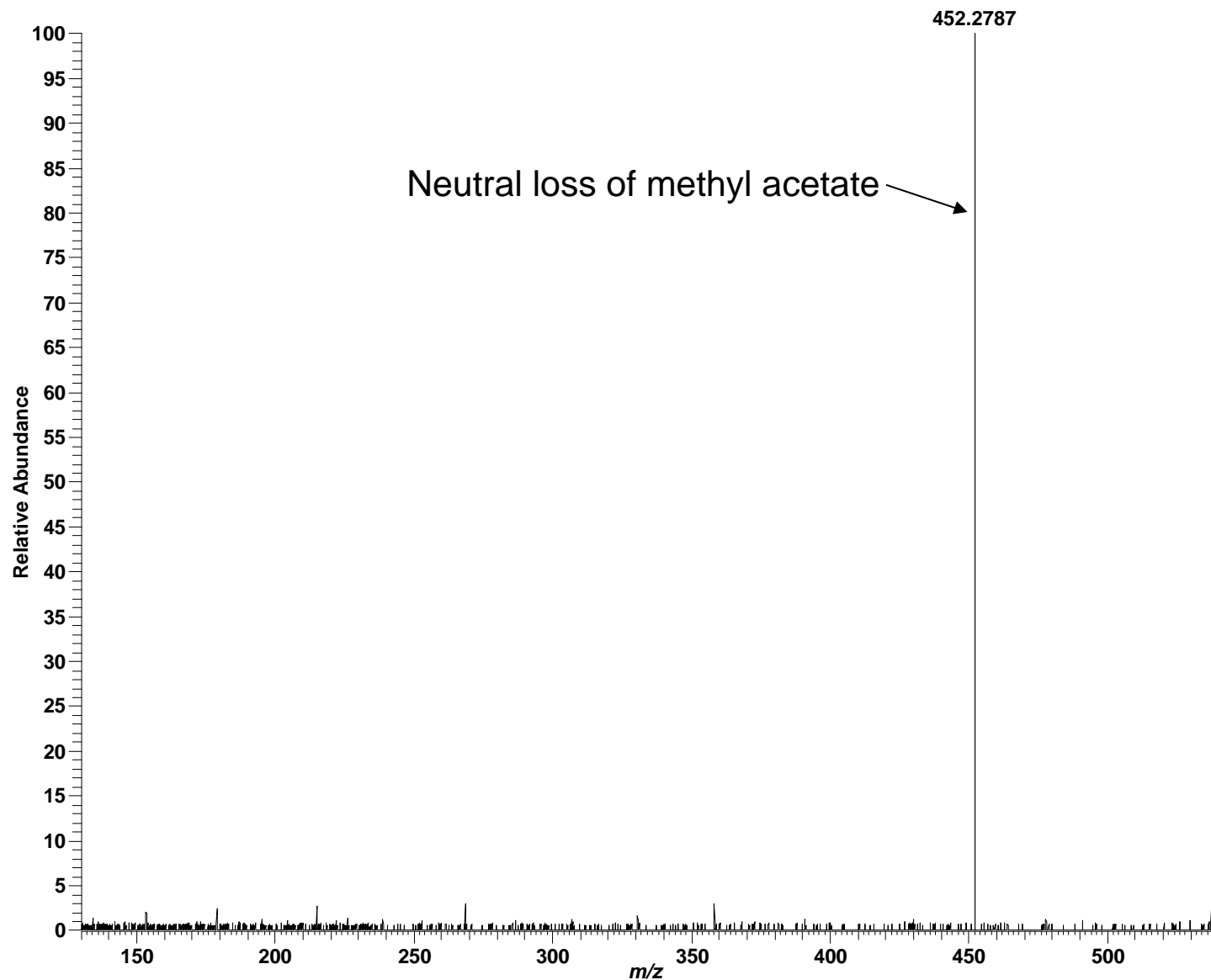
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 14:0; $C_{22}H_{46}NO_7P$; theoretical m/z 468.3090, $(M+H)^+$



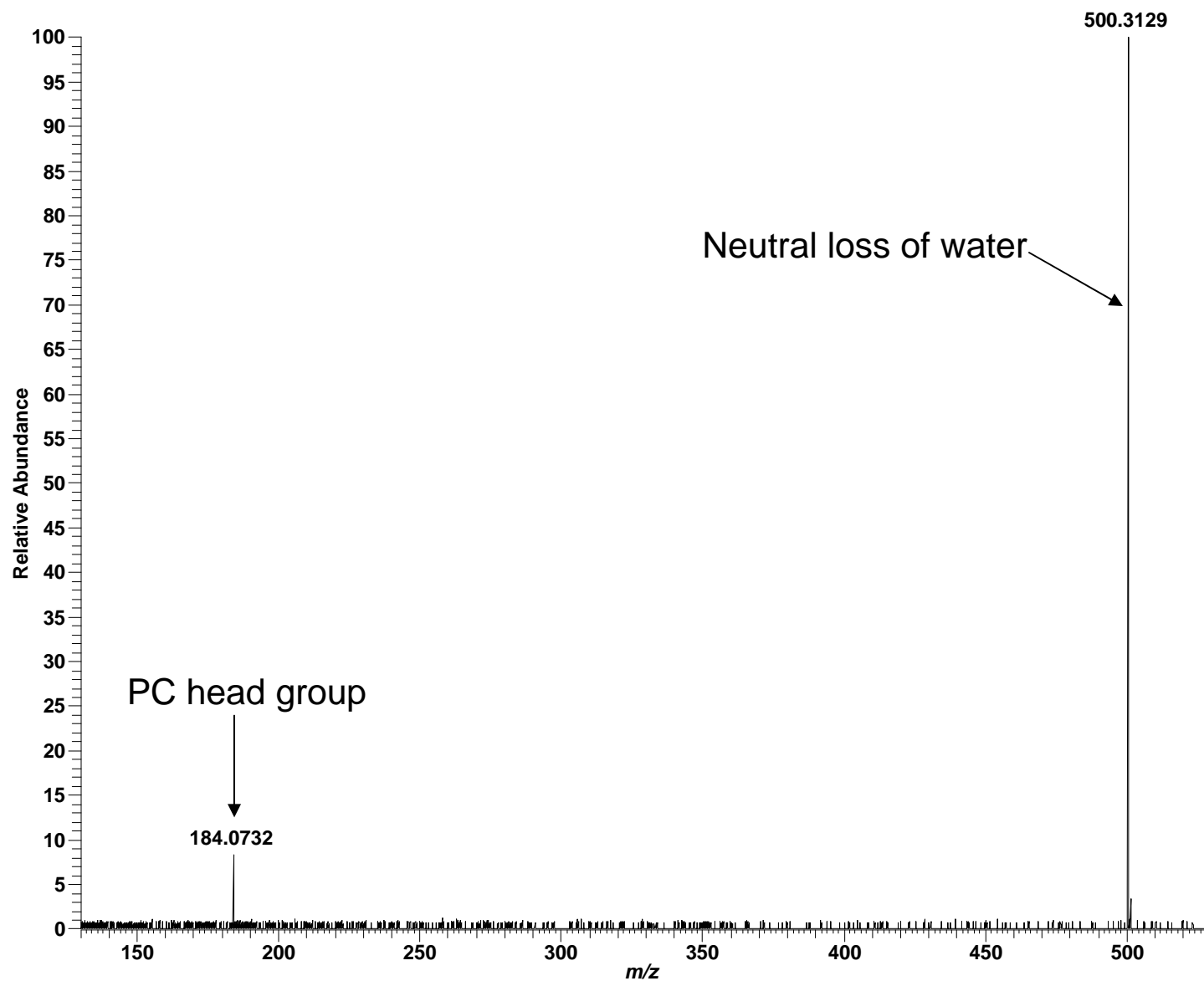
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 14:0; $C_{22}H_{46}NO_7P$; theoretical m/z 526.3145, $(M+CH_3COO)^-$



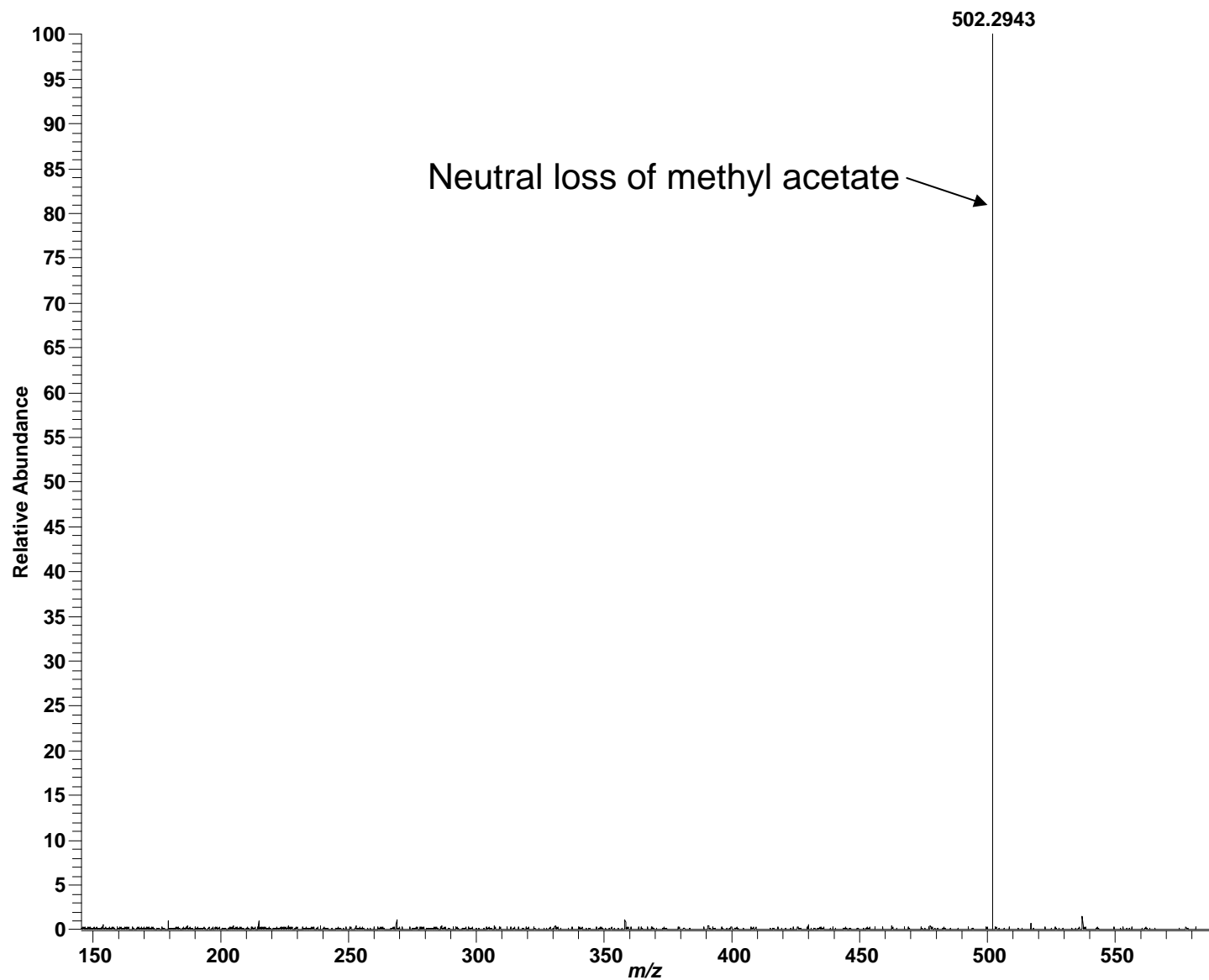
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 18:3; $C_{26}H_{48}NO_7P$; theoretical m/z 518.3246, $(M+H)^+$



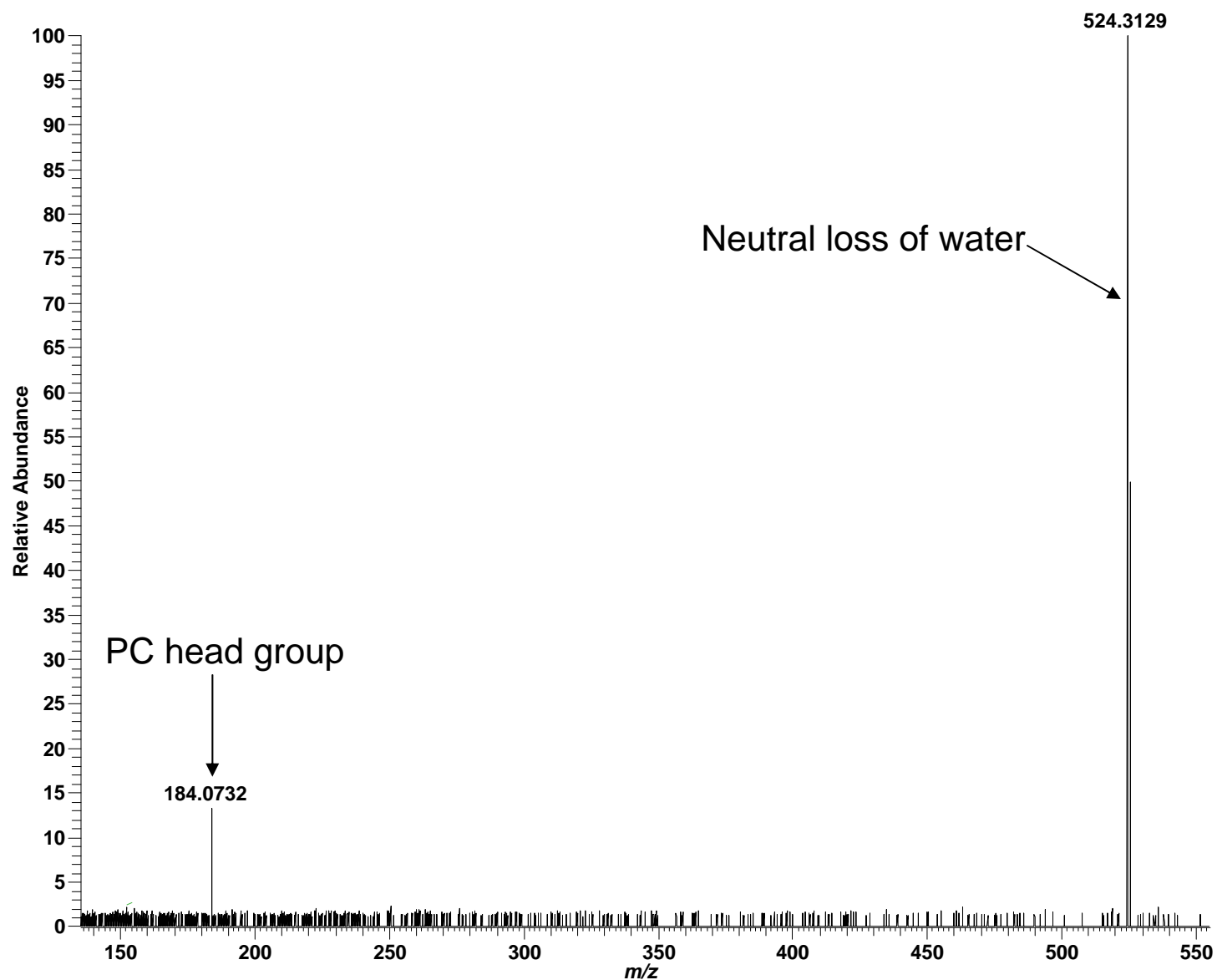
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 18:3; $C_{26}H_{48}NO_7P$; theoretical m/z 576.3301, $(M+CH_3COO)^-$



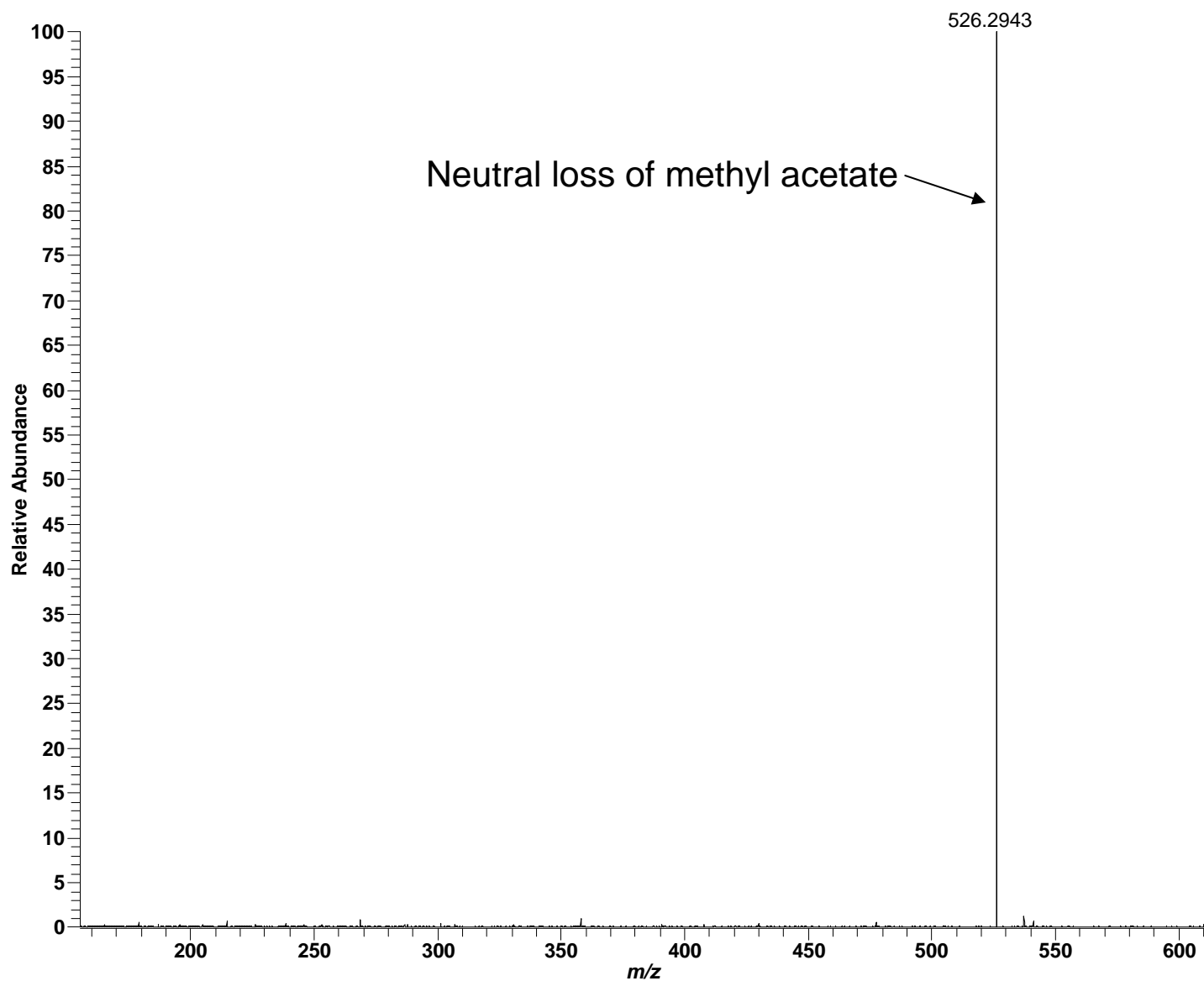
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 20:5; $C_{28}H_{48}NO_7P$; theoretical m/z 542.3246, $(M+H)^+$



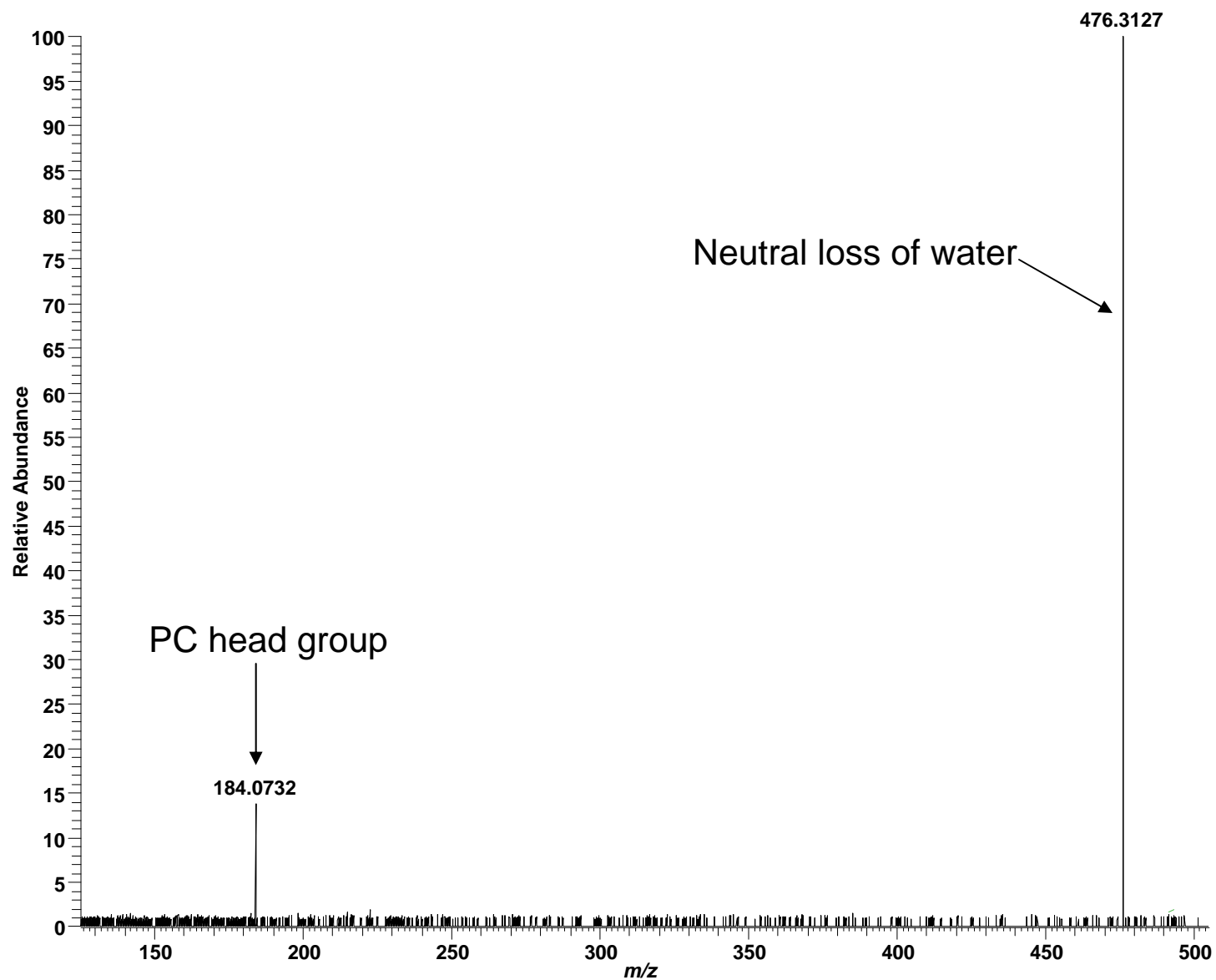
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 20:5; $C_{28}H_{48}NO_7P$; theoretical m/z 600.3301, $(M+CH_3COO)^-$



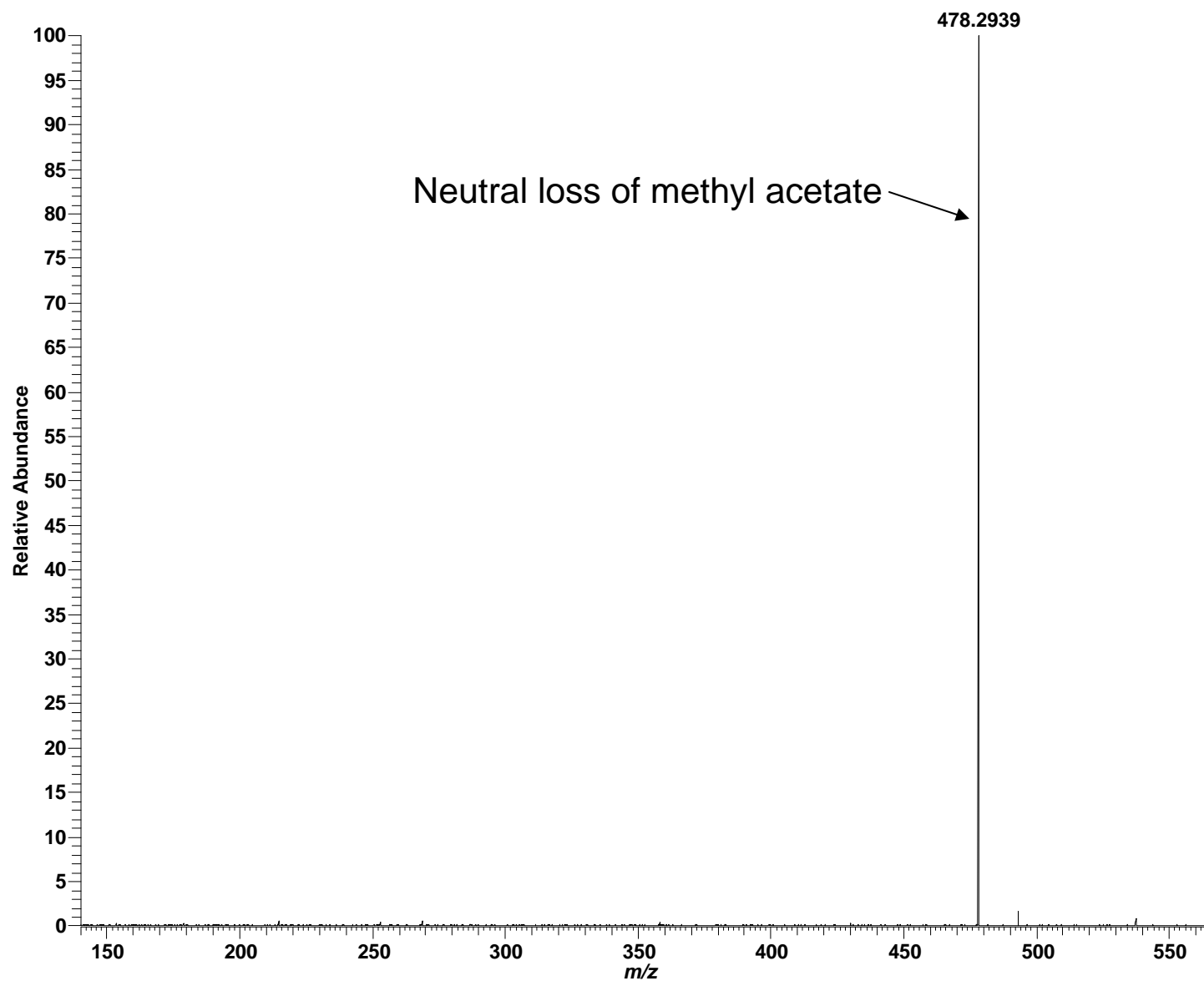
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 16:1; $C_{24}H_{48}NO_7P$; theoretical m/z 494.3247, $(M+H)^+$



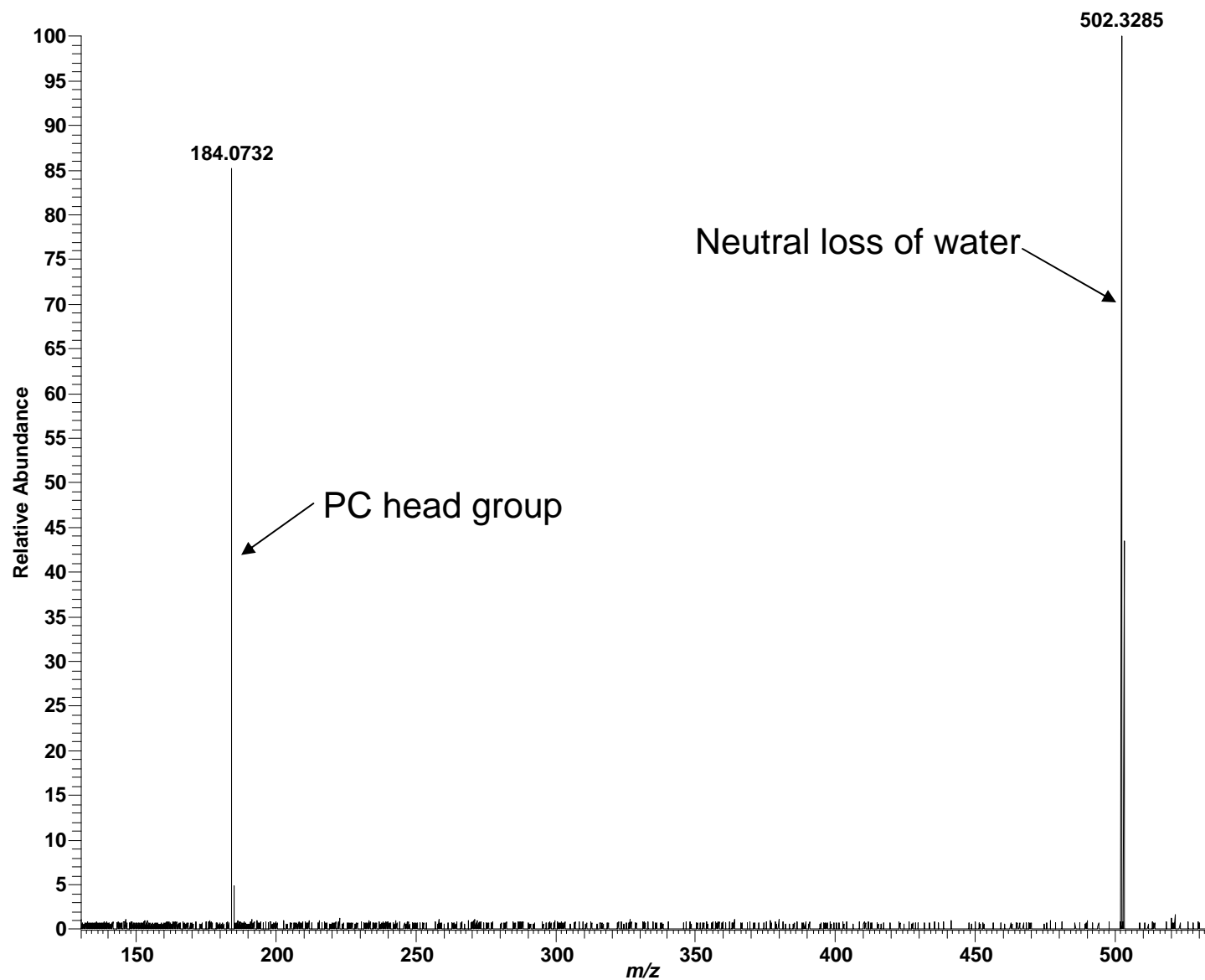
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 16:1; $C_{24}H_{48}NO_7P$; theoretical m/z 552.3301, $(M+CH_3COO)^-$



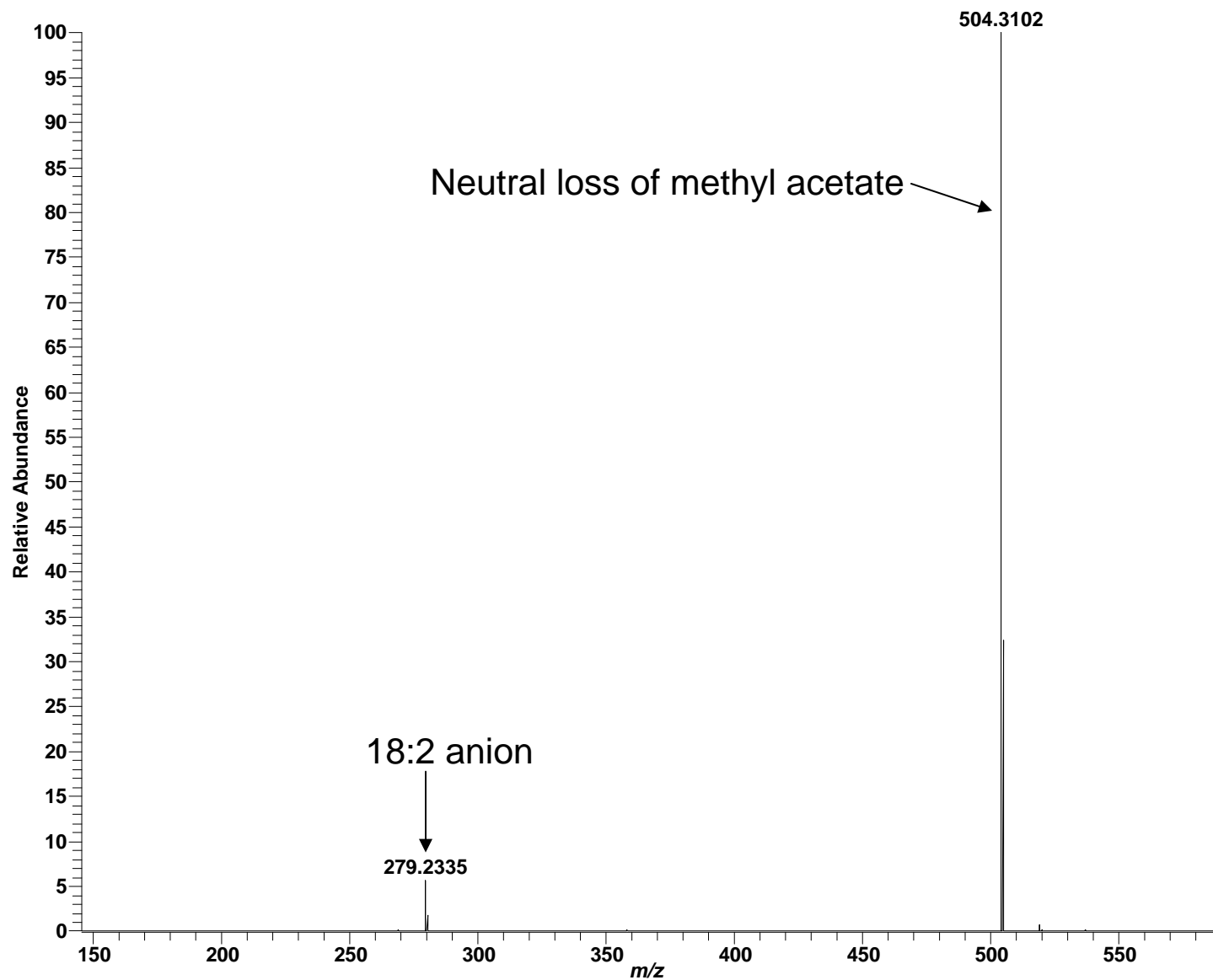
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 18:2; $C_{26}H_{50}NO_7P$; theoretical m/z 520.3403, $(M+H)^+$



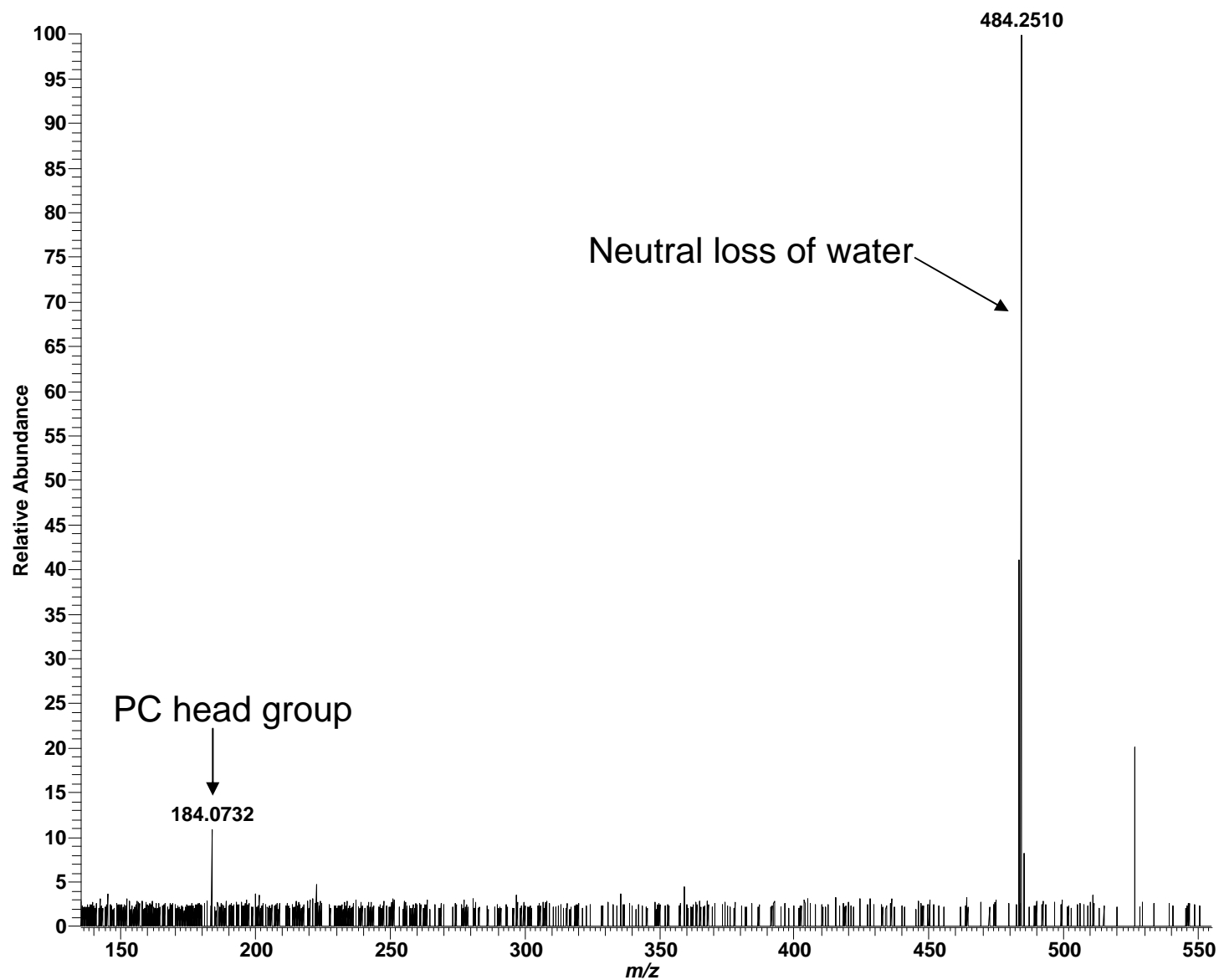
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 18:2; $C_{26}H_{50}NO_7P$; theoretical m/z 578.3458, $(M+CH_3COO)^-$



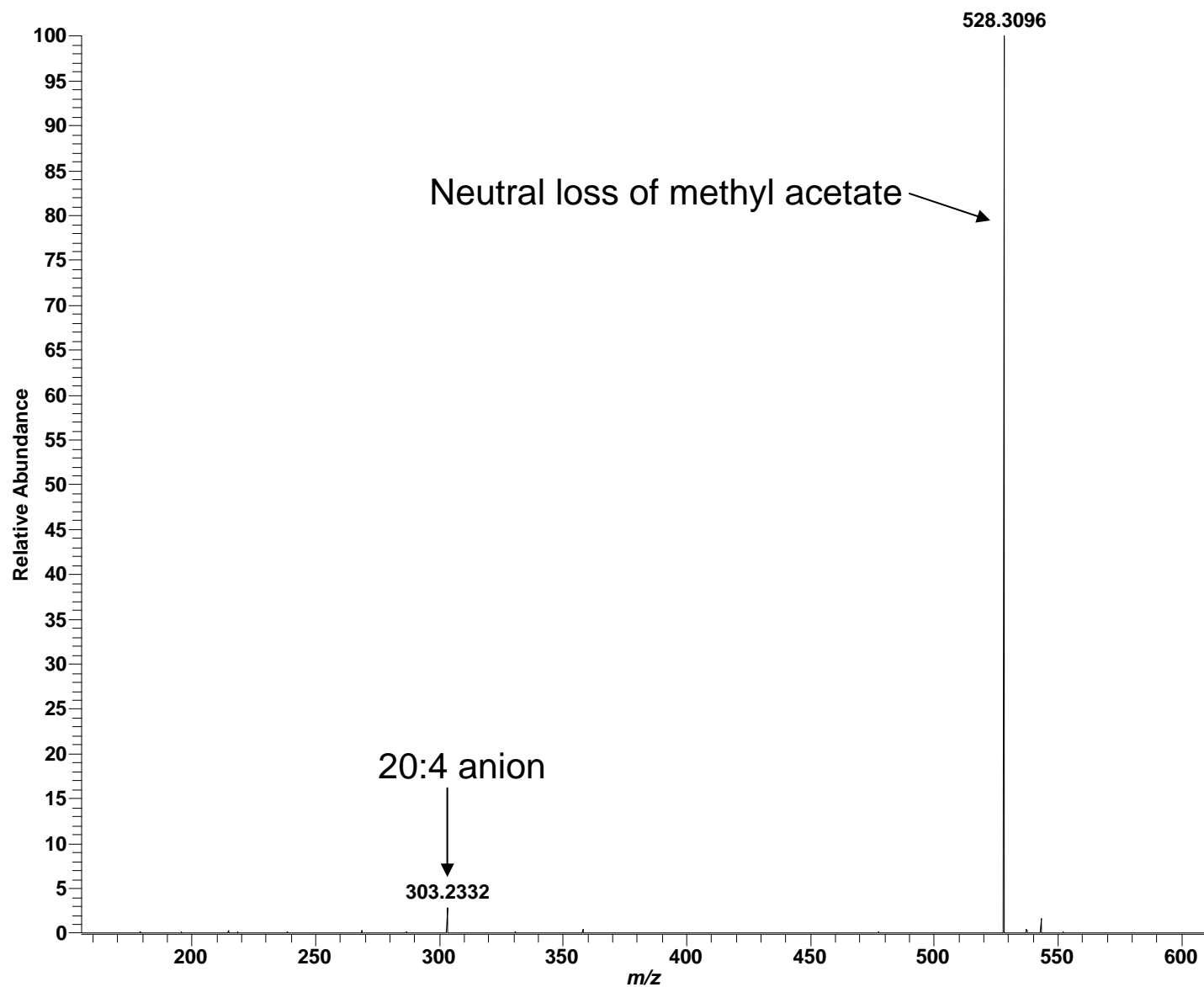
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 20:4; $C_{28}H_{50}NO_7P$; theoretical m/z 544.3403, $(M+H)^+$



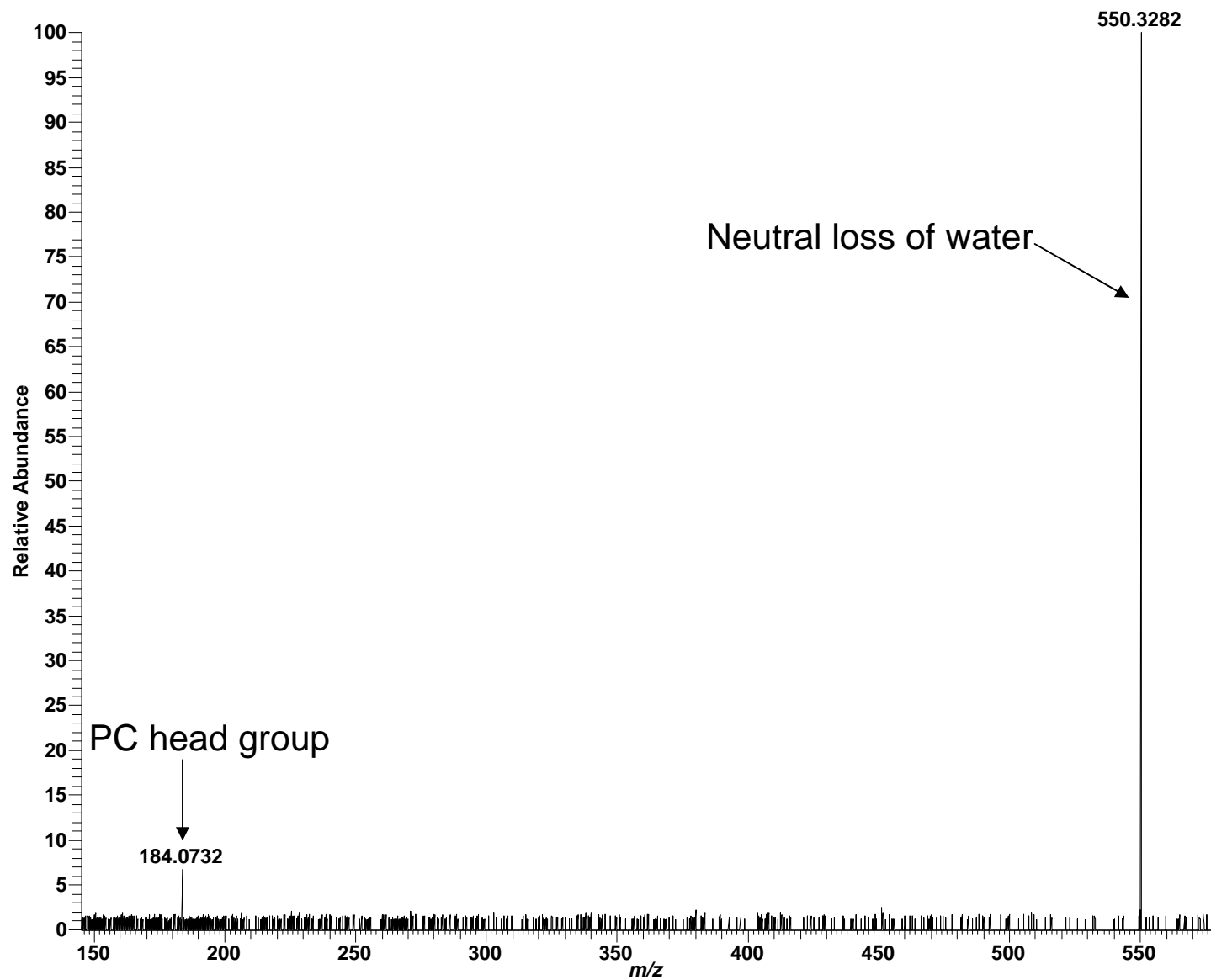
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 20:4; $C_{28}H_{50}NO_7P$; theoretical m/z 602.3458, $(M+CH_3COO)^-$



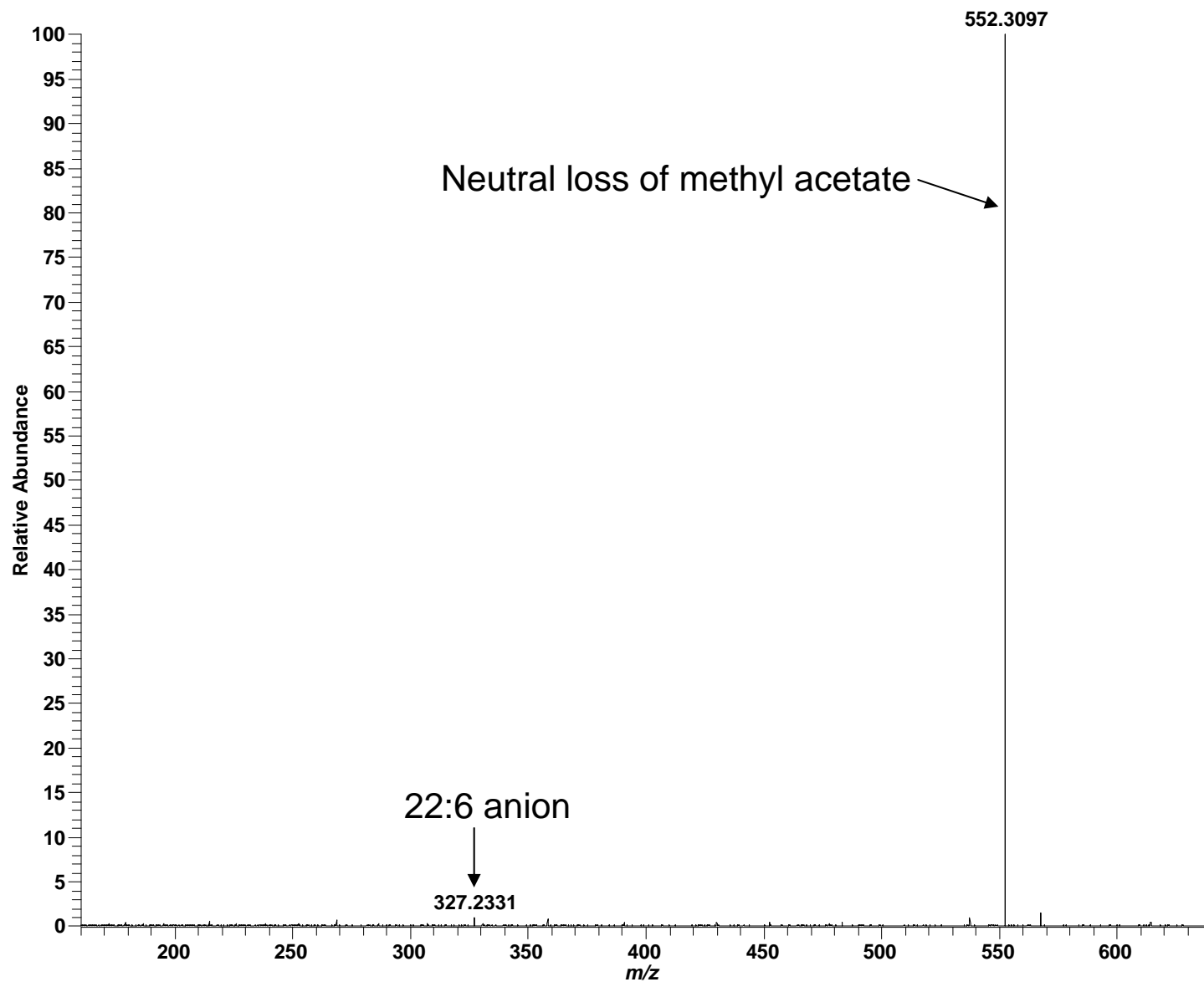
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 22:6; $C_{30}H_{50}NO_7P$; theoretical m/z 568.3403, $(M+H)^+$



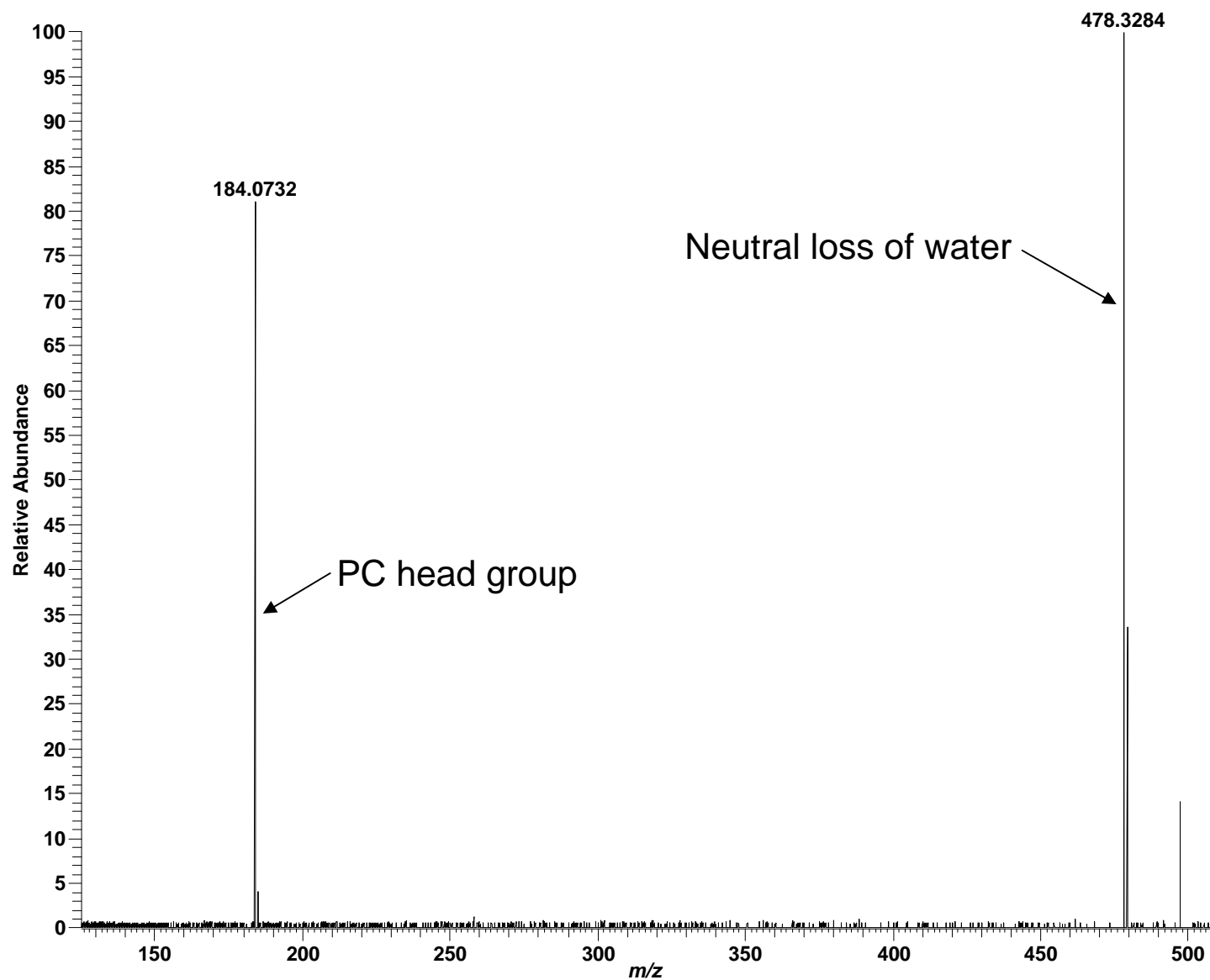
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 22:6; $C_{30}H_{50}NO_7P$; theoretical m/z 626.3458, $(M+CH_3COO)^-$



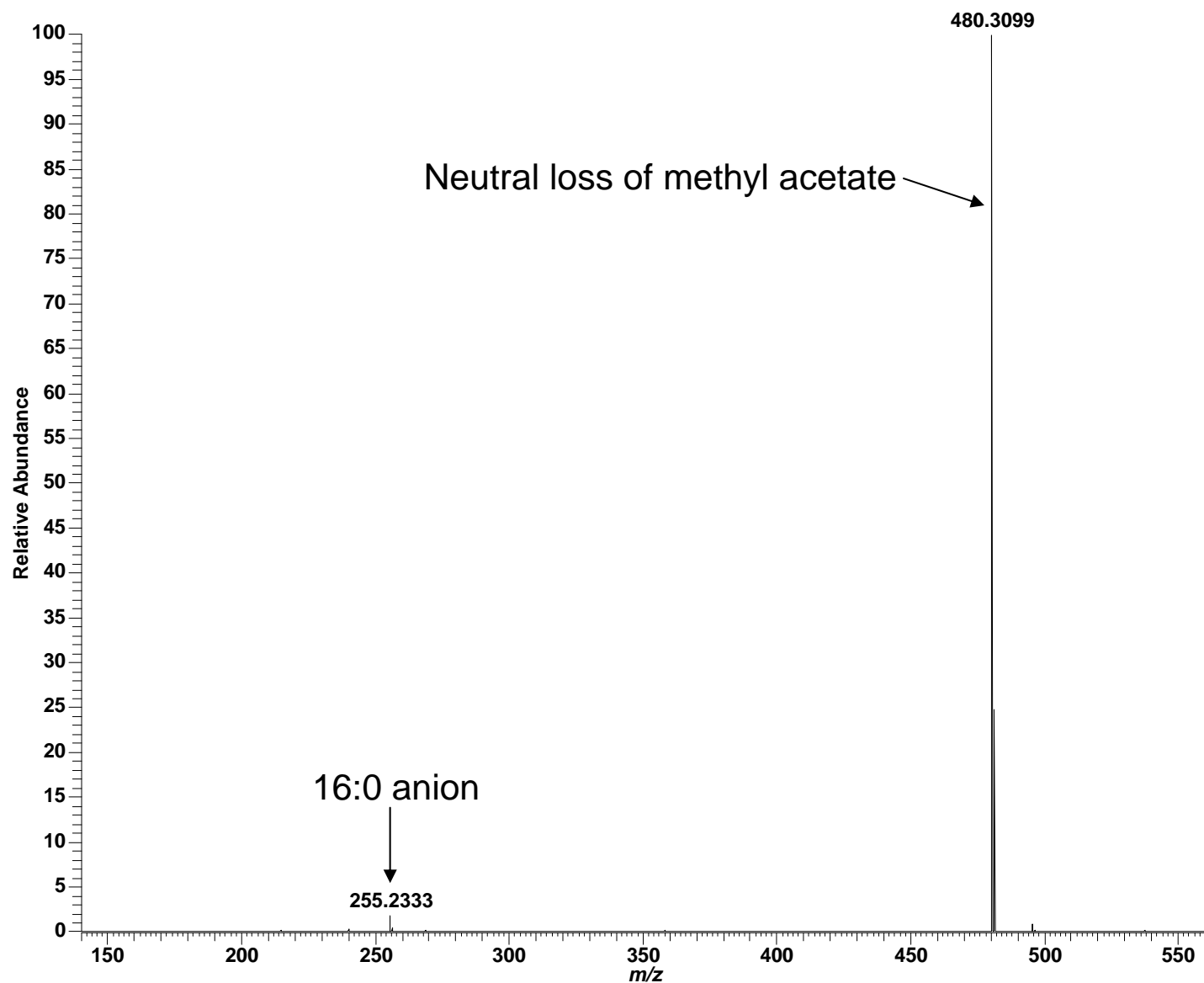
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 16:0; $C_{24}H_{50}NO_7P$; theoretical m/z 496.3403, $(M+H)^+$



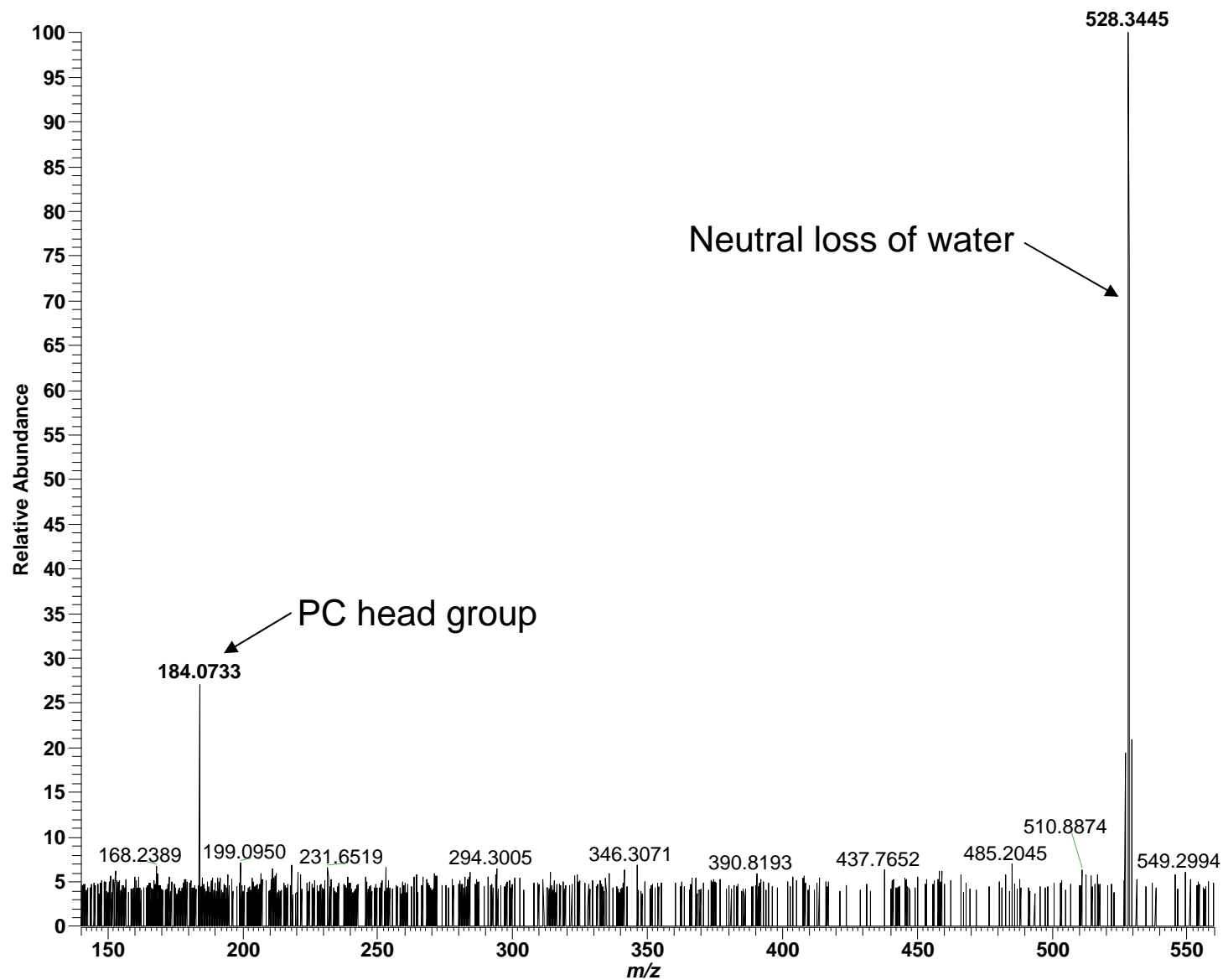
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 16:0; $C_{30}H_{50}NO_7P$; theoretical m/z 554.3458, $(M+CH_3COO)^-$



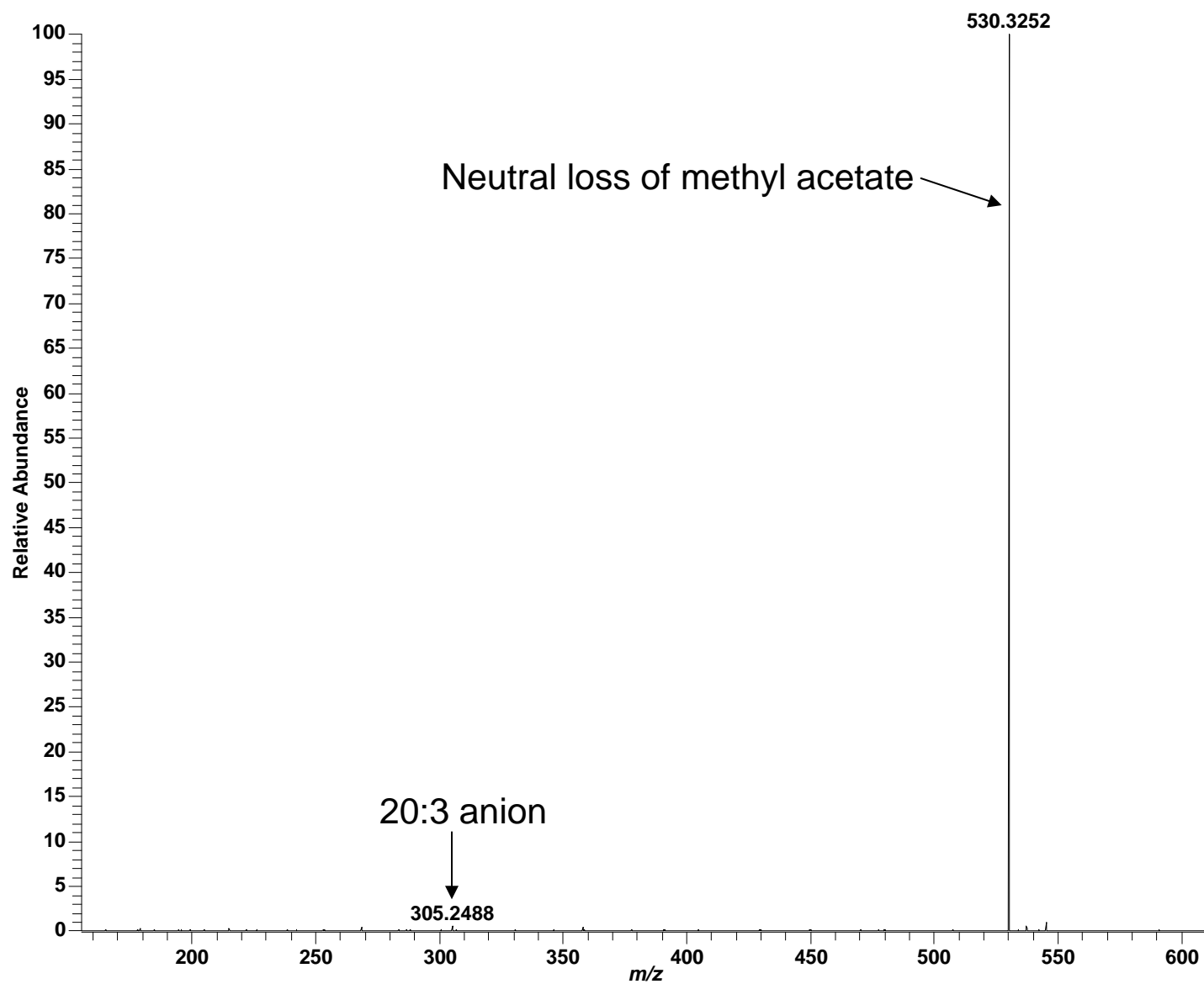
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 20:3; $C_{28}H_{52}NO_7P$; theoretical m/z 546.3559, $(M+H)^+$



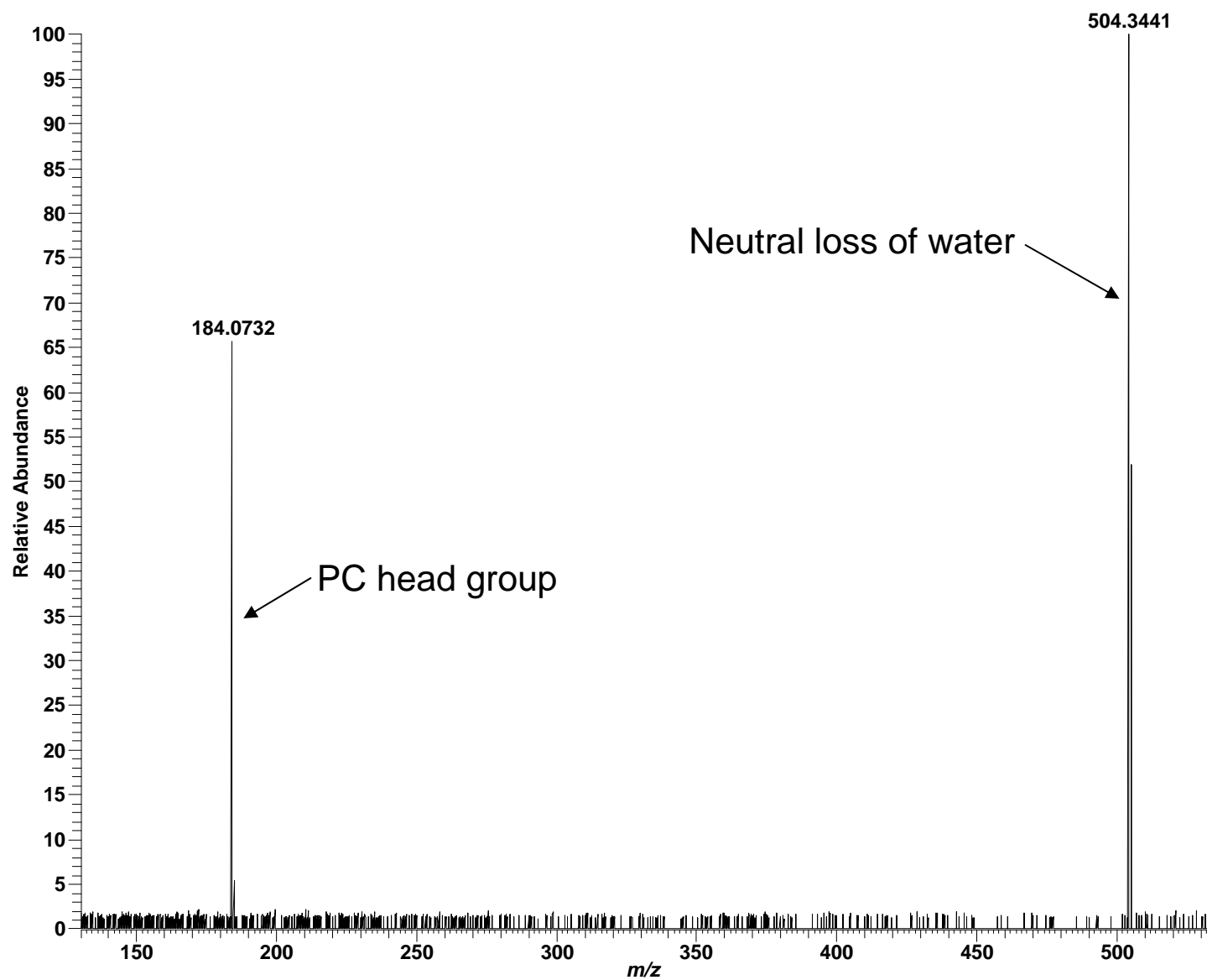
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 20:3; $C_{28}H_{52}NO_7P$; theoretical m/z 604.3614, $(M+CH_3COO)^-$



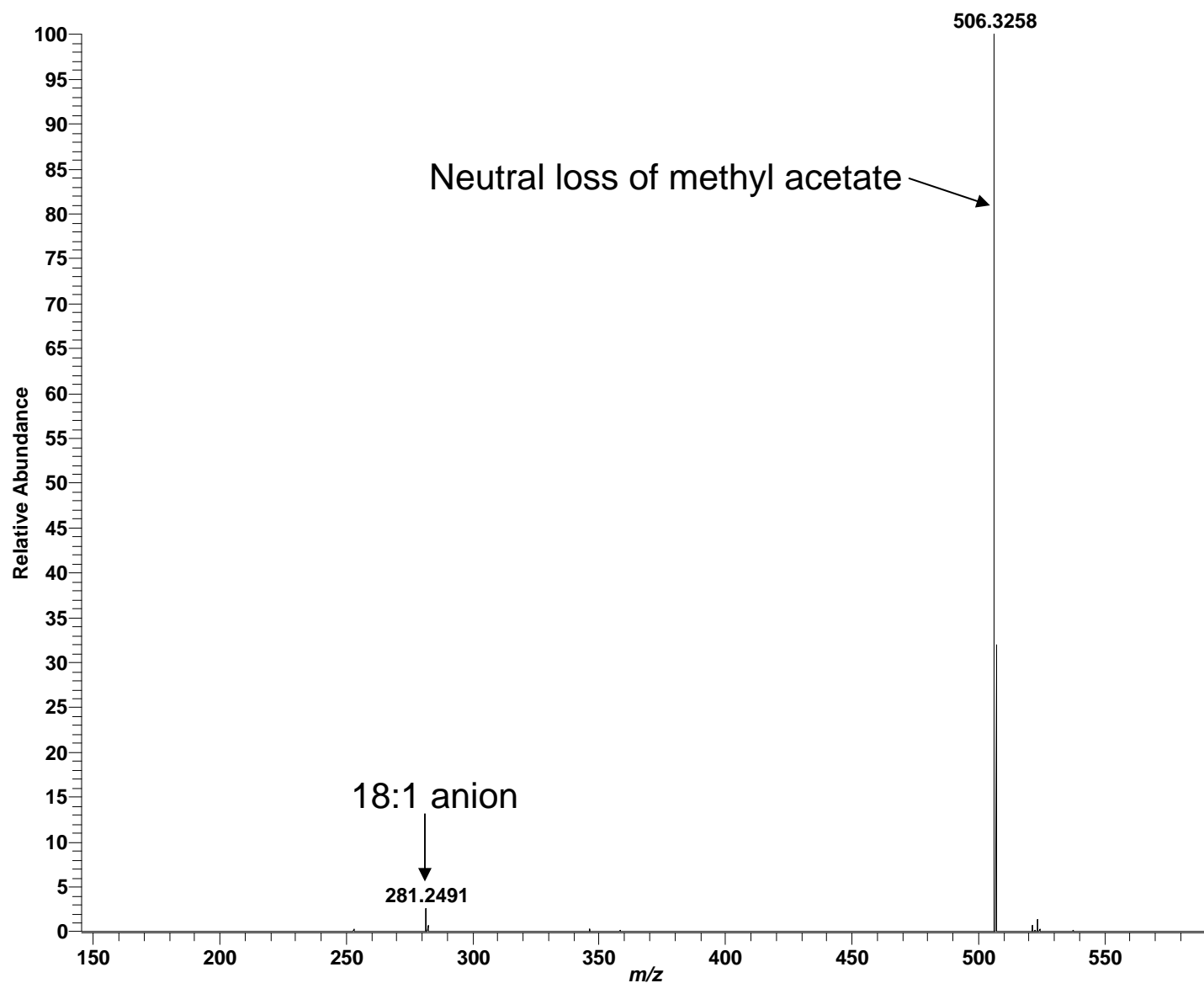
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 18:1; $C_{26}H_{52}NO_7P$; theoretical m/z 522.3559, $(M+H)^+$



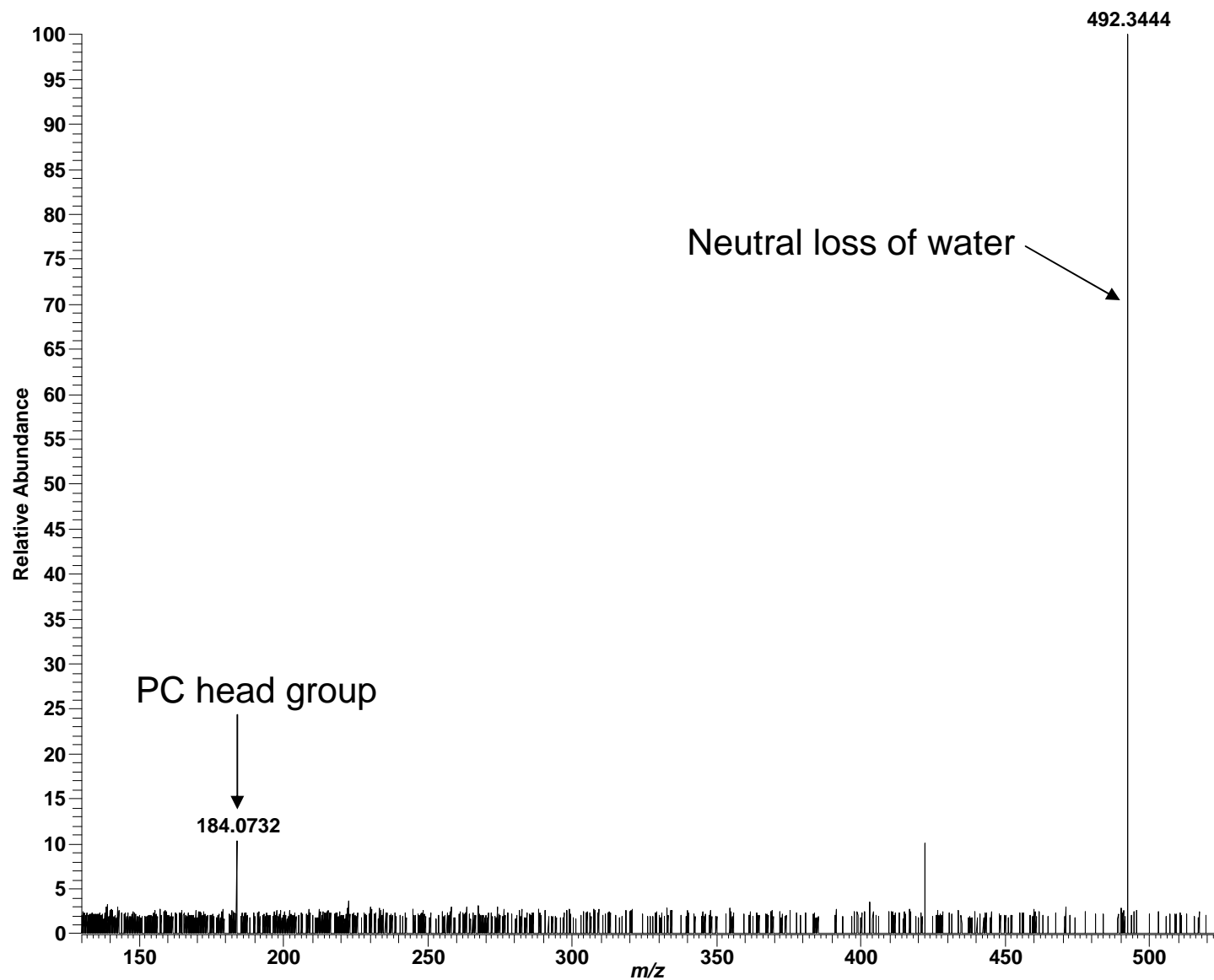
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 18:1; $C_{26}H_{52}NO_7P$; theoretical m/z 580.3614, $(M+CH_3COO)^-$



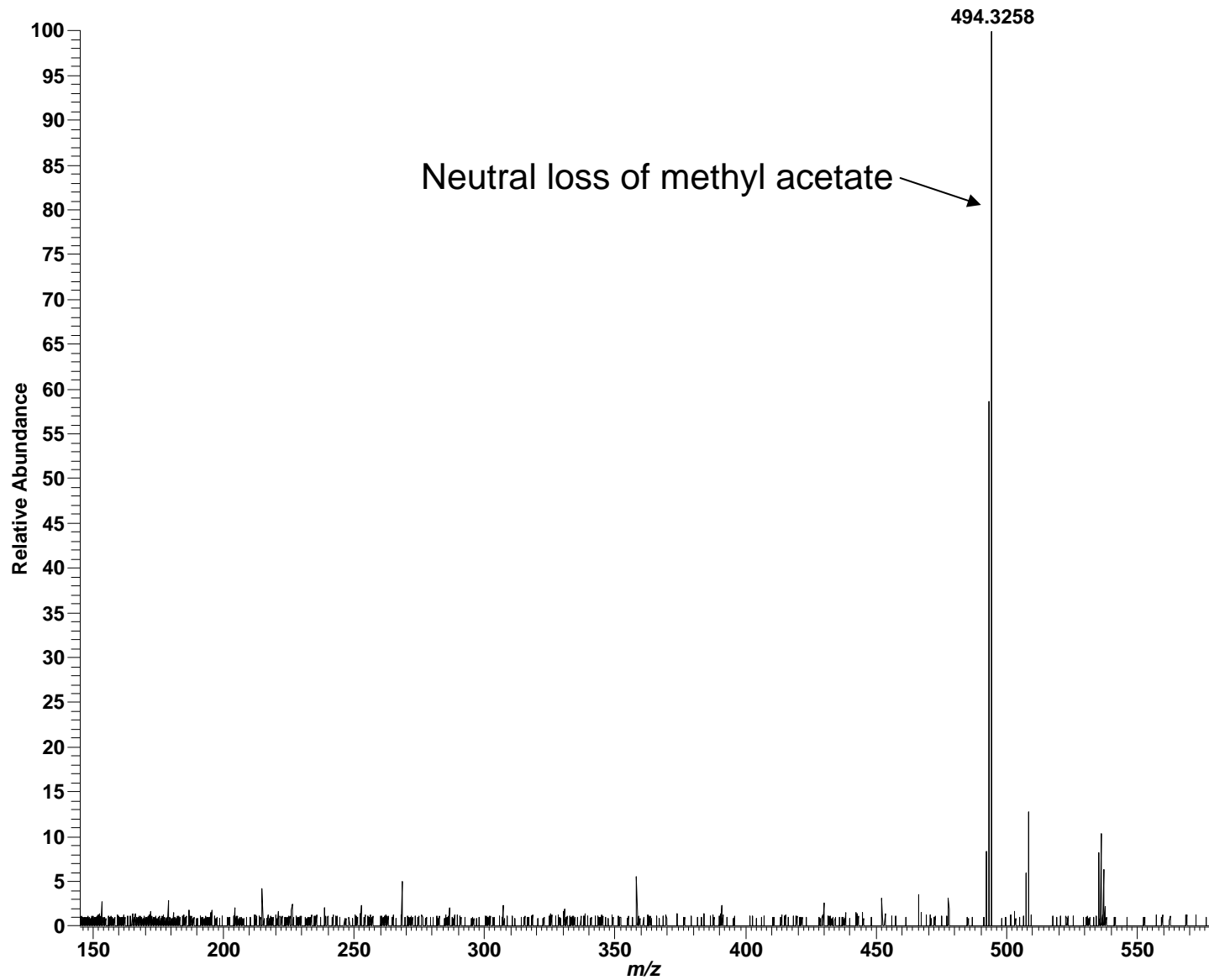
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 17:0; $C_{25}H_{52}NO_7P$; theoretical m/z 510.3559, $(M+H)^+$



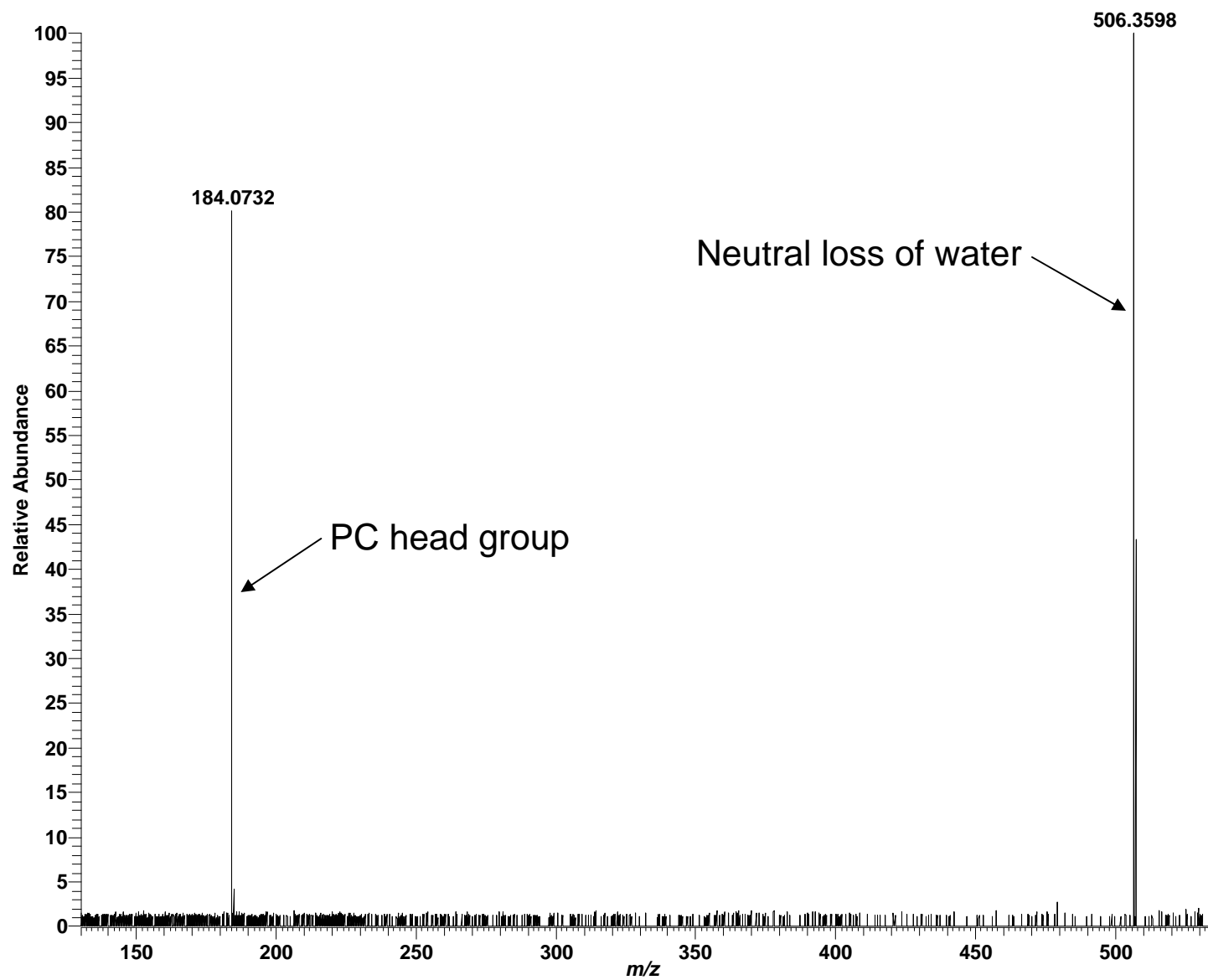
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 17:0; $C_{25}H_{52}NO_7P$; theoretical m/z 568.3614, $(M+CH_3COO)^-$



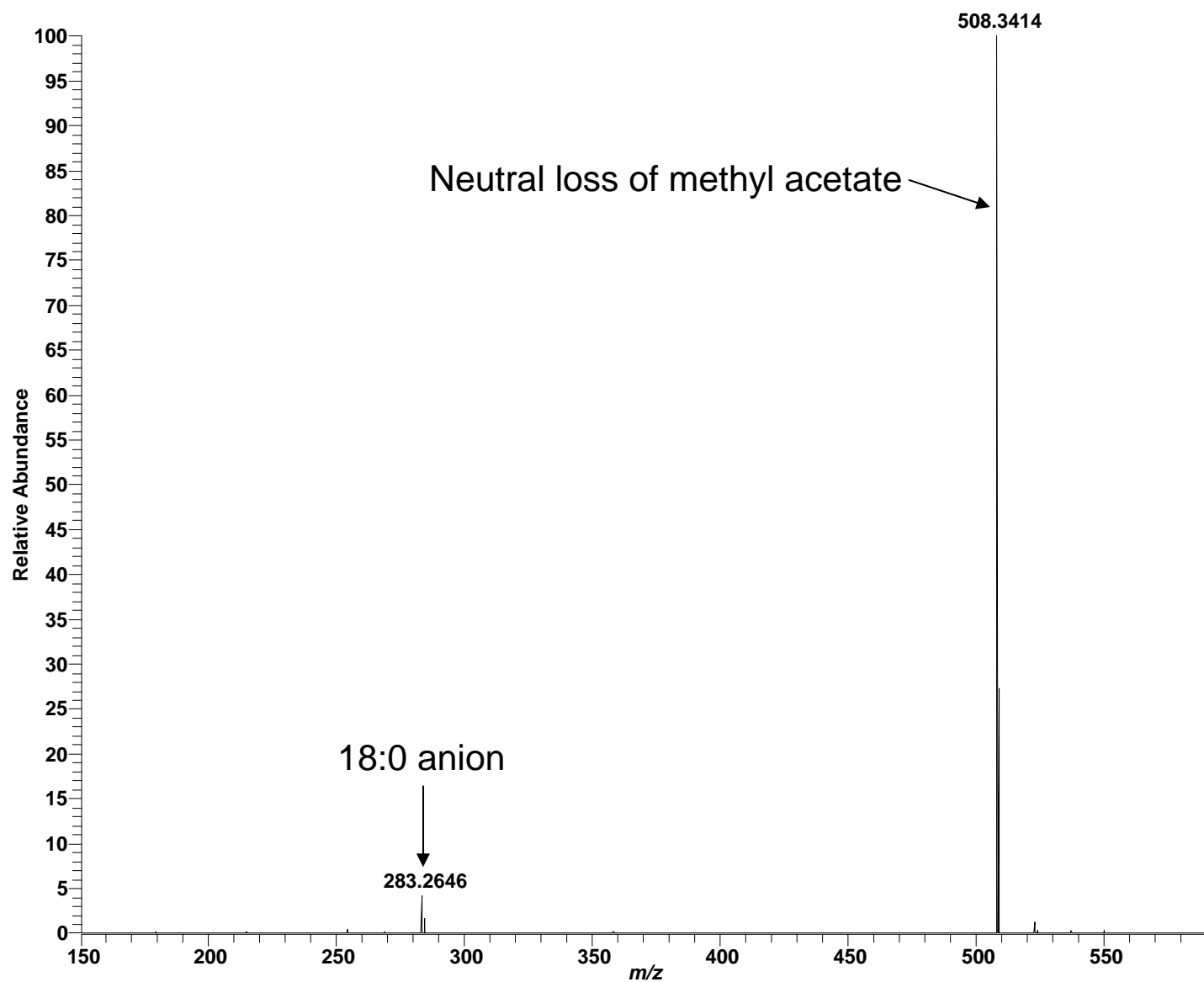
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: LPC 18:0; $C_{26}H_{54}NO_7P$; theoretical m/z 524.3716, (M+H)⁺



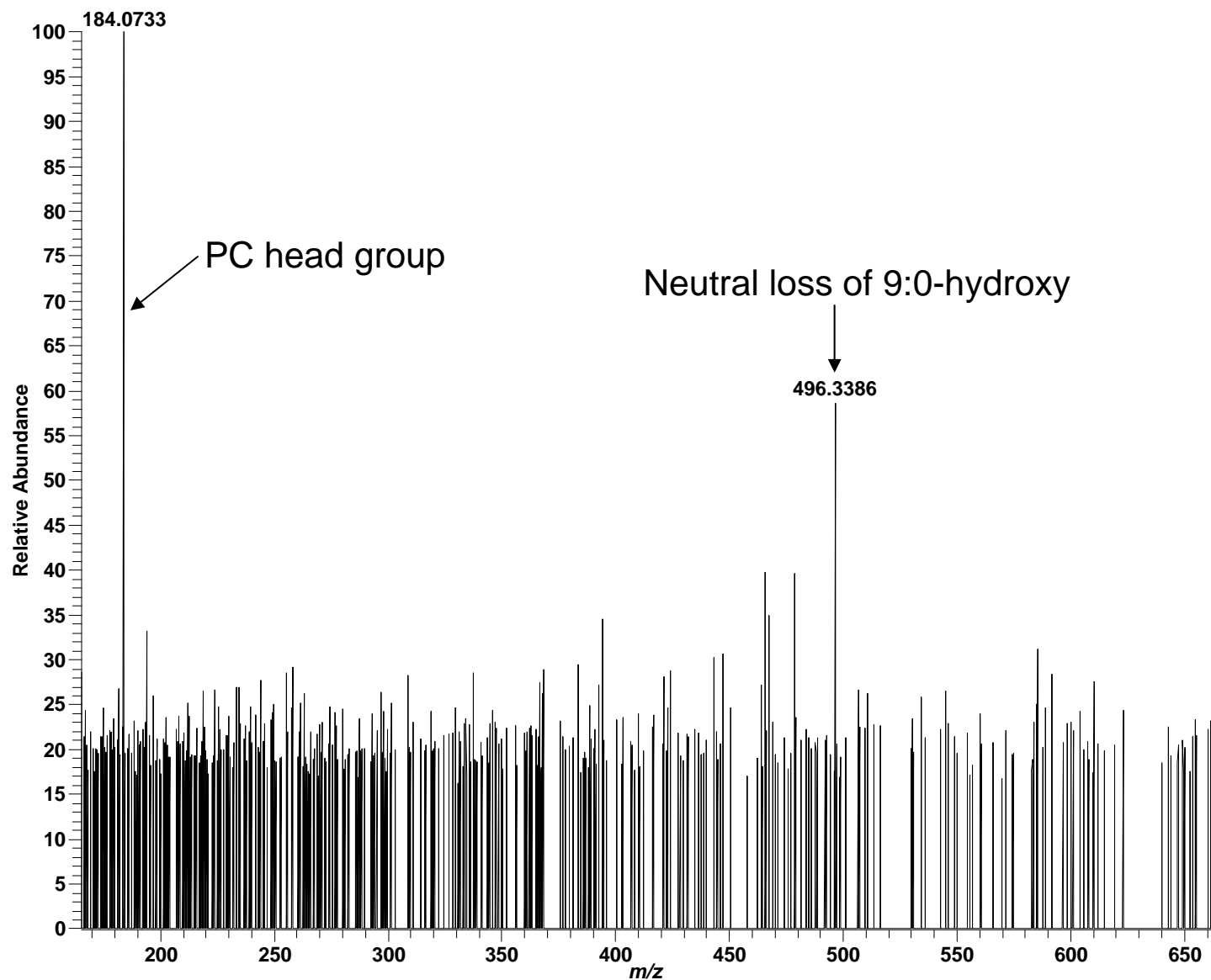
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: LPC 18:0; $C_{26}H_{54}NO_7P$; theoretical m/z 582.3771, $(M+CH_3COO)^-$



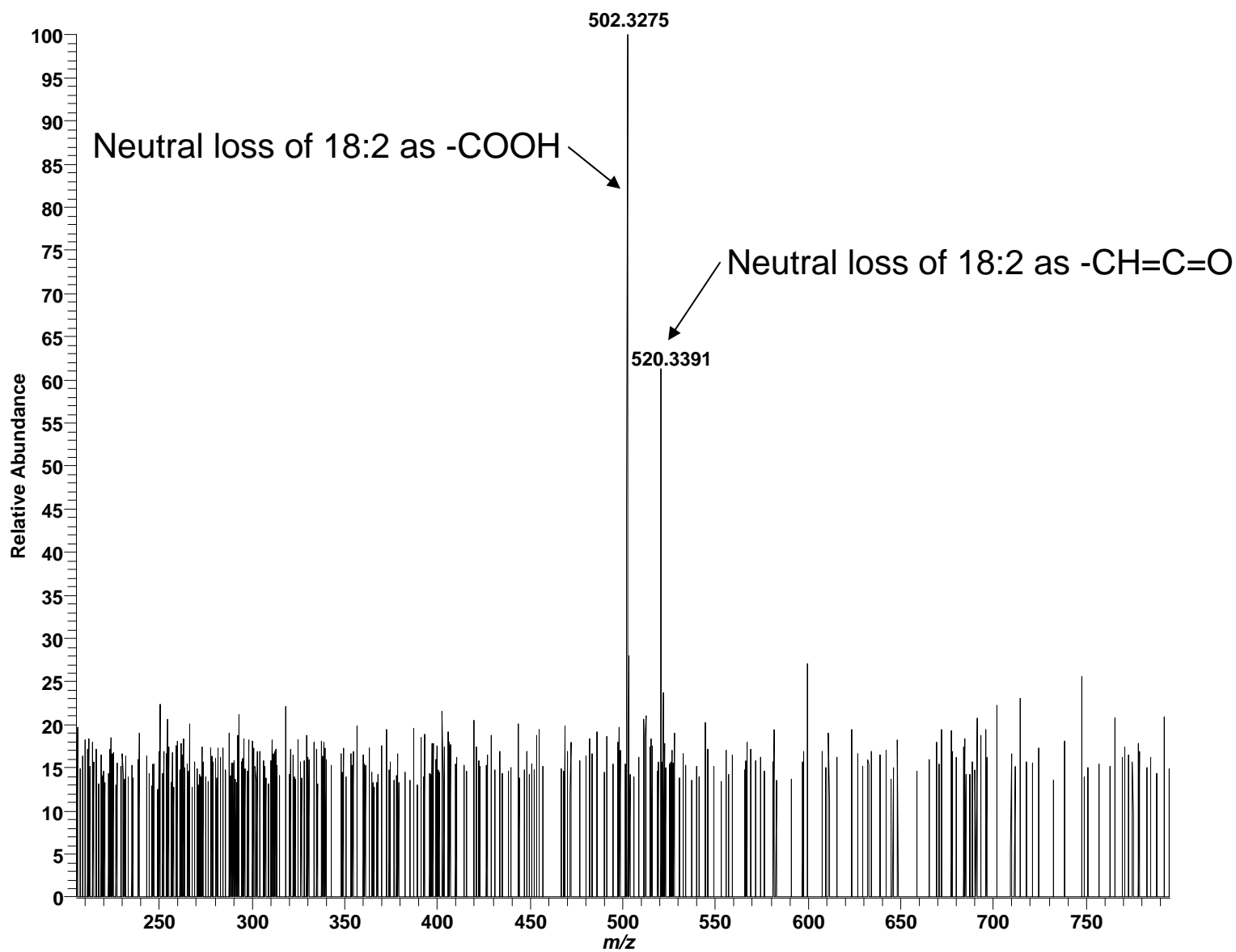
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: Oxidized PC 16:0/9:0-hydroxy; $C_{33}H_{64}NO_9P$; theoretical m/z 650.4397, $(M+H)^+$



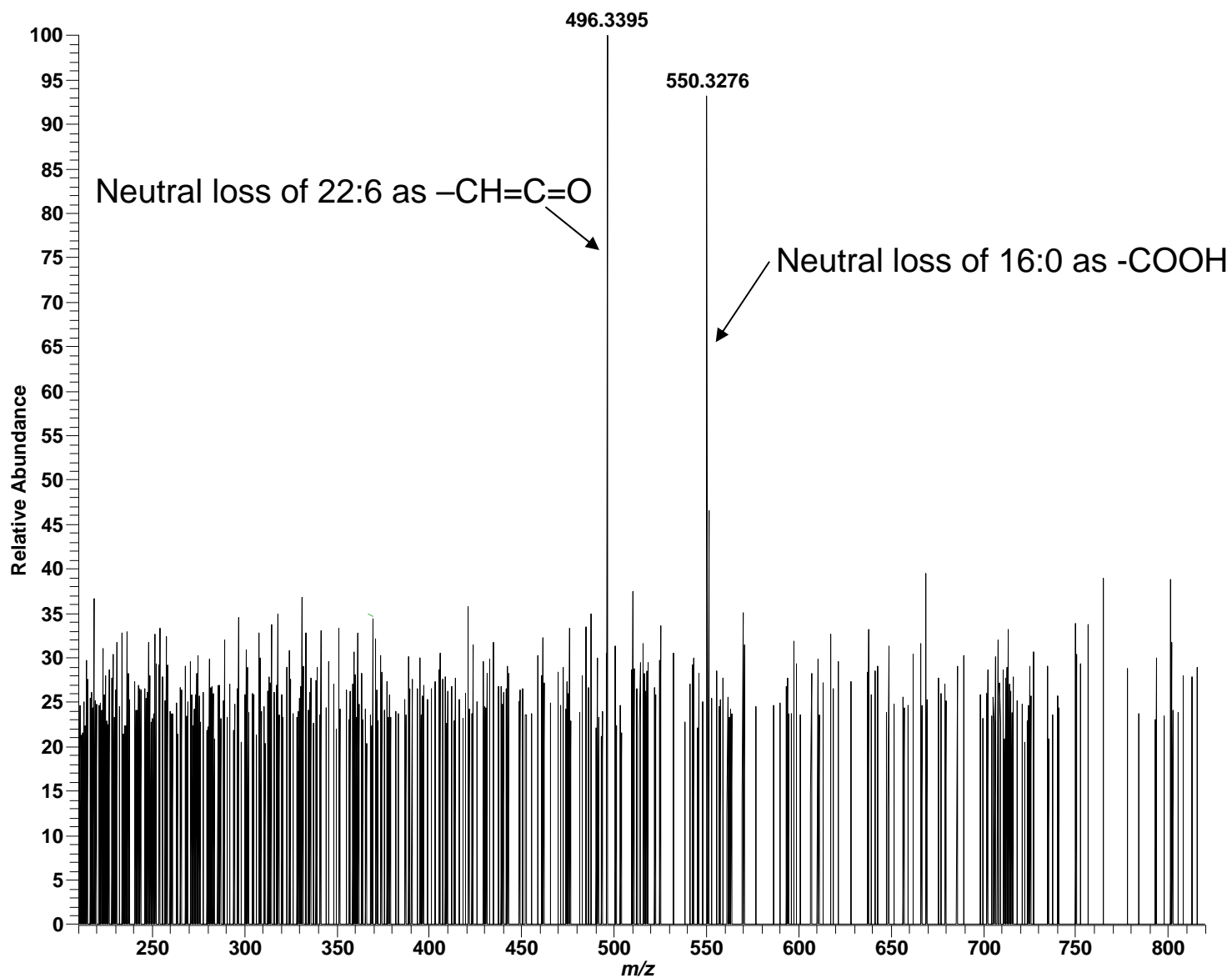
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PC 18:2/18:2; $C_{44}H_{80}NO_8P$; theoretical m/z 782.5699, $(M+H)^+$



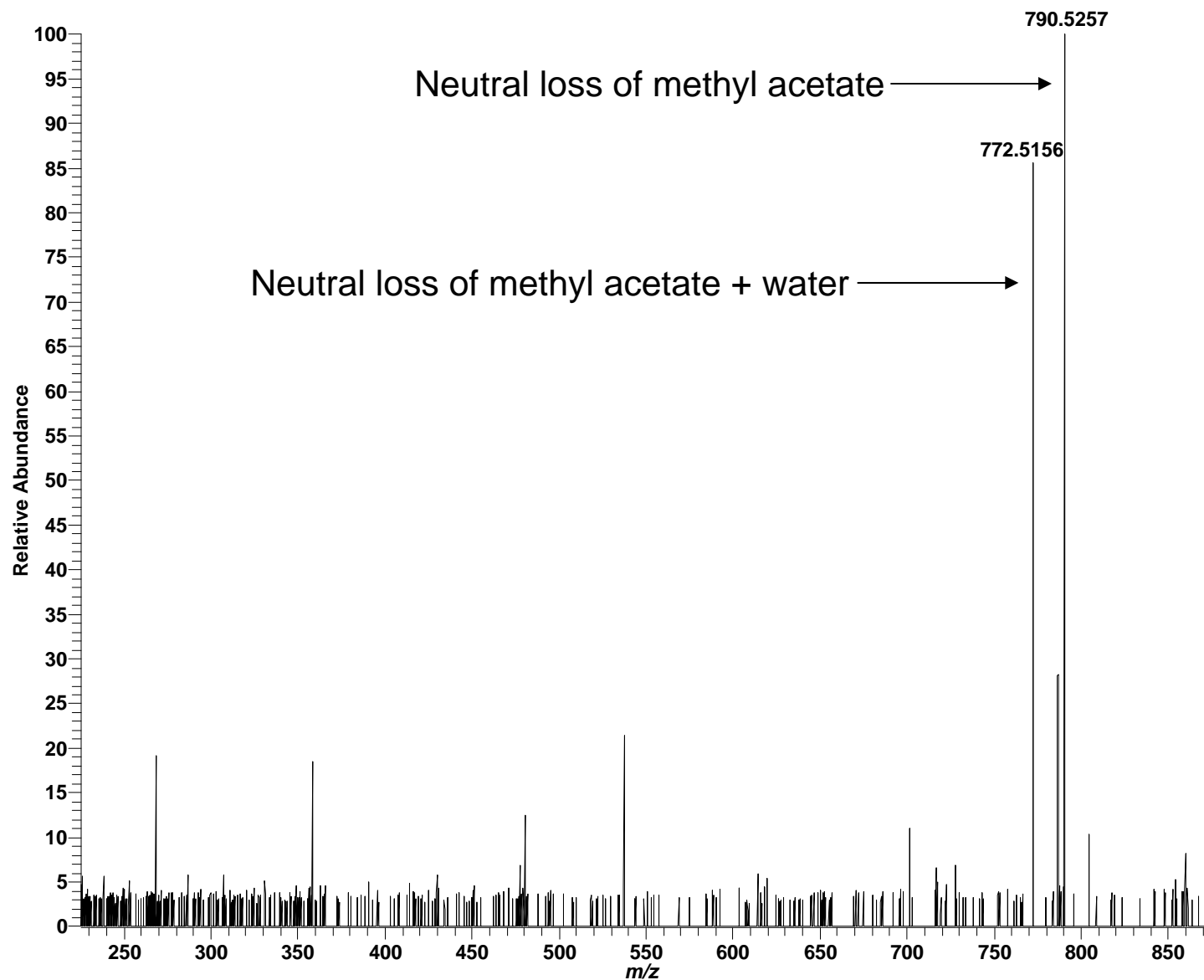
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PC 16:0/22:6; $C_{46}H_{80}NO_8P$; theoretical m/z 806.5699, $(M+H)^+$



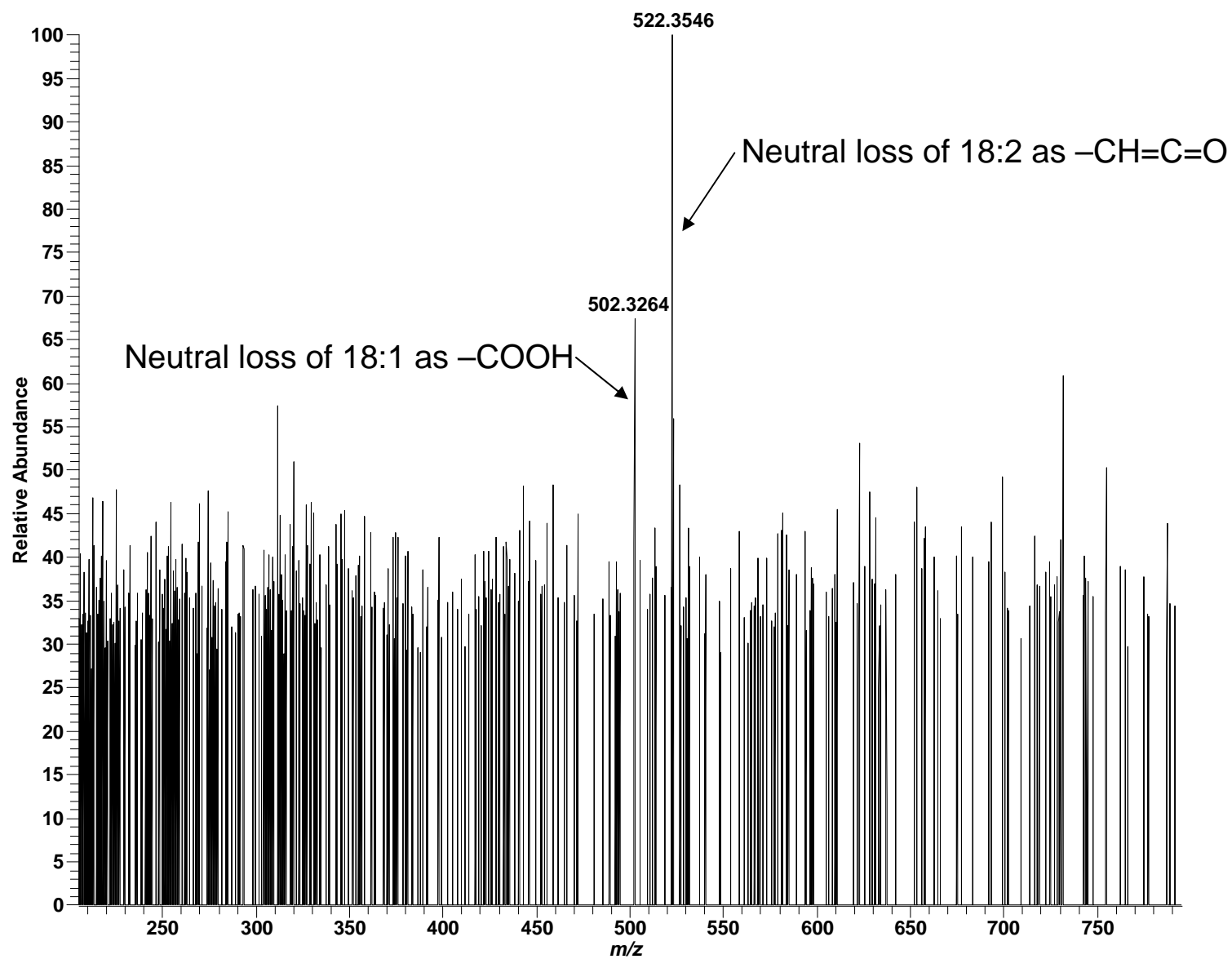
High mass measurement accuracy MS/MS utilizing LTQ-FT

Negative ESI: PC 16:0/22:6; $C_{46}H_{80}NO_8P$; theoretical m/z 864.5754, $(M+CH_3COO)^-$



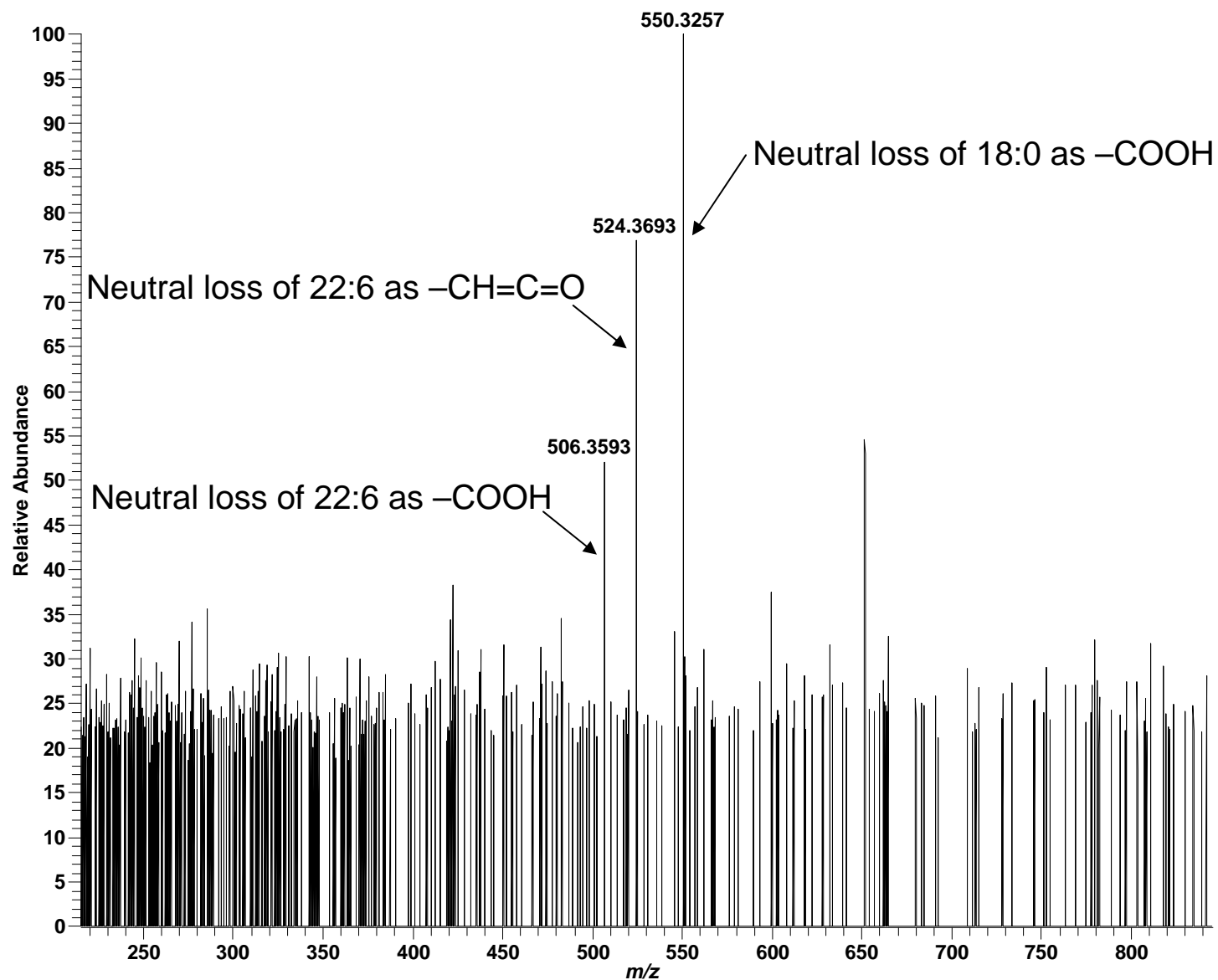
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PC 18:1/18:2; $C_{44}H_{82}NO_8P$; theoretical m/z 784.5856, $(M+H)^+$



High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: PC 18:0/22:6; $C_{48}H_{84}NO_8P$; theoretical m/z 834.6013, $(M+H)^+$

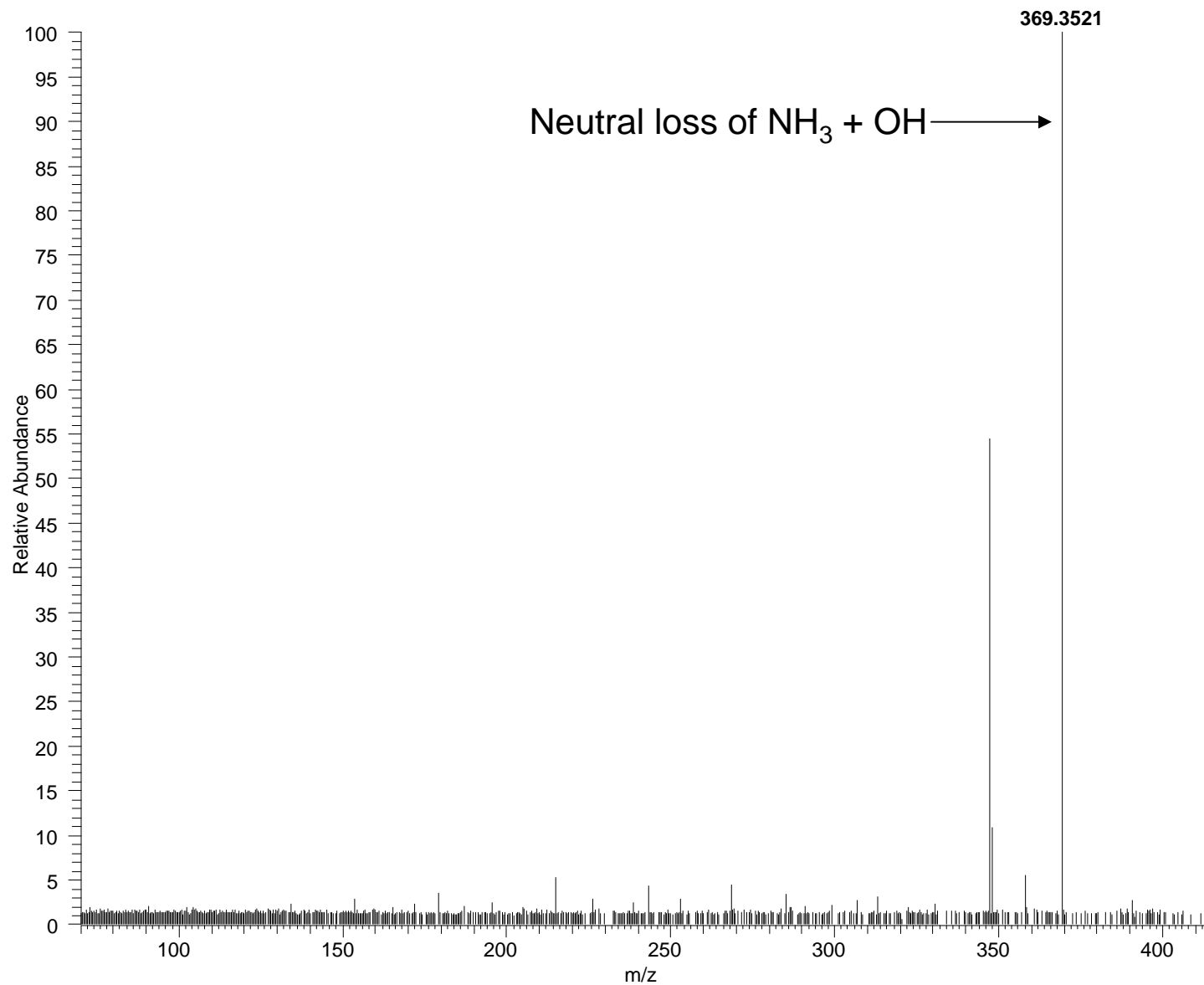


Cholesterol and its esters

Characteristic daughter ion: 369.3521
(Neutral loss of $\text{NH}_4 + \text{OH}$)

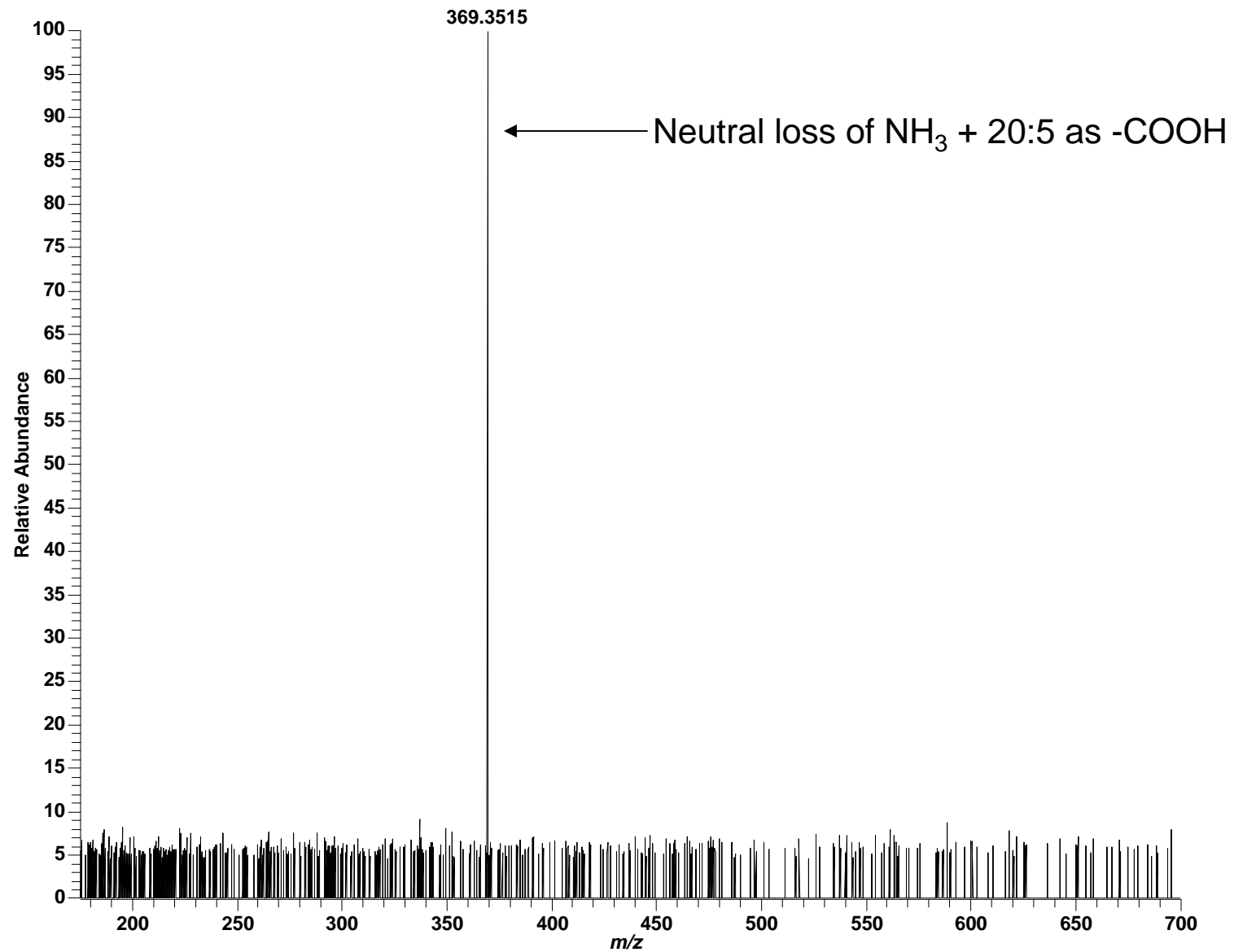
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: Cholesterol; $C_{27}H_{46}O$; theoretical m/z 404.3892, $(M+NH_4)^+$



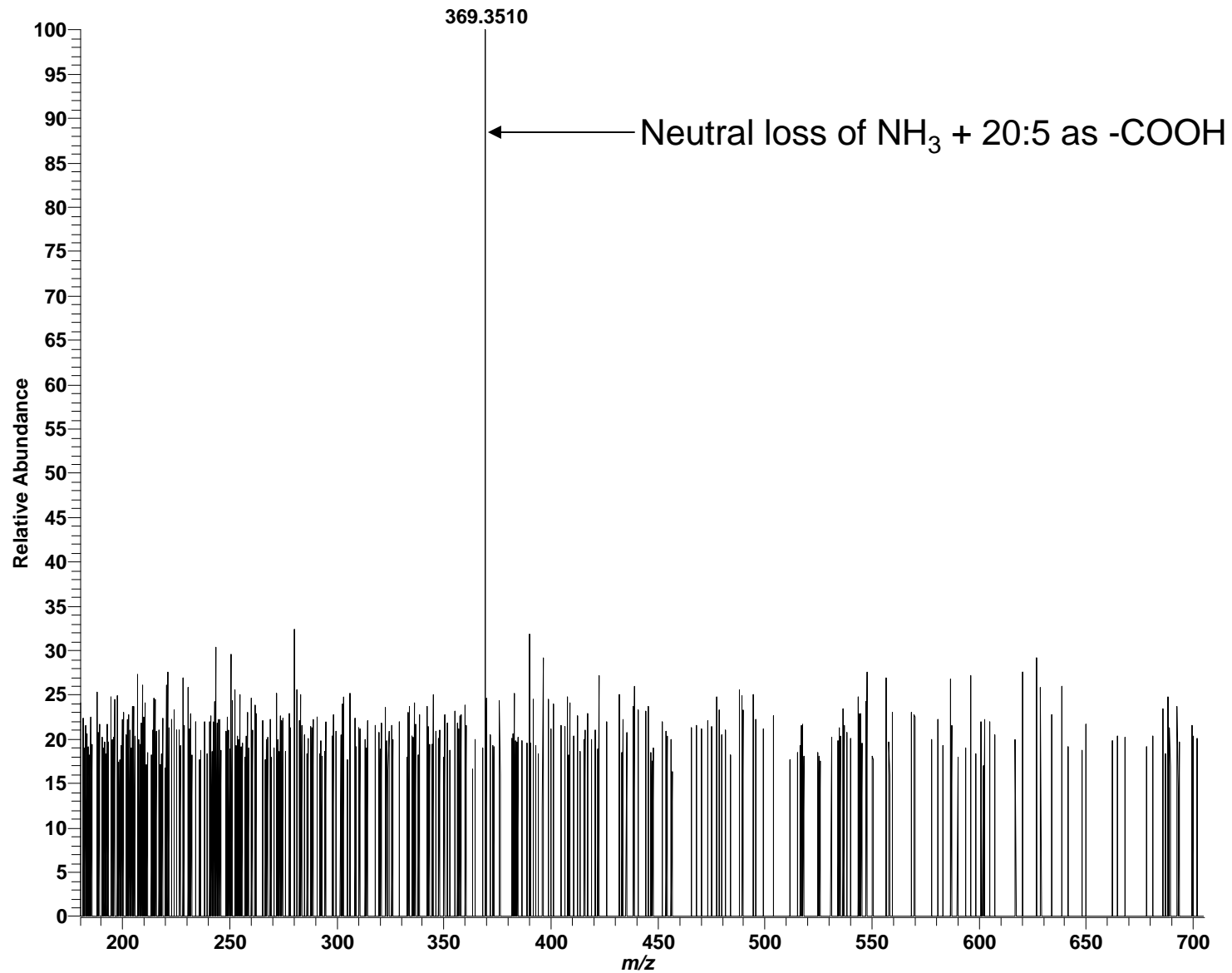
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: CE 20:5; $C_{47}H_{74}O_2$; theoretical m/z 688.6032, $(M+NH_4)^+$



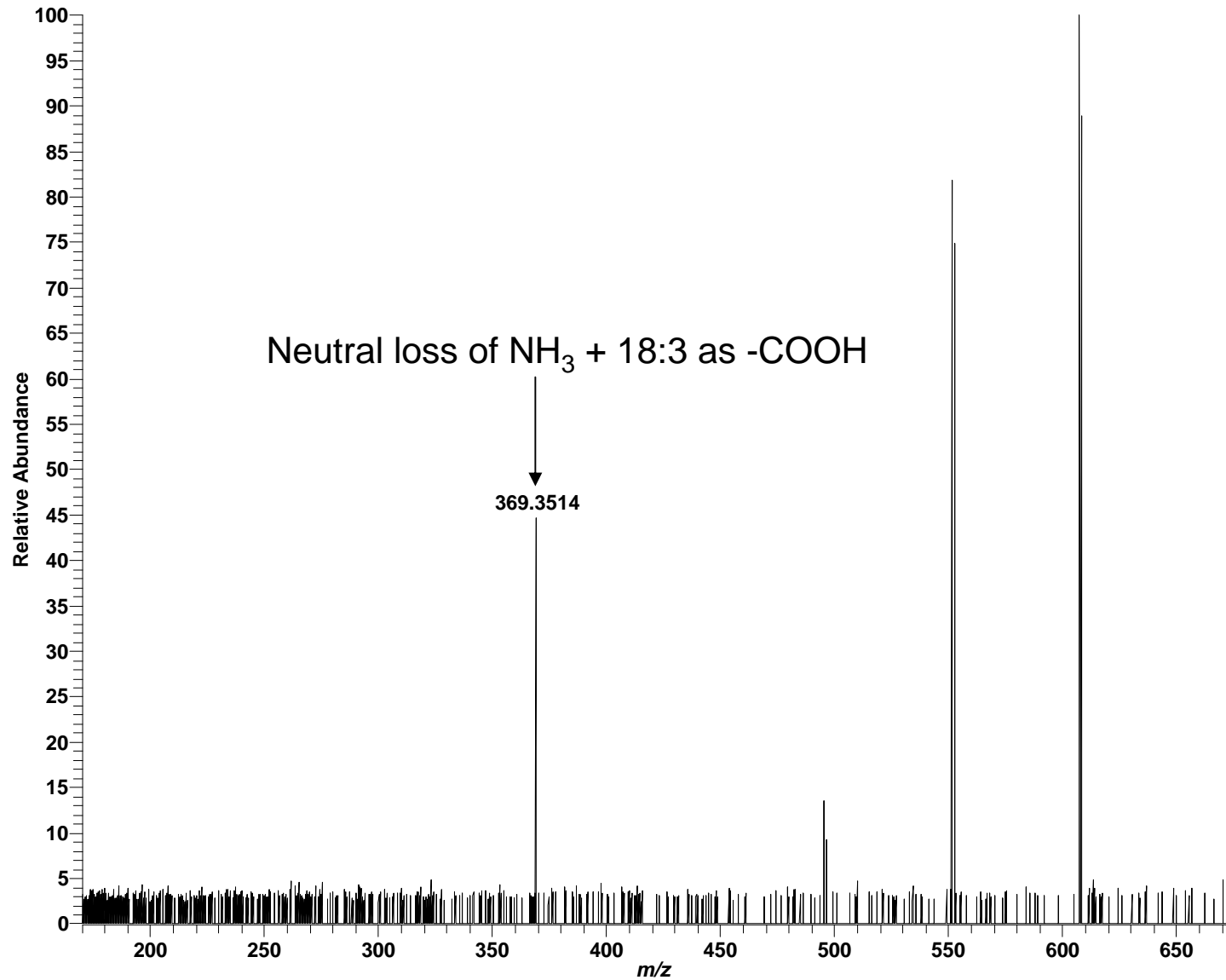
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: CE 20:4; $C_{47}H_{76}O_2$; theoretical m/z 690.6189, $(M+NH_4)^+$



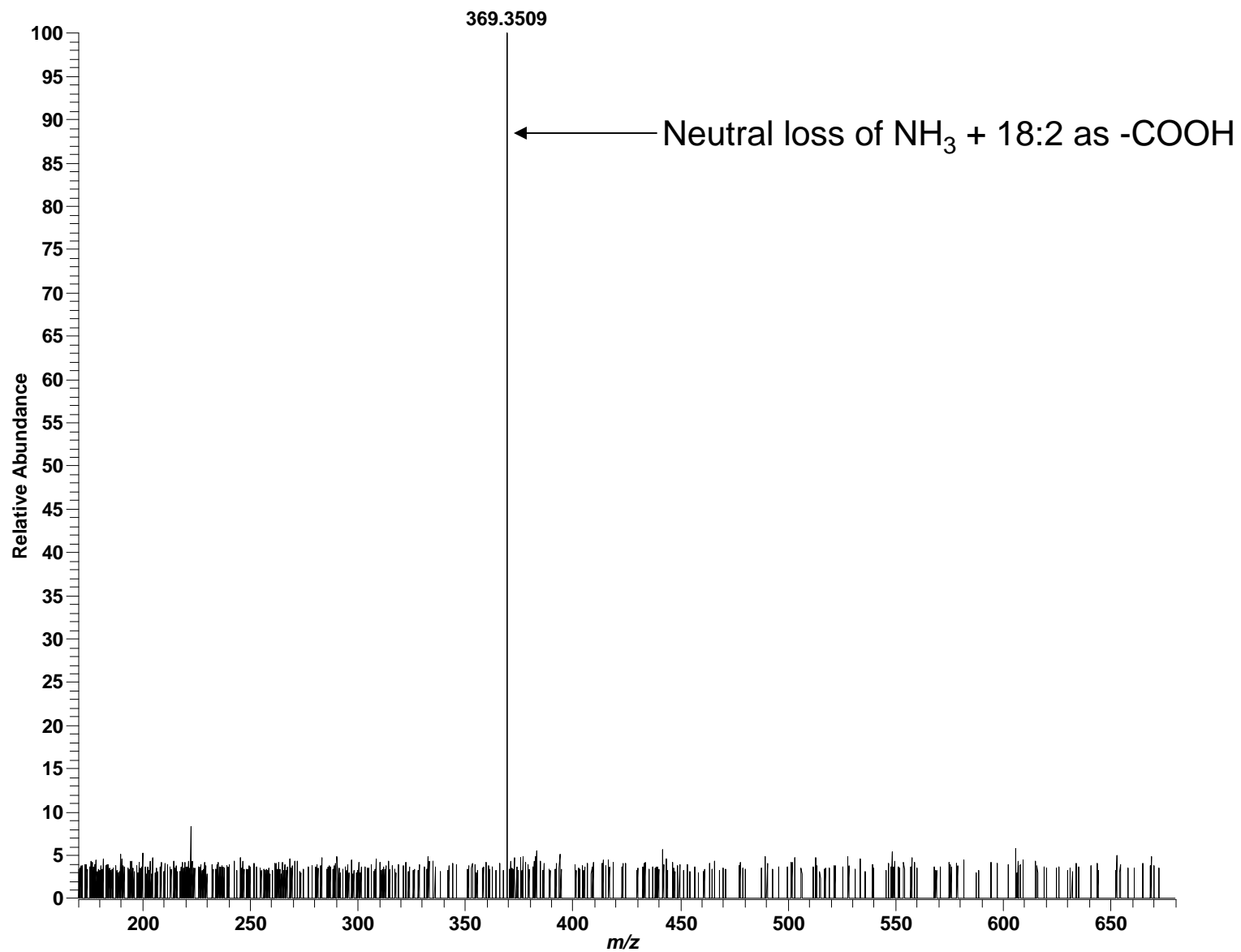
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: CE 18:3; C₄₅H₇₄O₂; theoretical *m/z* 664.6032, (M+NH₄)⁺



High mass measurement accuracy MS/MS utilizing LTQ-FT

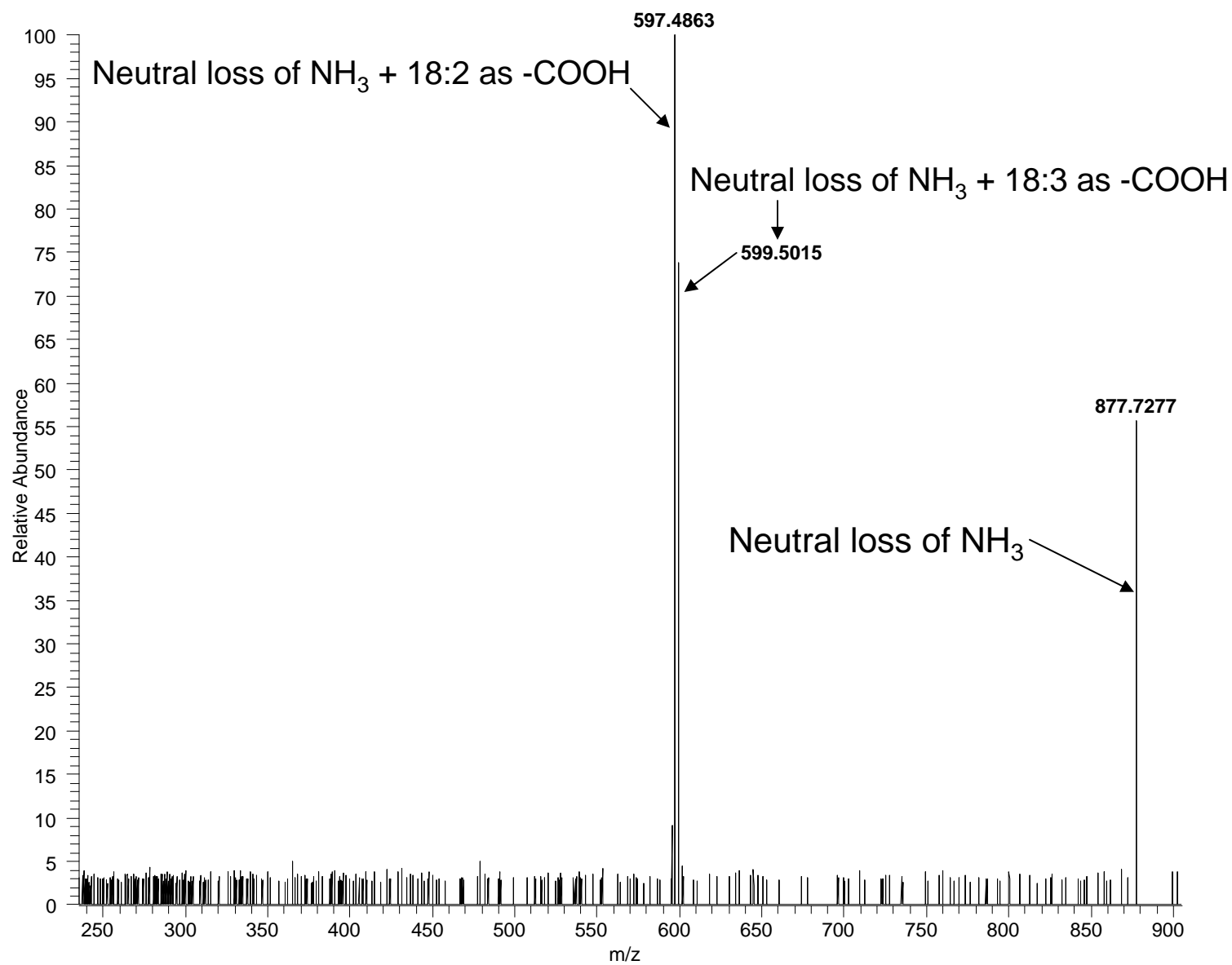
Positive ESI: CE 18:2; $C_{45}H_{76}O_2$; theoretical m/z 666.6189, $(M+NH_4)^+$



Triacylglycerols

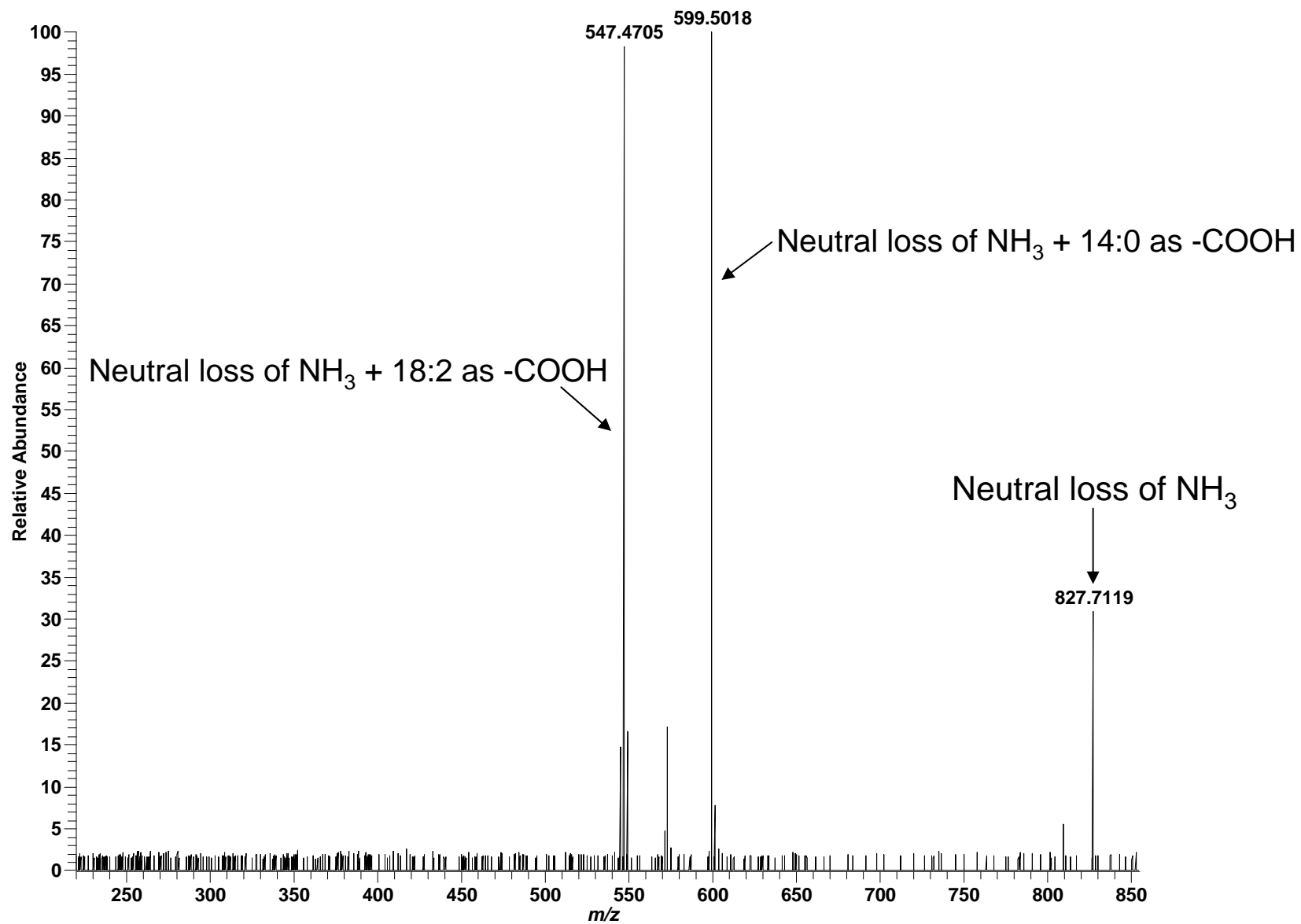
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:2,18:2,18:3); $C_{57}H_{96}O_6$; theoretical m/z 894.7551, $(M+NH_4)^+$



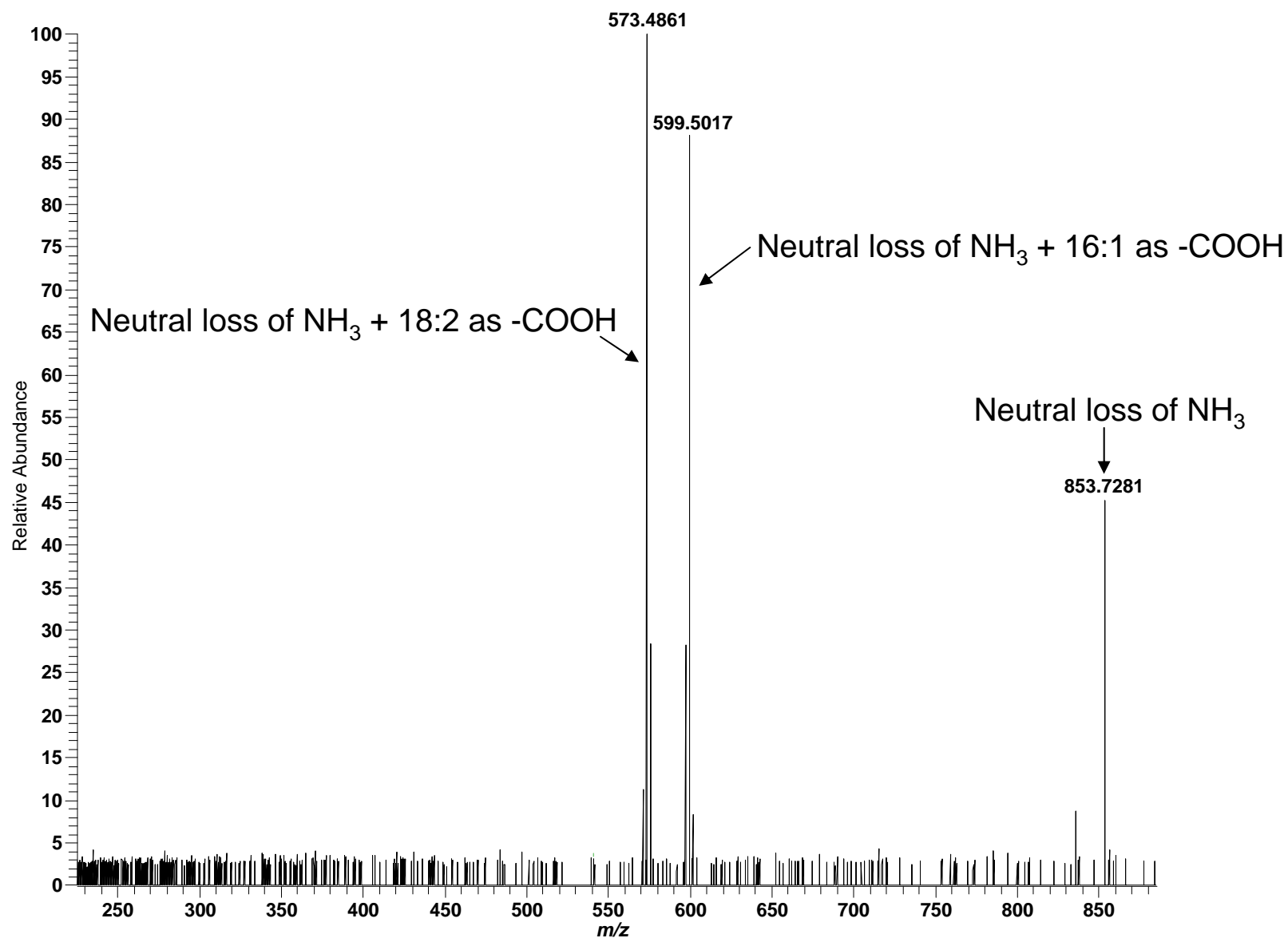
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (14:0,18:2,18:2); $C_{53}H_{94}O_6$; theoretical m/z 844.7394, $(M+NH_4)^+$



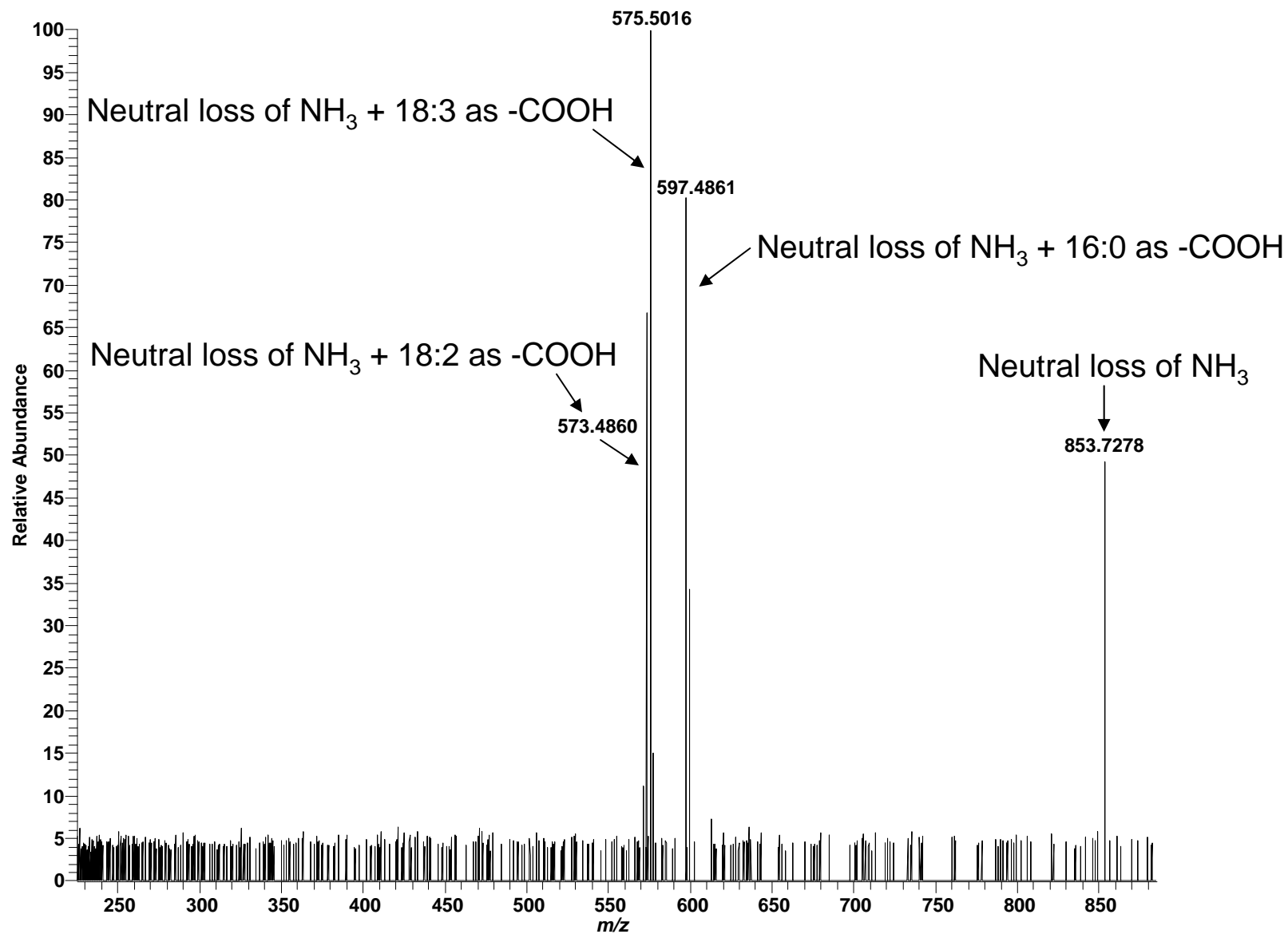
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:1,18:2,18:2); $C_{55}H_{96}O_6$; theoretical m/z 870.7550, $(M+NH_4)^+$



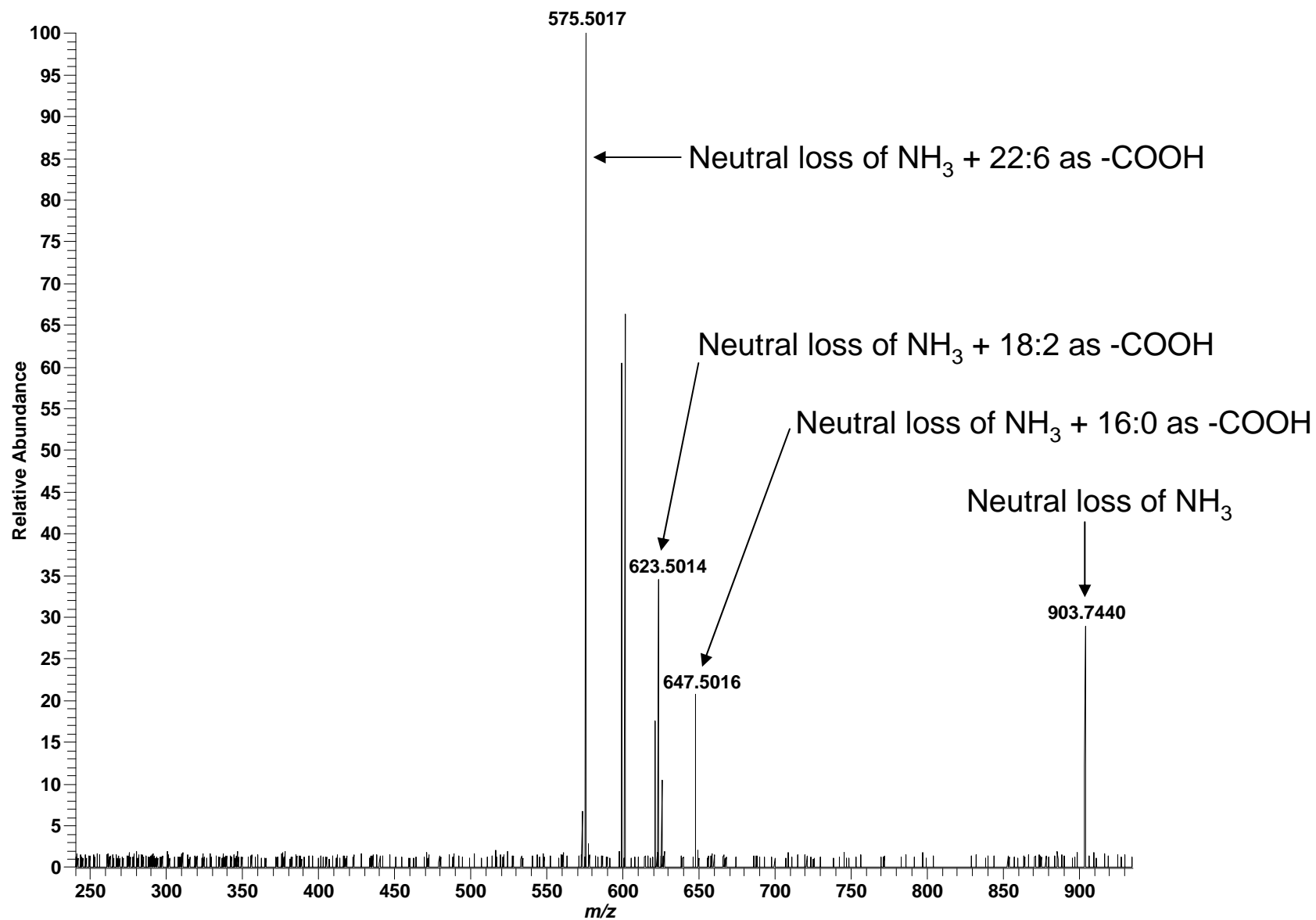
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:2,18:3); $C_{55}H_{96}O_6$; theoretical m/z 870.7550, $(M+NH_4)^+$



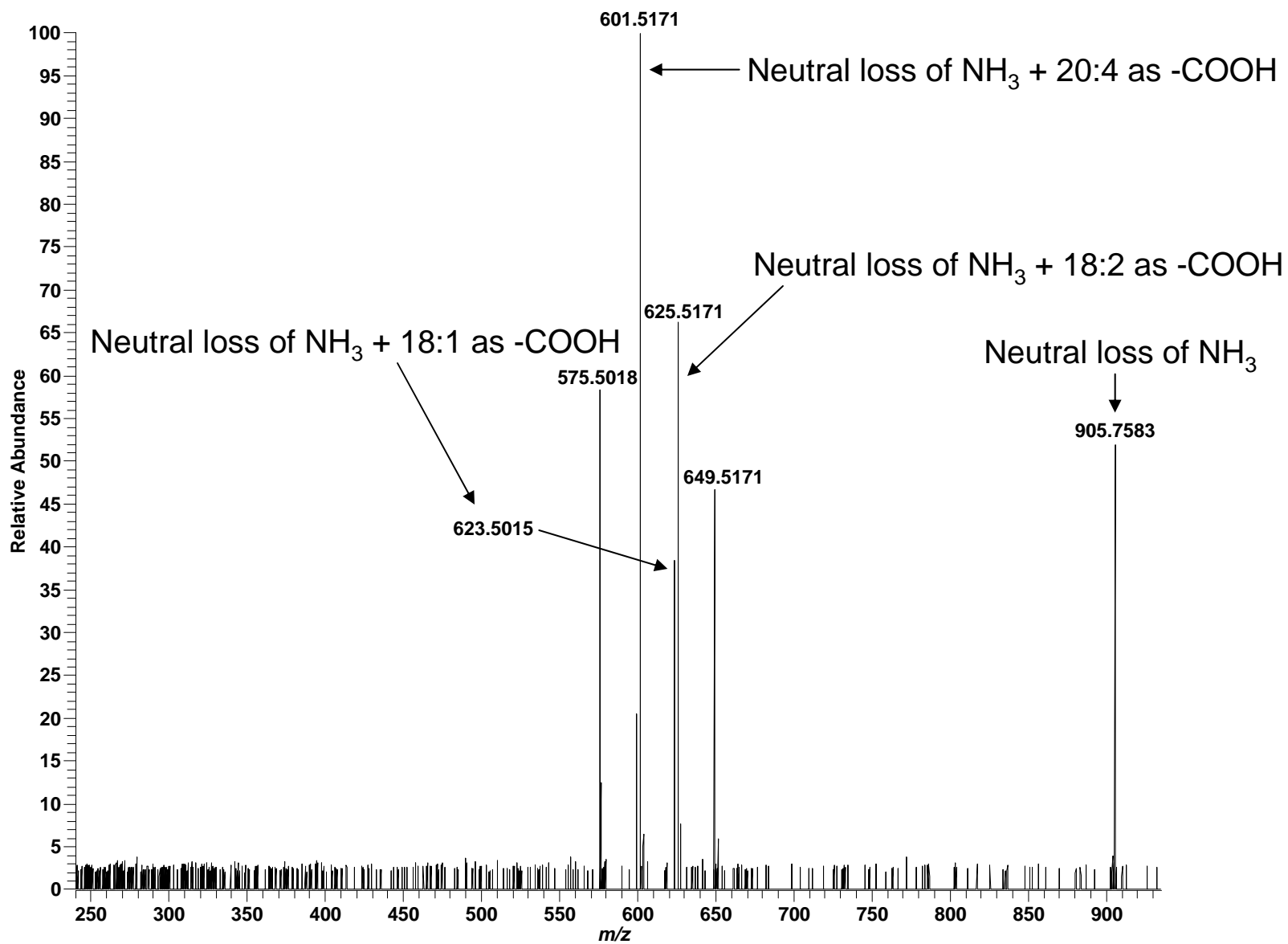
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:2,22:6); $C_{59}H_{98}O_6$; theoretical m/z 920.7707, $(M+NH_4)^+$



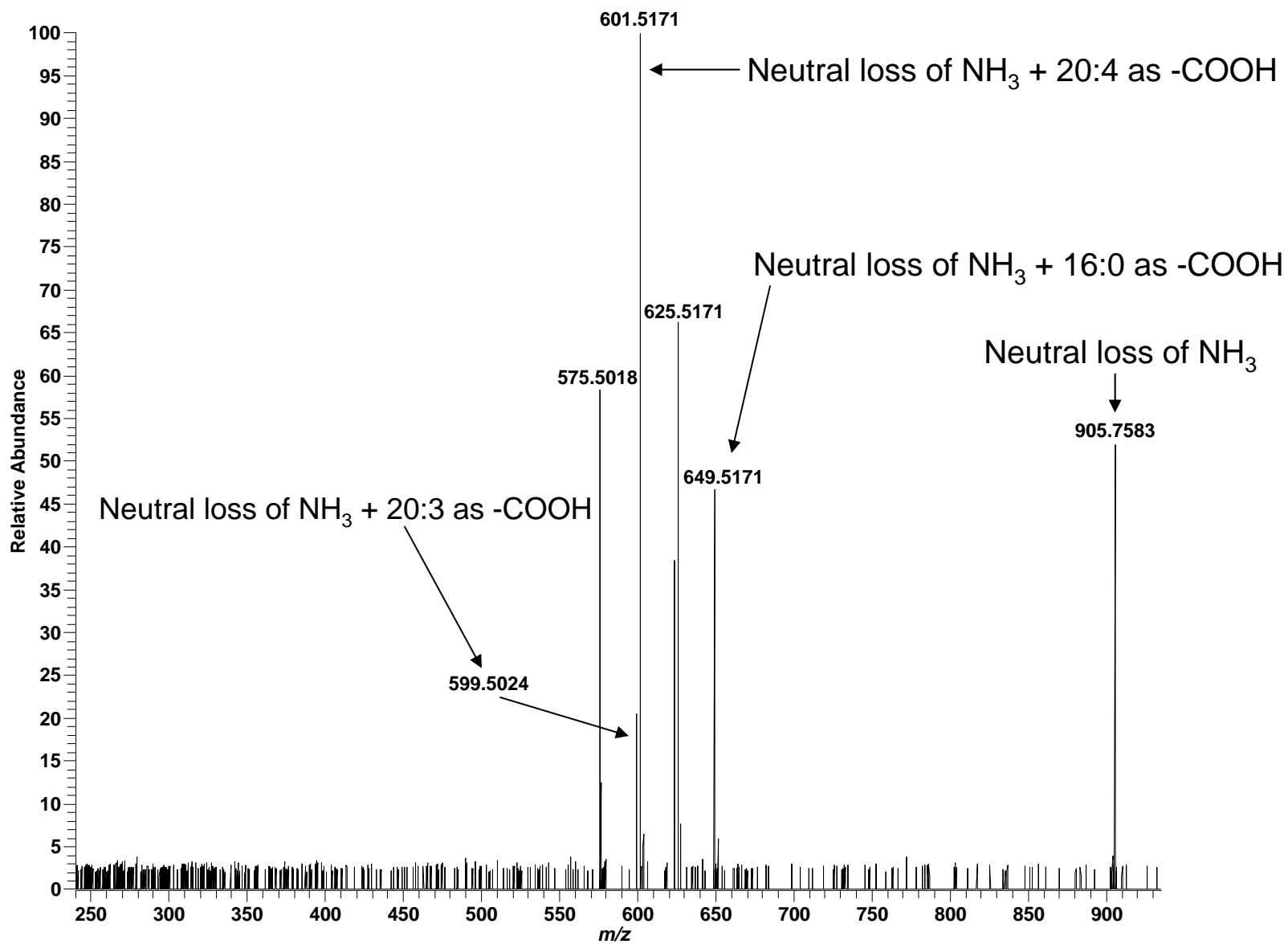
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:1,18:2,20:4); $C_{59}H_{100}O_6$; theoretical m/z 922.7864, $(M+NH_4)^+$



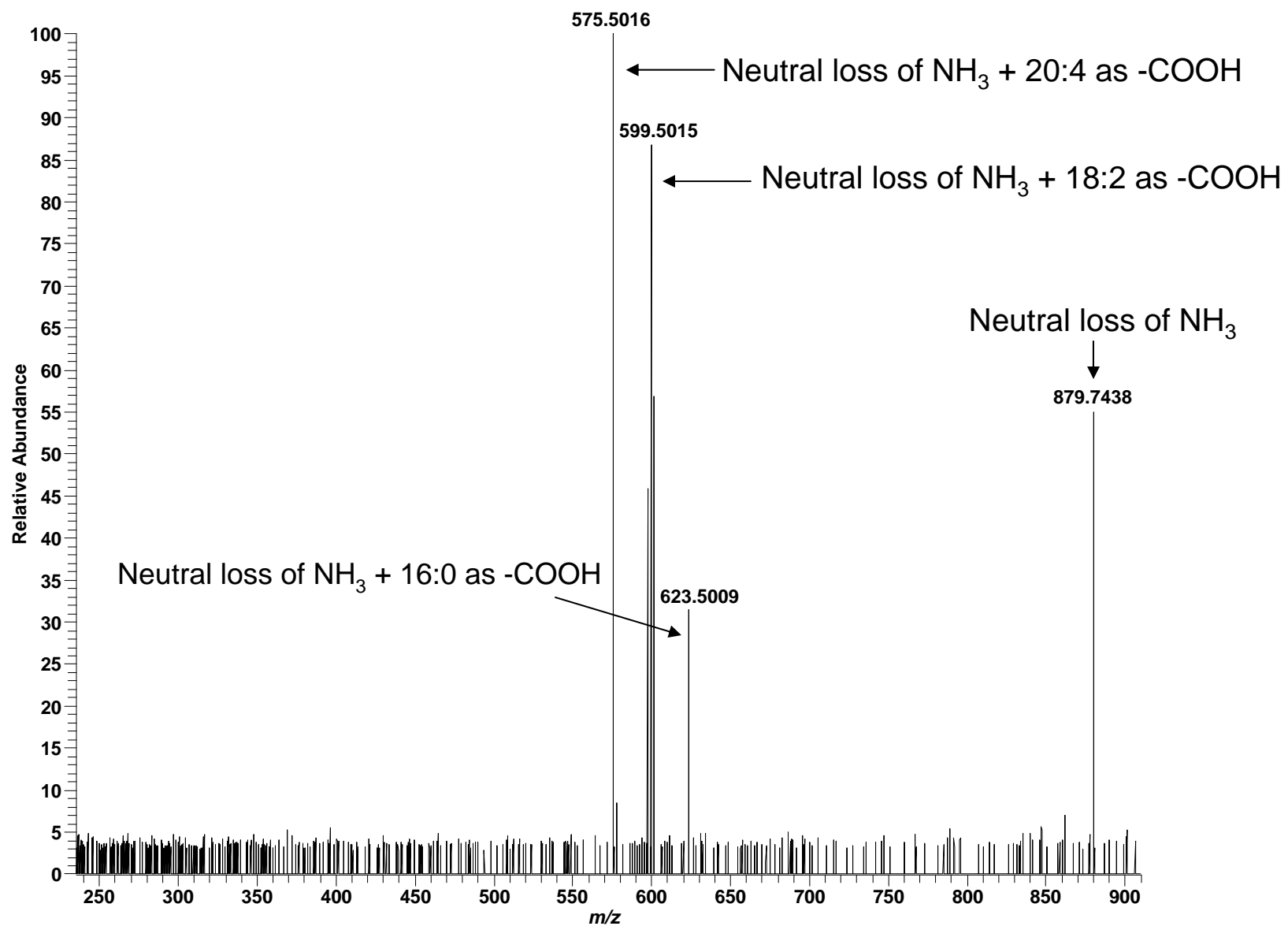
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,20:3,20:4); $C_{59}H_{100}O_6$; theoretical m/z 922.7864, $(M+NH_4)^+$



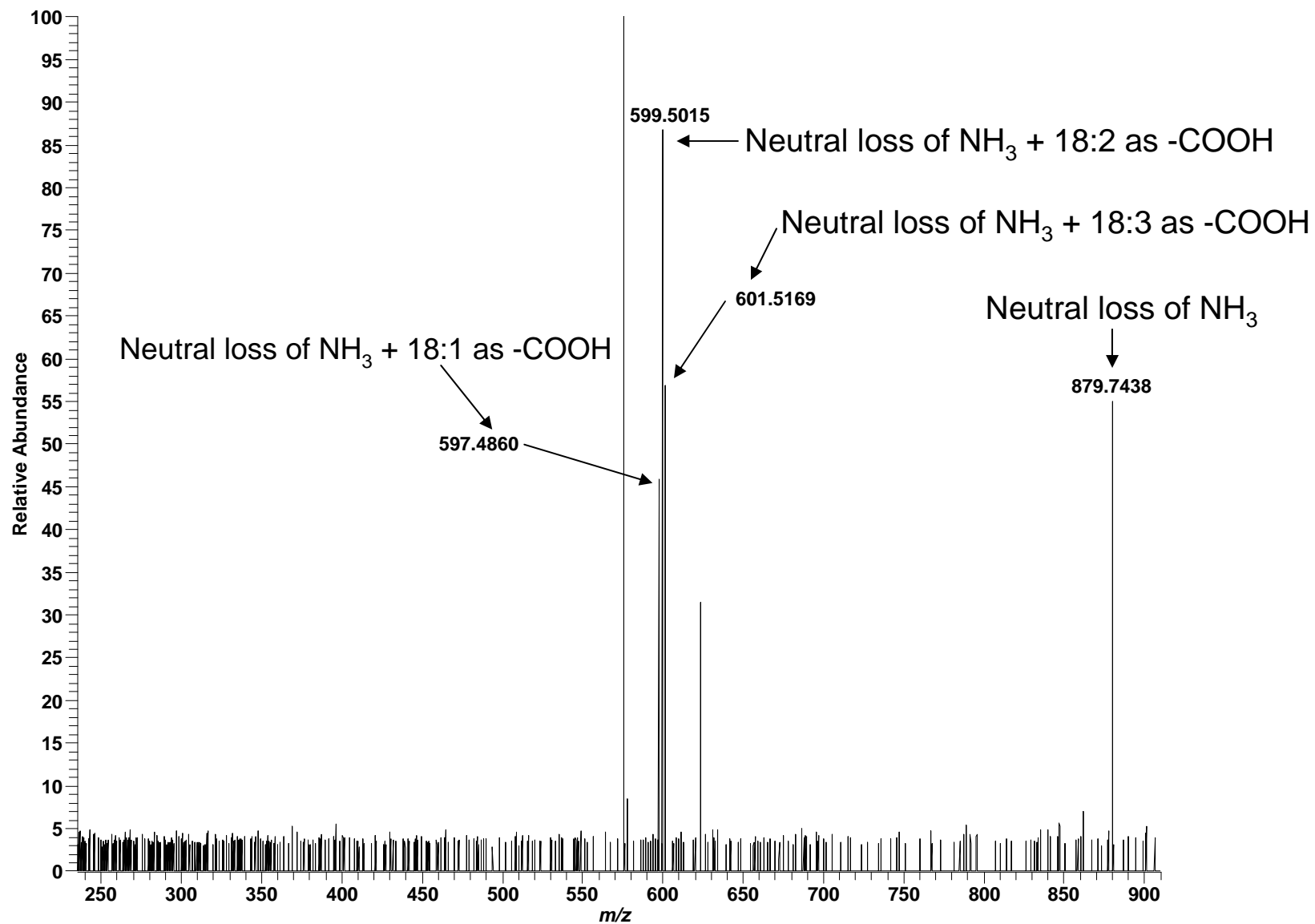
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:2,20:4); $C_{57}H_{98}O_6$; theoretical m/z 896.7707, $(M+NH_4)^+$



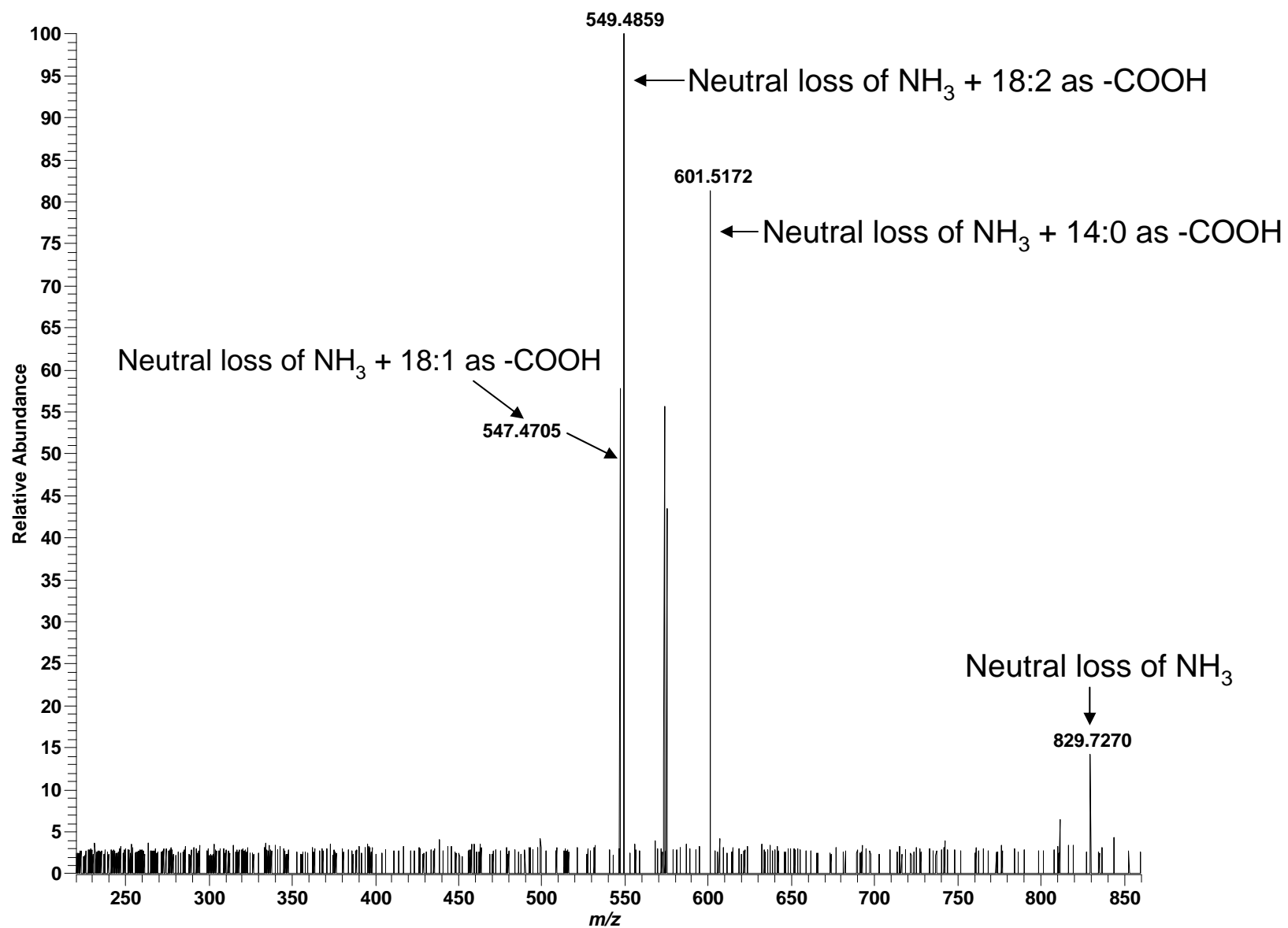
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:1,18:2,18:3); $C_{57}H_{98}O_6$; theoretical m/z 896.7707, $(M+NH_4)^+$



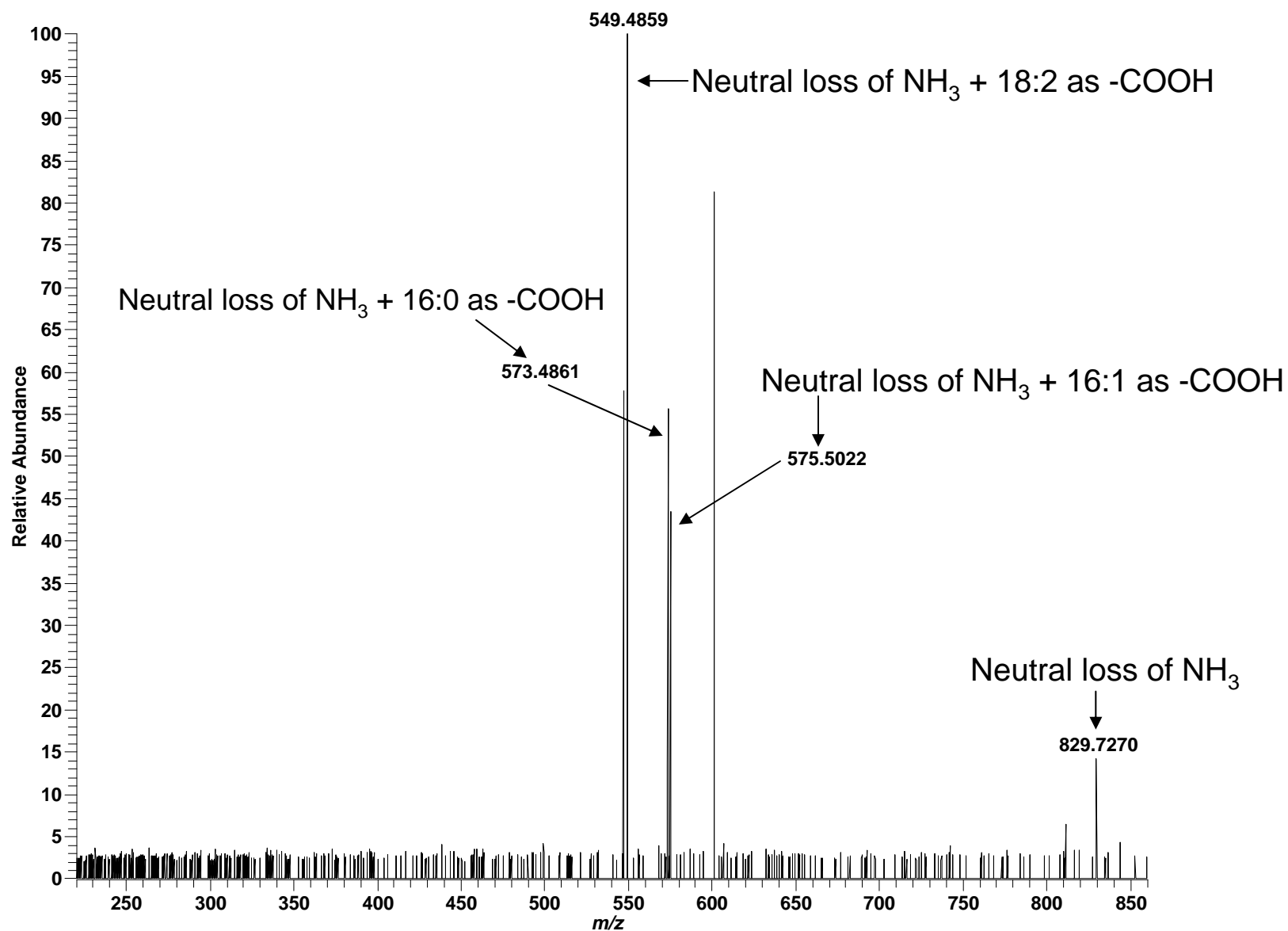
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (14:0,18:1,18:2); $C_{53}H_{96}O_6$; theoretical m/z 846.7551, $(M+NH_4)^+$



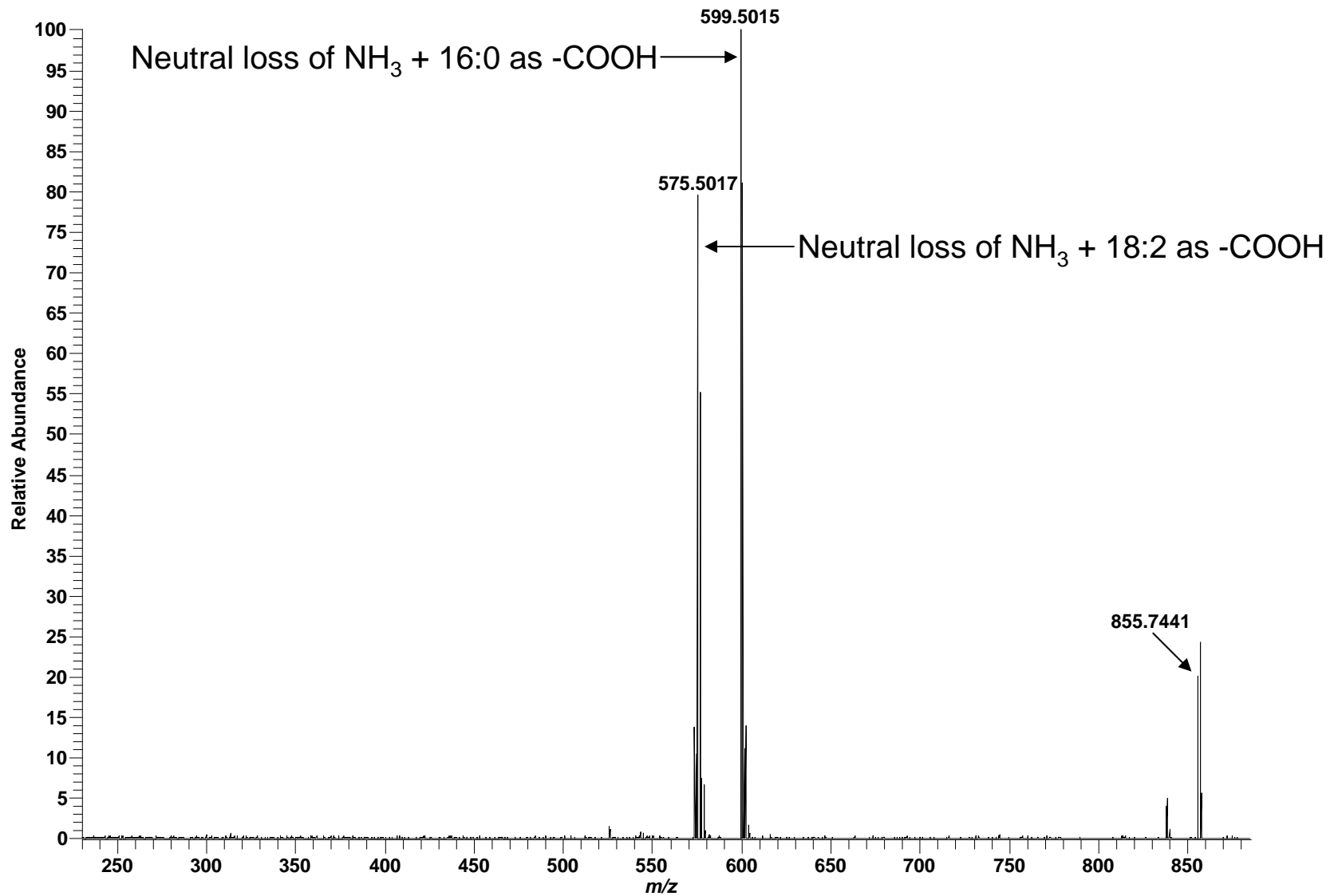
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,16:1,18:2); $C_{53}H_{96}O_6$; theoretical m/z 846.7551, $(M+NH_4)^+$



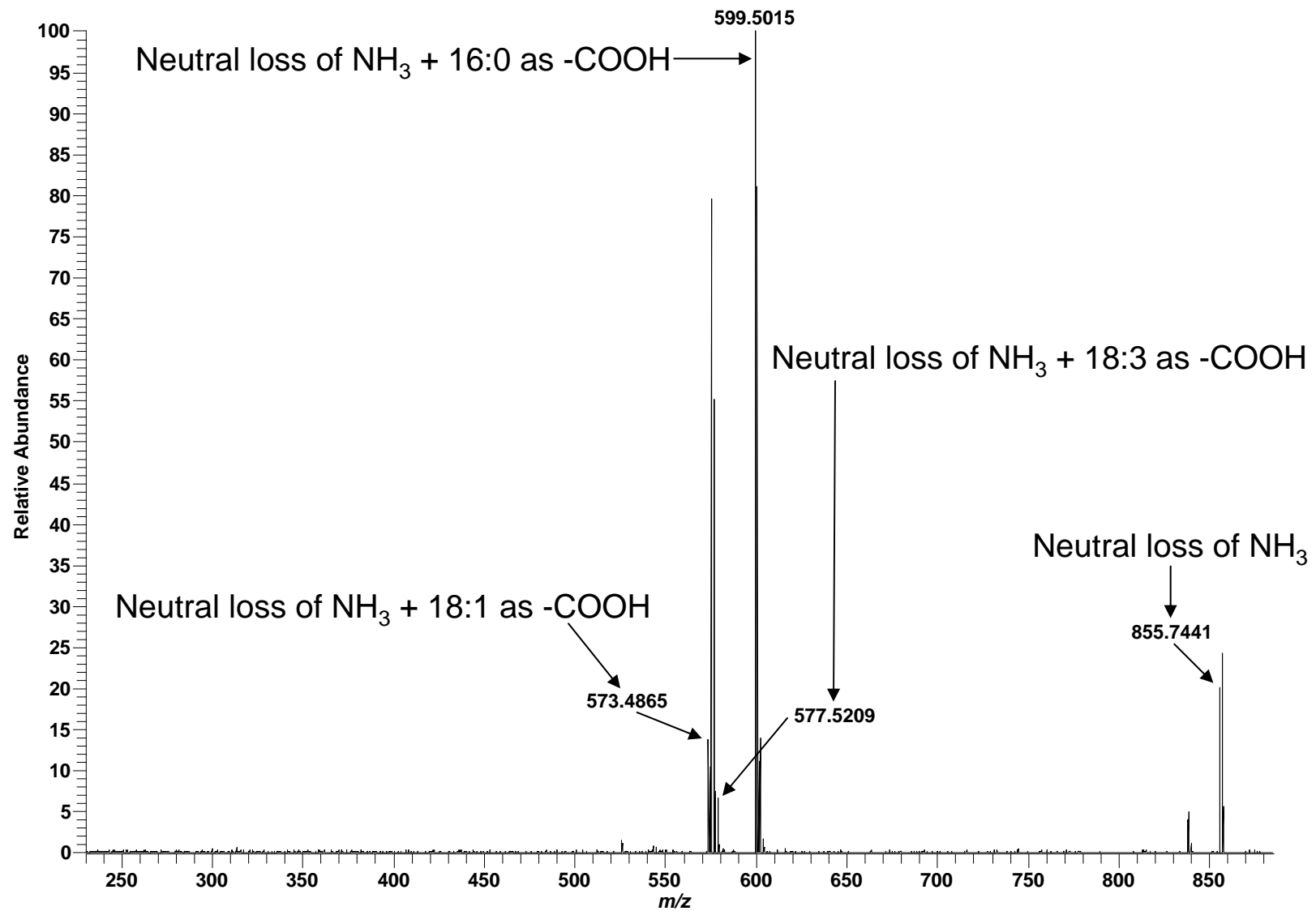
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:2,18:2); $C_{55}H_{98}O_6$; theoretical m/z 872.7707, $(M+NH_4)^+$



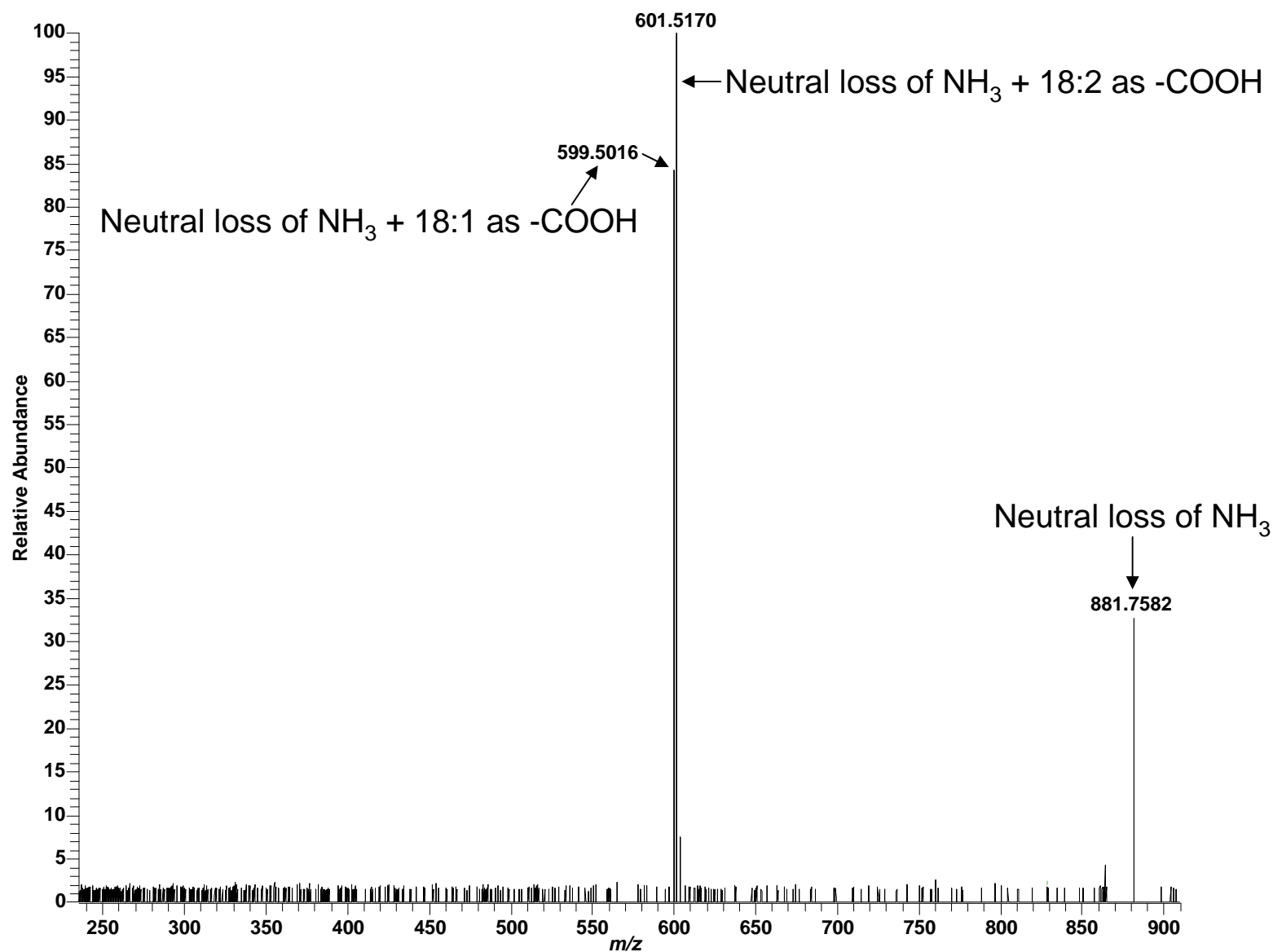
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:2,18:3); $C_{55}H_{98}O_6$; theoretical m/z 872.7707, $(M+NH_4)^+$



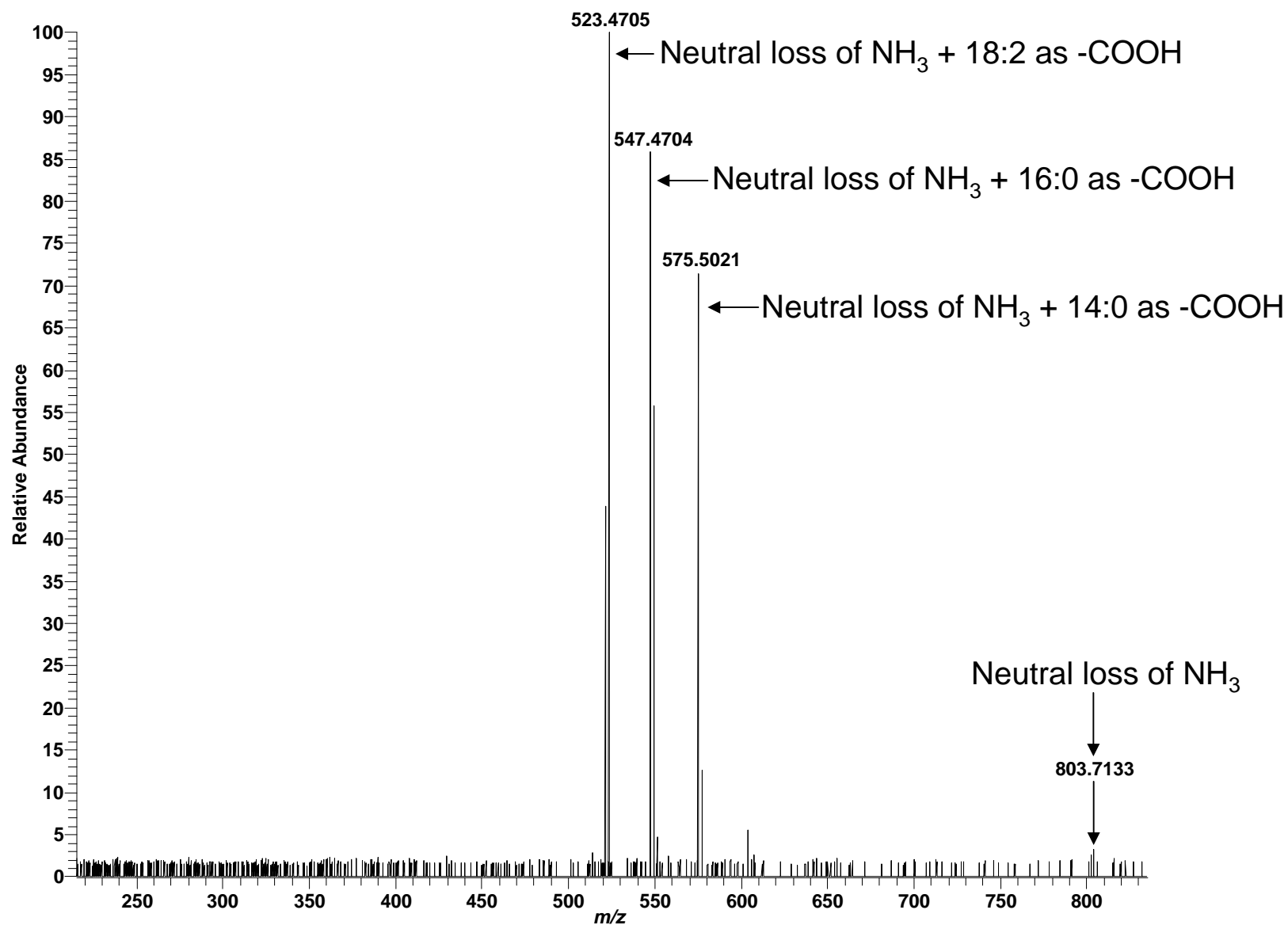
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:1,18:2,18:2); $C_{57}H_{100}O_6$; theoretical m/z 898.7864, $(M+NH_4)^+$



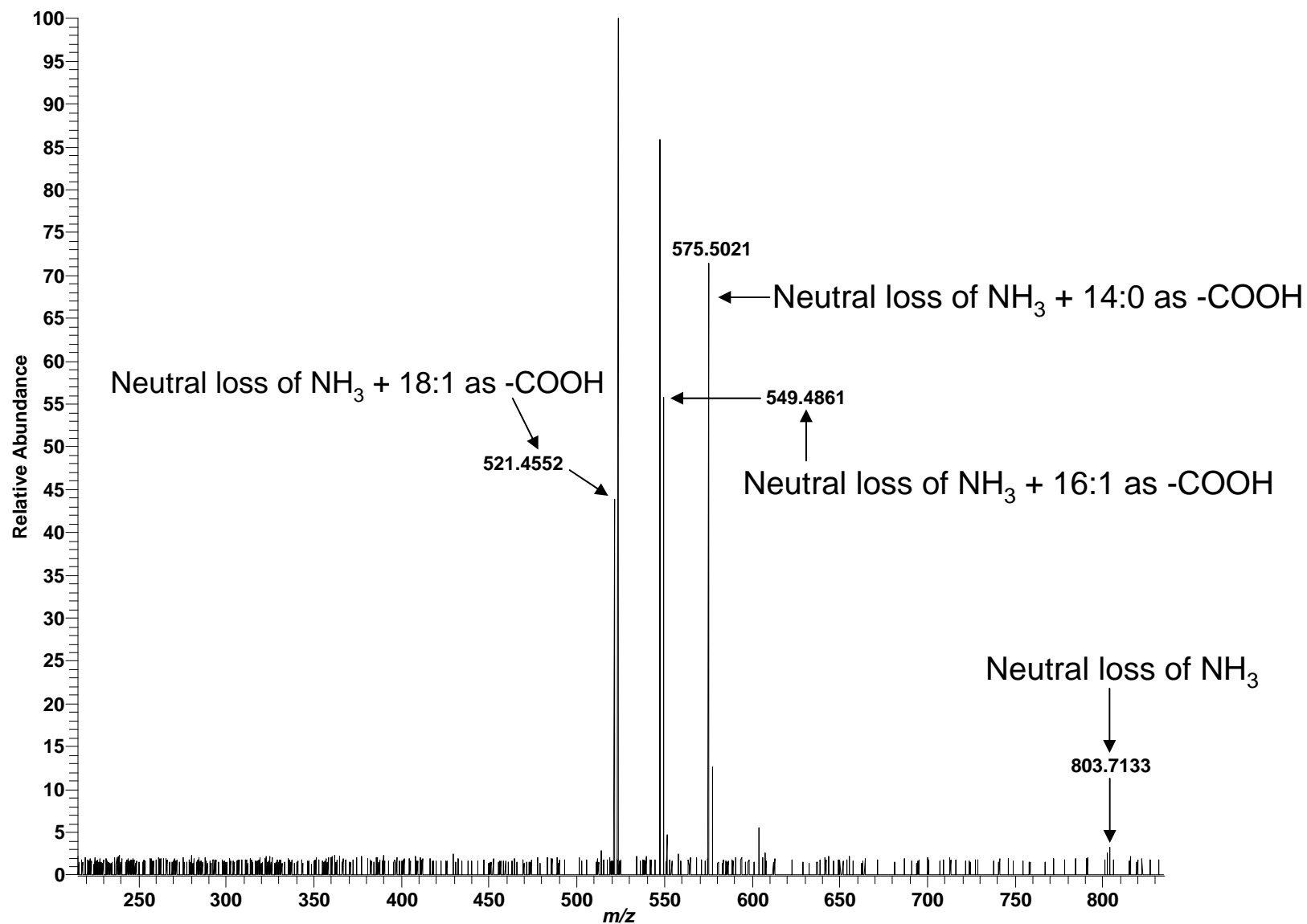
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (14:0,16:0,18:2); $C_{51}H_{94}O_6$; theoretical m/z 820.7394, $(M+NH_4)^+$



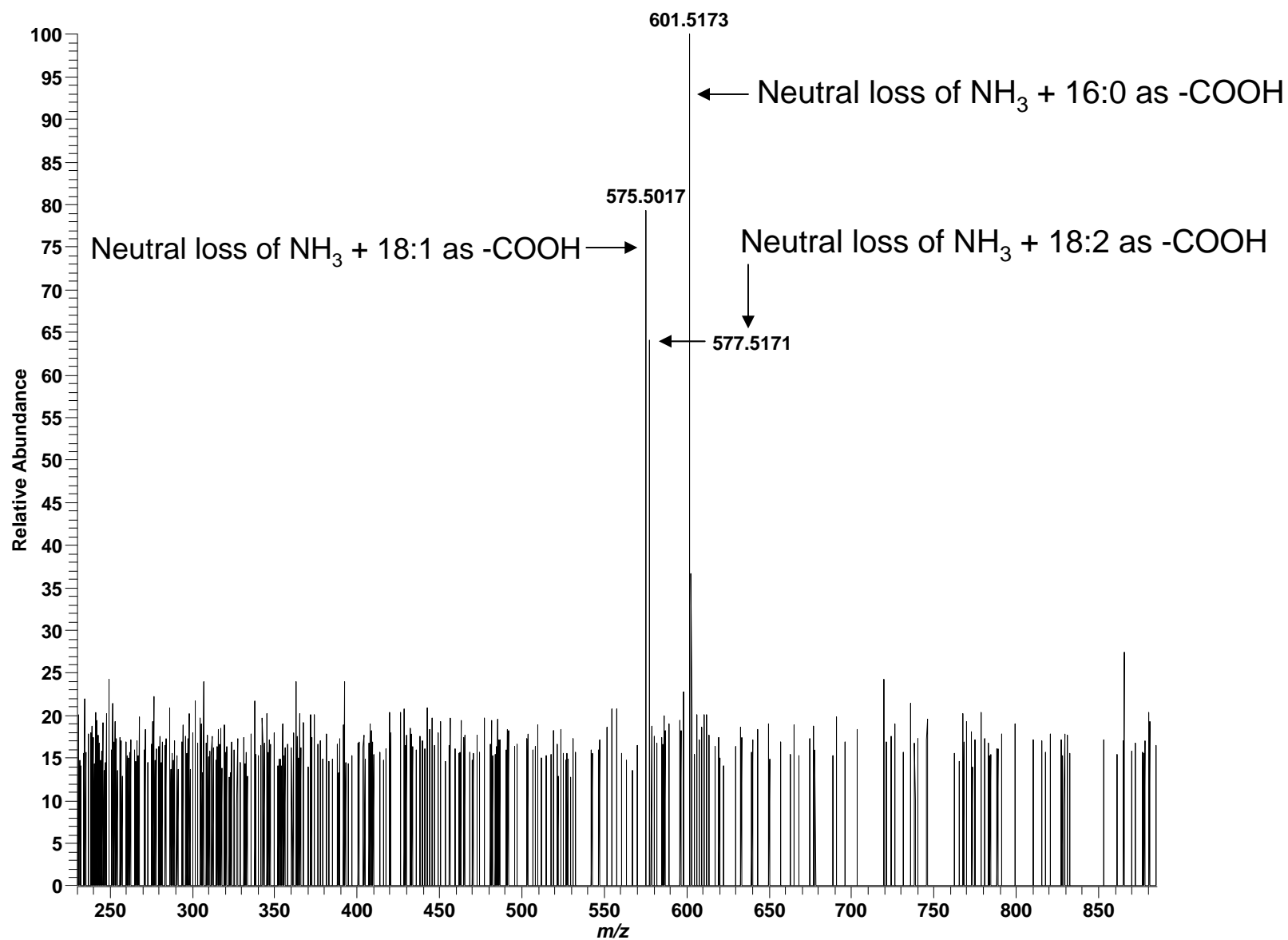
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (14:0,16:1,18:1); $C_{51}H_{94}O_6$; theoretical m/z 820.7394, $(M+NH_4)^+$



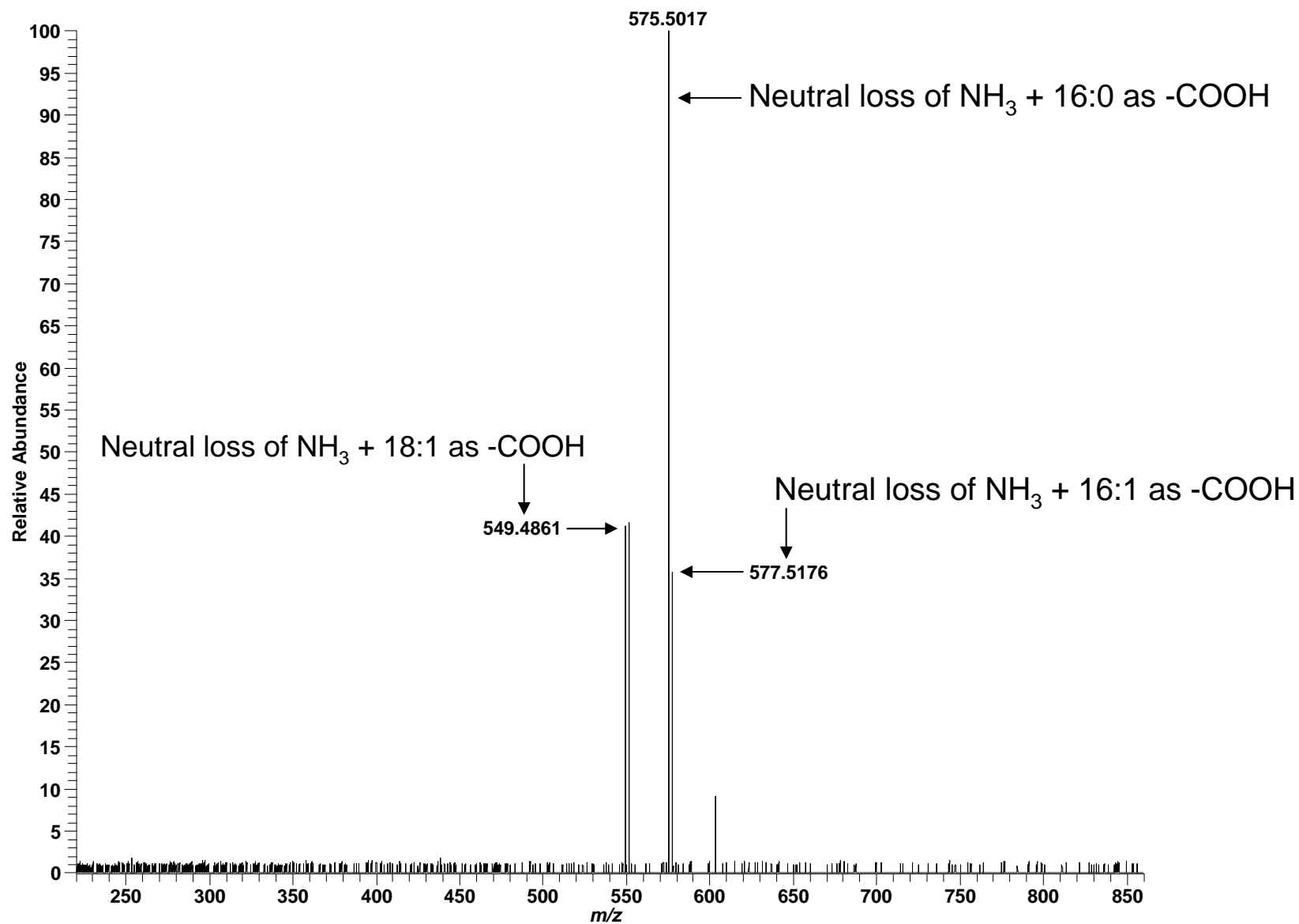
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:1,18:2); $C_{55}H_{100}O_6$; theoretical m/z 874.7864, $(M+NH_4)^+$



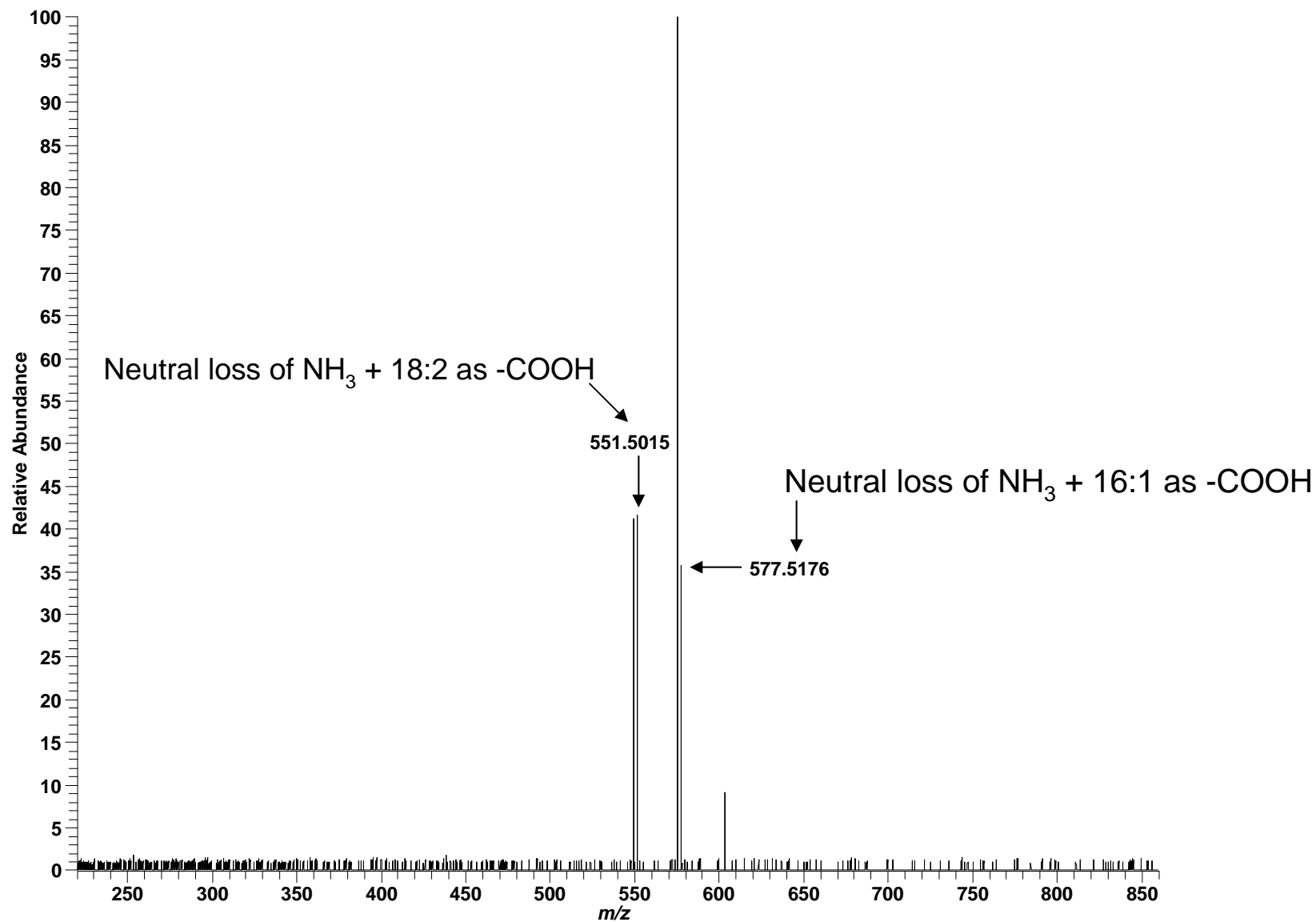
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,16:1,18:1); $C_{53}H_{98}O_6$; theoretical m/z 848.7707, $(M+NH_4)^+$



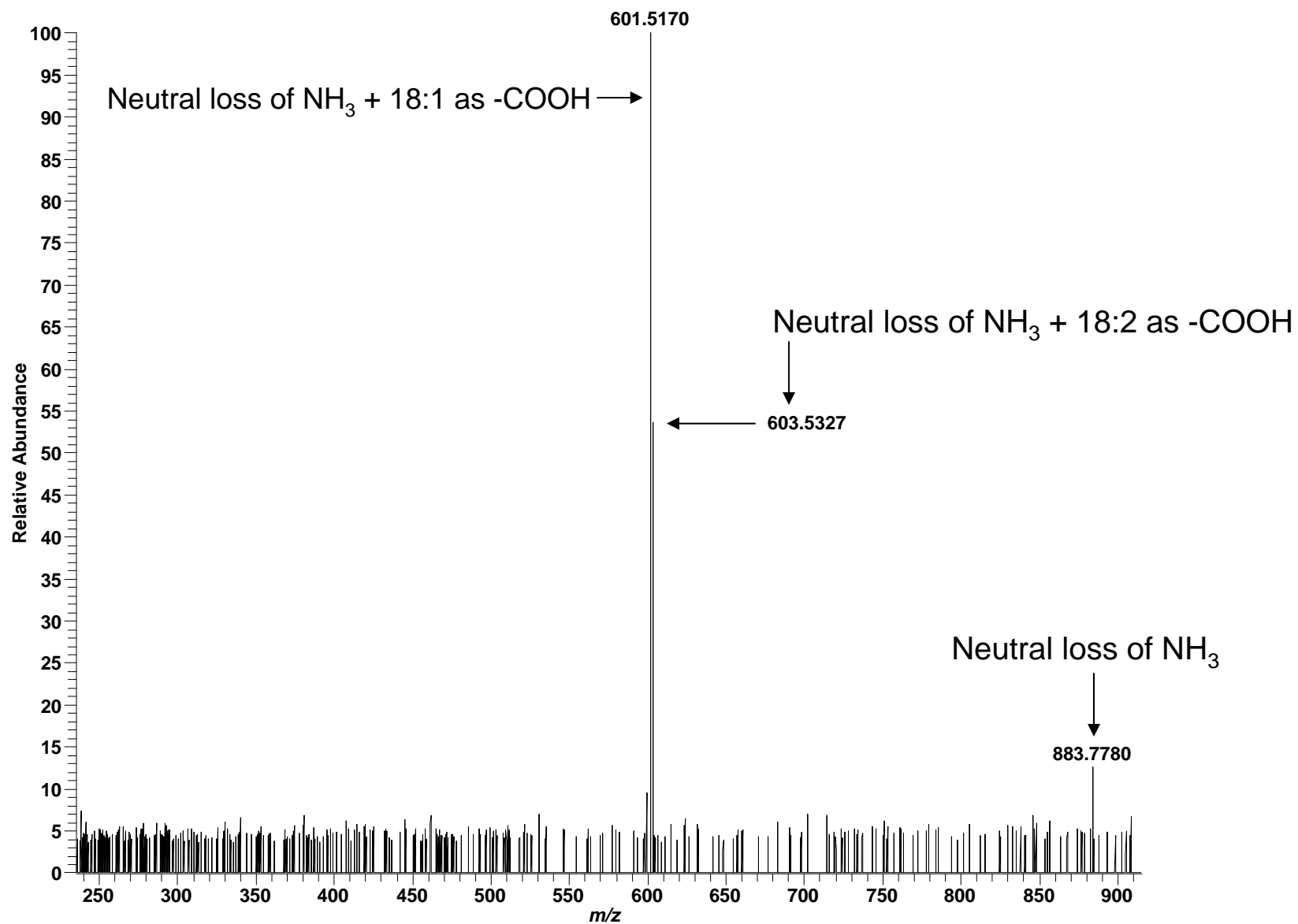
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,16:0,18:2); $C_{57}H_{102}O_6$; theoretical m/z 848.7707, $(M+NH_4)^+$



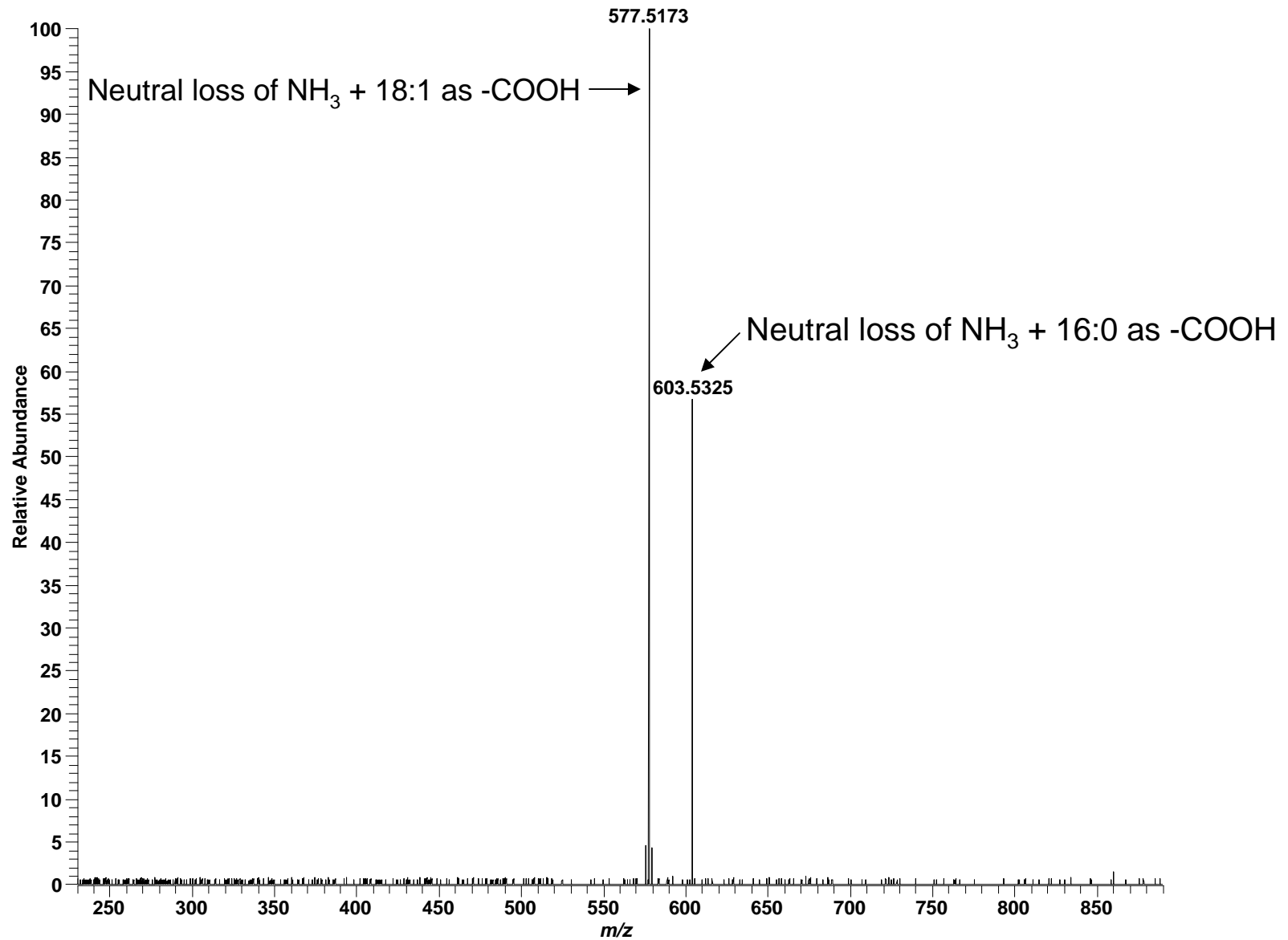
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:1,18:1,18:2); $C_{57}H_{102}O_6$; theoretical m/z 900.8020, $(M+NH_4)^+$



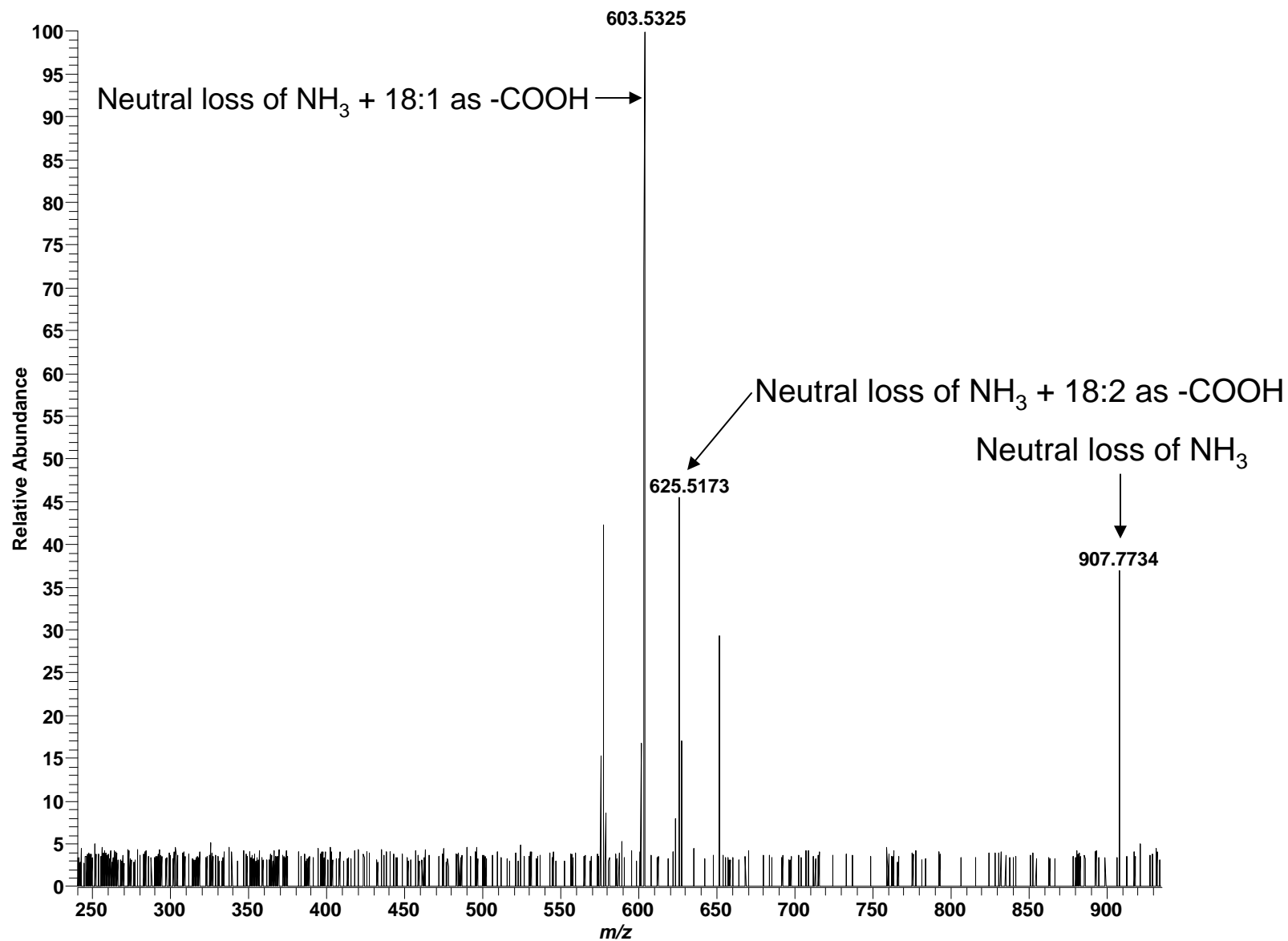
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:1,18:1); $C_{55}H_{102}O_6$; theoretical m/z 876.8020, $(M+NH_4)^+$



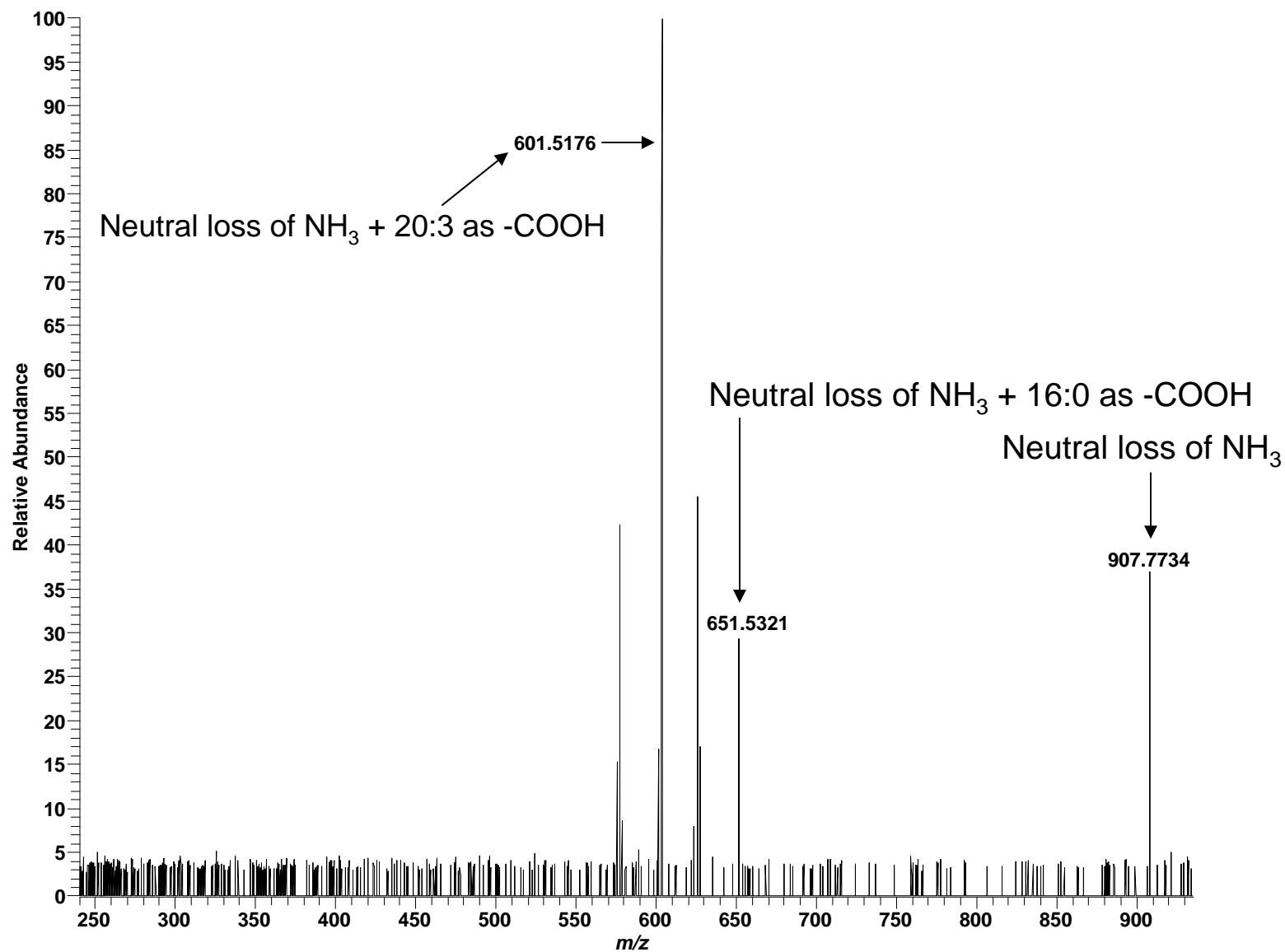
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:1,18:1,20:4); $C_{59}H_{102}O_6$; theoretical m/z 924.8020, $(M+NH_4)^+$



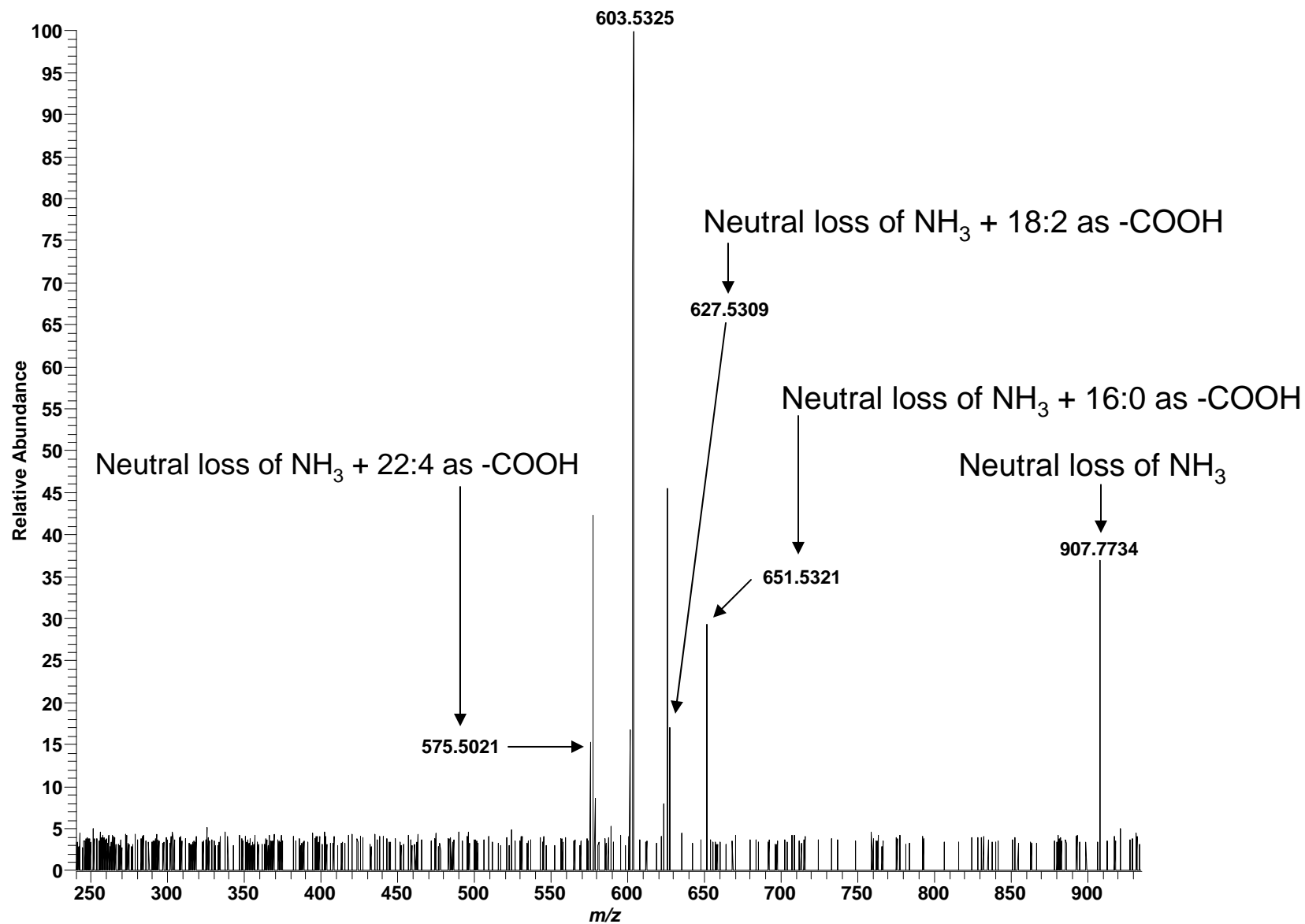
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,20:3,20:3); $C_{59}H_{102}O_6$; theoretical m/z 924.8020, $(M+NH_4)^+$



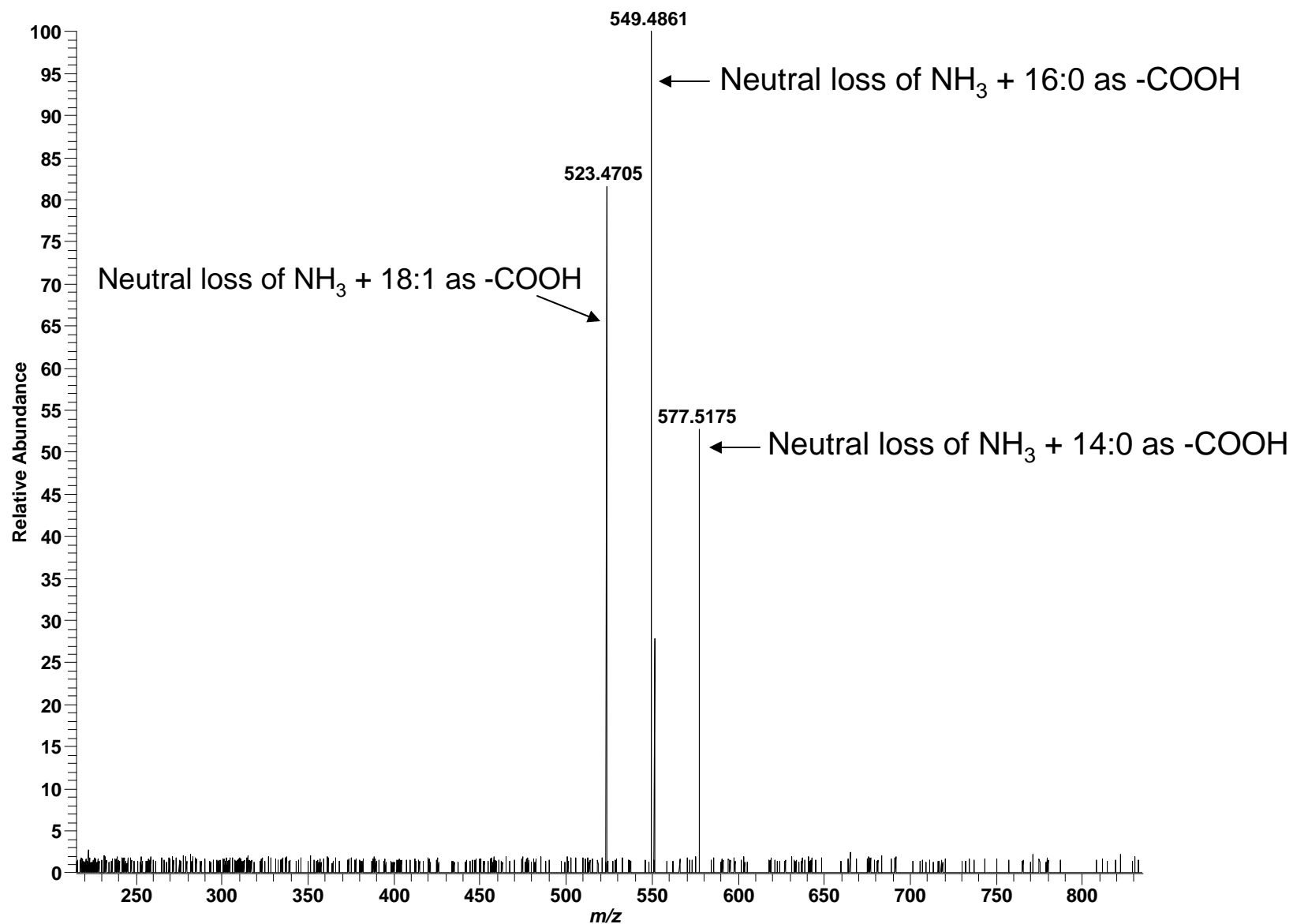
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,18:2,22:4); $C_{59}H_{102}O_6$; theoretical m/z 924.8020, $(M+NH_4)^+$



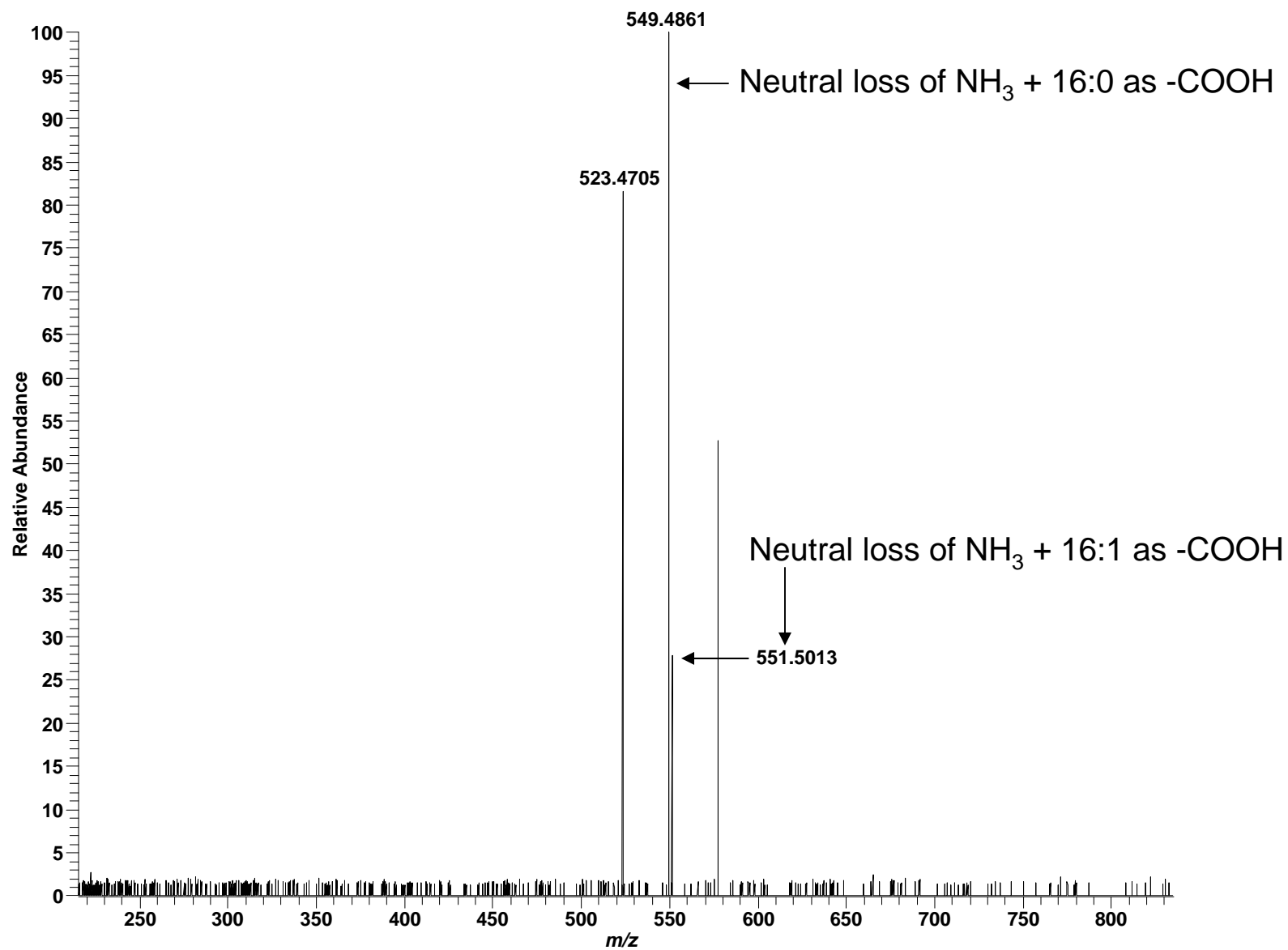
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (14:0,16:0,18:1); $C_{51}H_{96}O_6$; theoretical m/z 822.7550, $(M+NH_4)^+$



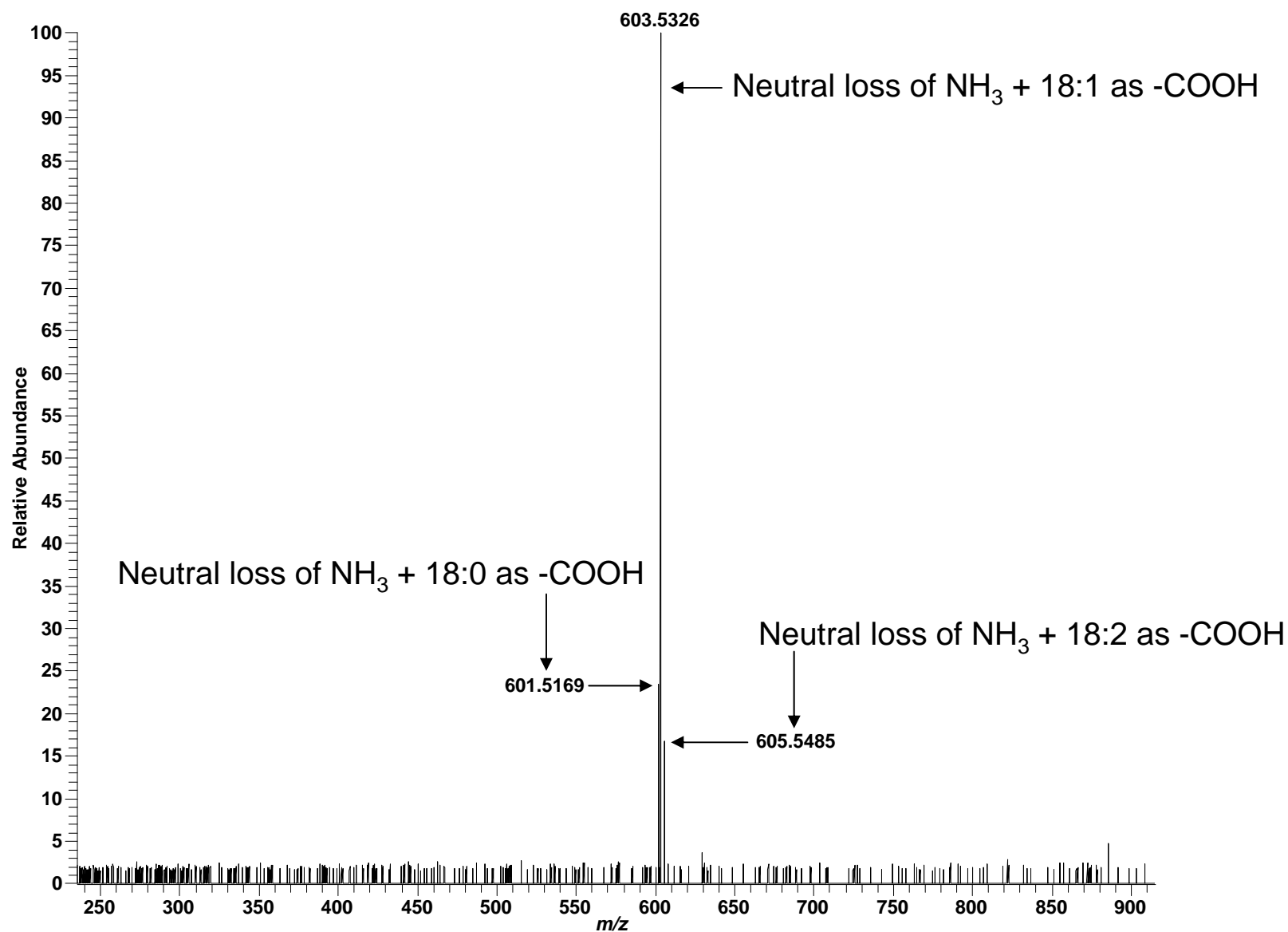
High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,16:0,16:1); $C_{51}H_{96}O_6$; theoretical m/z 822.7550, $(M+NH_4)^+$



High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (18:0,18:1,18:2); $C_{57}H_{104}O_6$; theoretical m/z 902.8177, $(M+NH_4)^+$



High mass measurement accuracy MS/MS utilizing LTQ-FT

Positive ESI: TAG (16:0,16:0,18:1); $C_{53}H_{100}O_6$; theoretical m/z 850.7864, $(M+NH_4)^+$

