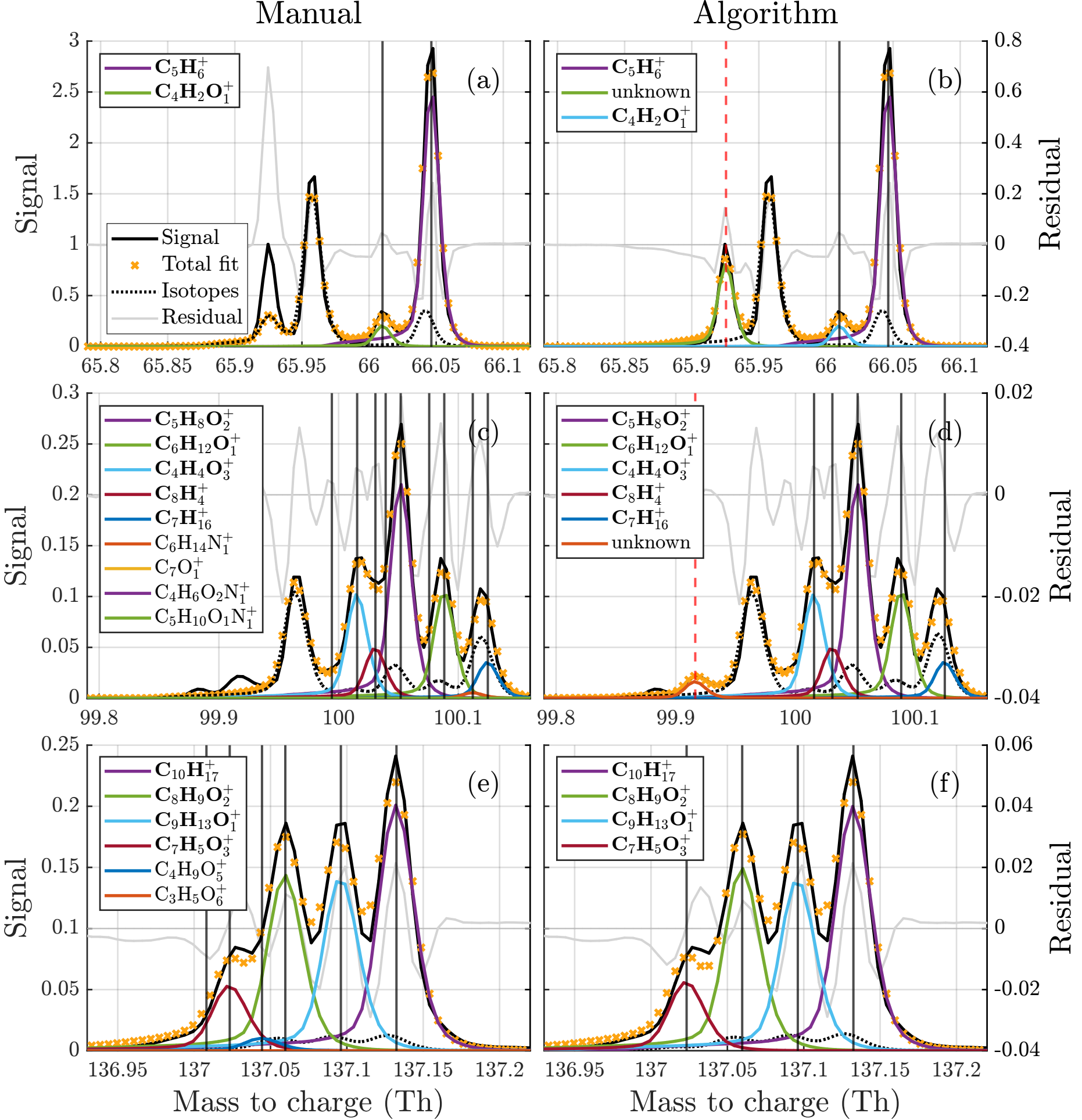
Manual
Algorithm
(a)
(b)
(c)
(d)
(e)
(f)
Signal
Residual
Signal
Total fit
Isotopes
Residual
unknown
$C_5H_6^+$
$C_4H_2O_1^+$
$C_5H_8O_2^+$
$C_6H_{12}O_1^+$
$C_4H_4O_3^+$
$C_8H_4^+$
$C_7H_{16}^+$
$C_6H_{14}N_1^+$
$C_7O_1^+$
$C_4H_6O_2N_1^+$
$C_5H_{10}O_1N_1^+$
$C_{10}H_{17}^+$
$C_8H_9O_2^+$
$C_9H_{13}O_1^+$
$C_7H_5O_3^+$
$C_4H_9O_5^+$
$C_3H_5O_6^+$
Mass to charge (Th)
Mass to charge (Th)