

One-Pot Oxidative N-Demethylation of Tropane Alkaloids with Hydrogen Peroxide and an Fe^{III}-TAML Catalyst

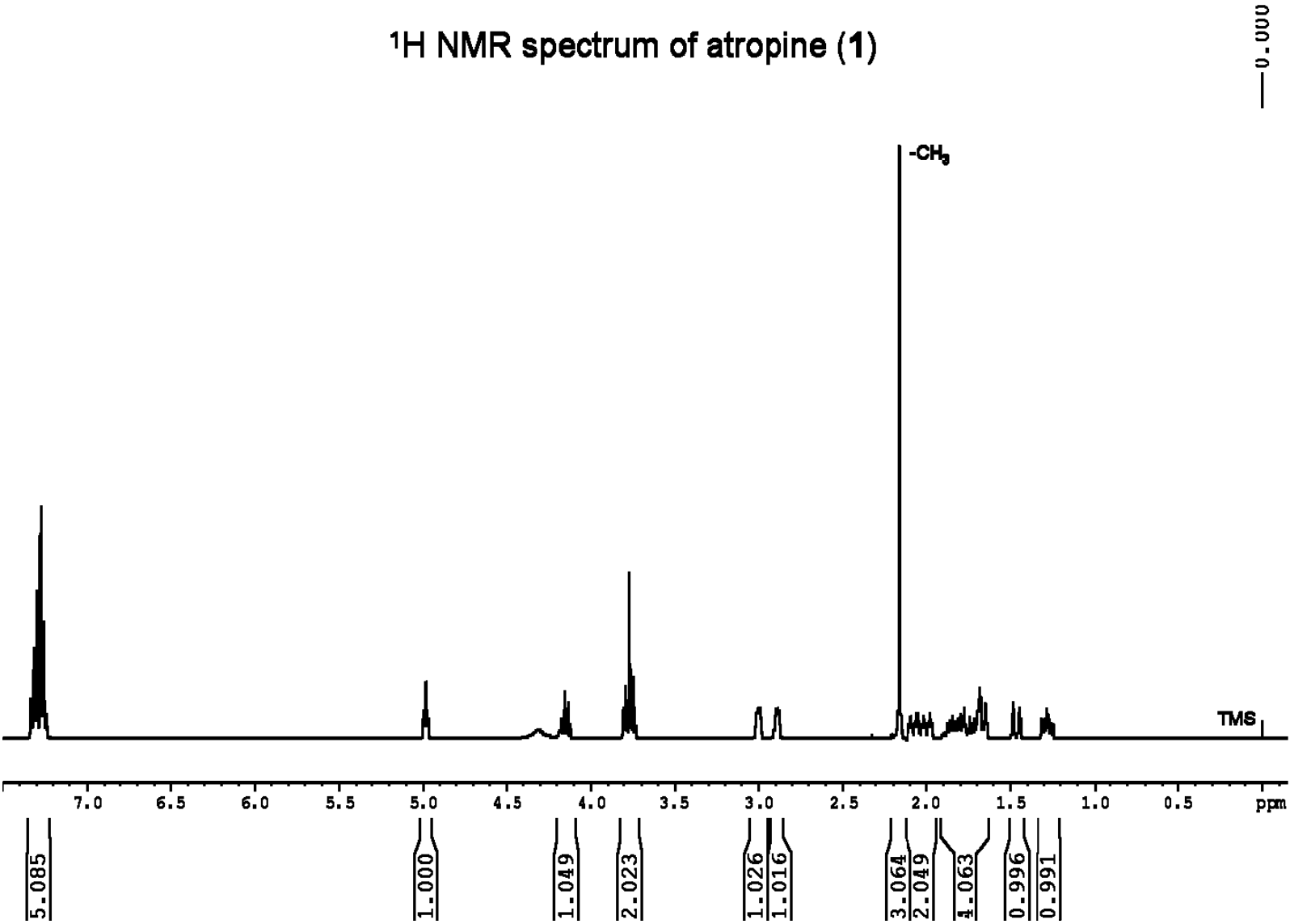
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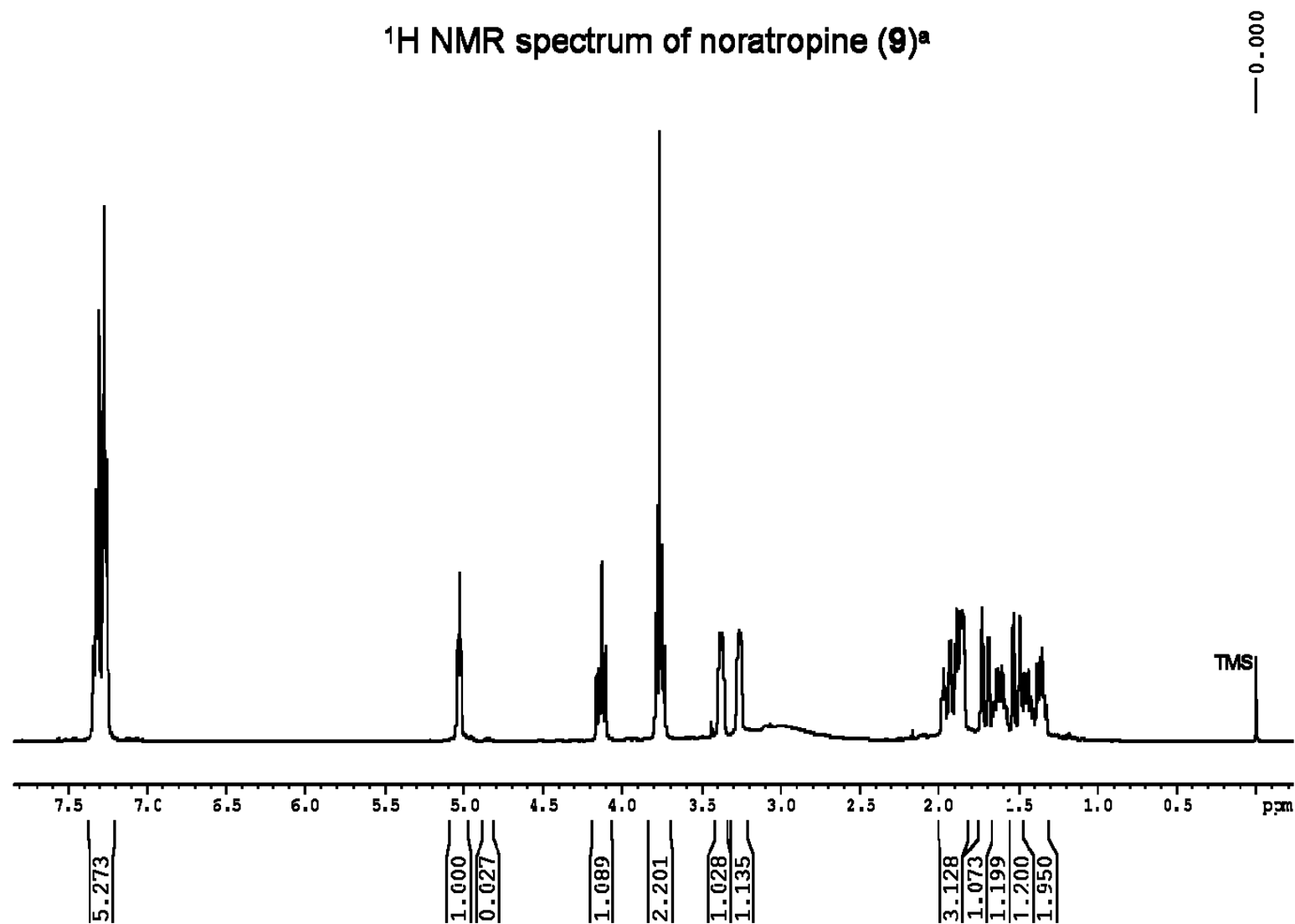
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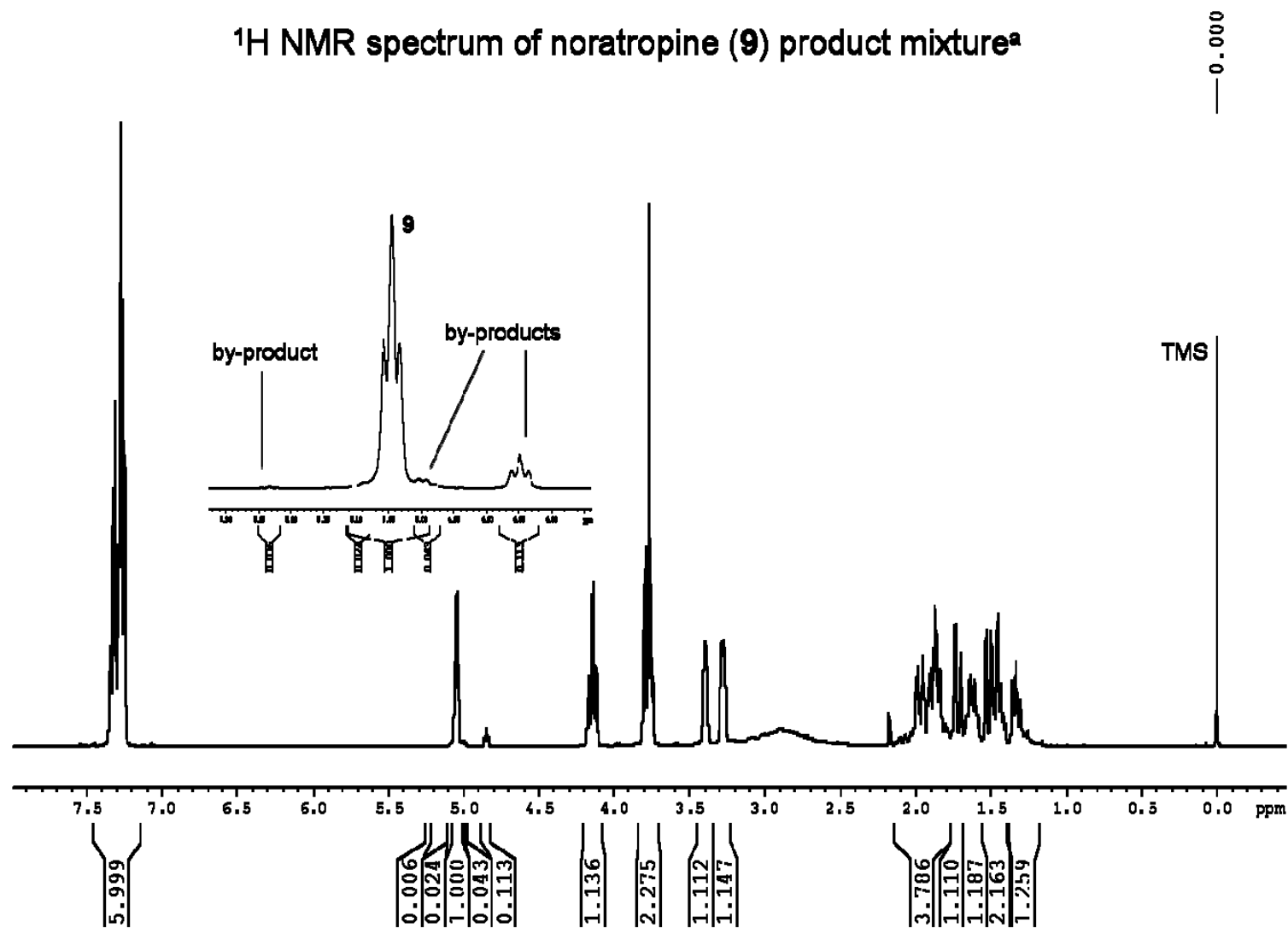
2. 2. ¹H NMR spectrum of atropine (**1**)
3. 4. ¹H NMR spectrum of noratropine (**9**)
4. 5. ¹H NMR spectrum of noratropine (**9**) product mixture
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6. 7. MS/MS fragmentation of noratropine (**9**)
7. 8. MS/MS fragmentation of atropine (**1**)
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14. 15. ¹H NMR spectrum of nortropine (**10**) product mixture
15. 16. LC-MS of nortropine (**10**) product mixture



¹H NMR spectrum of noratropine (9)^a

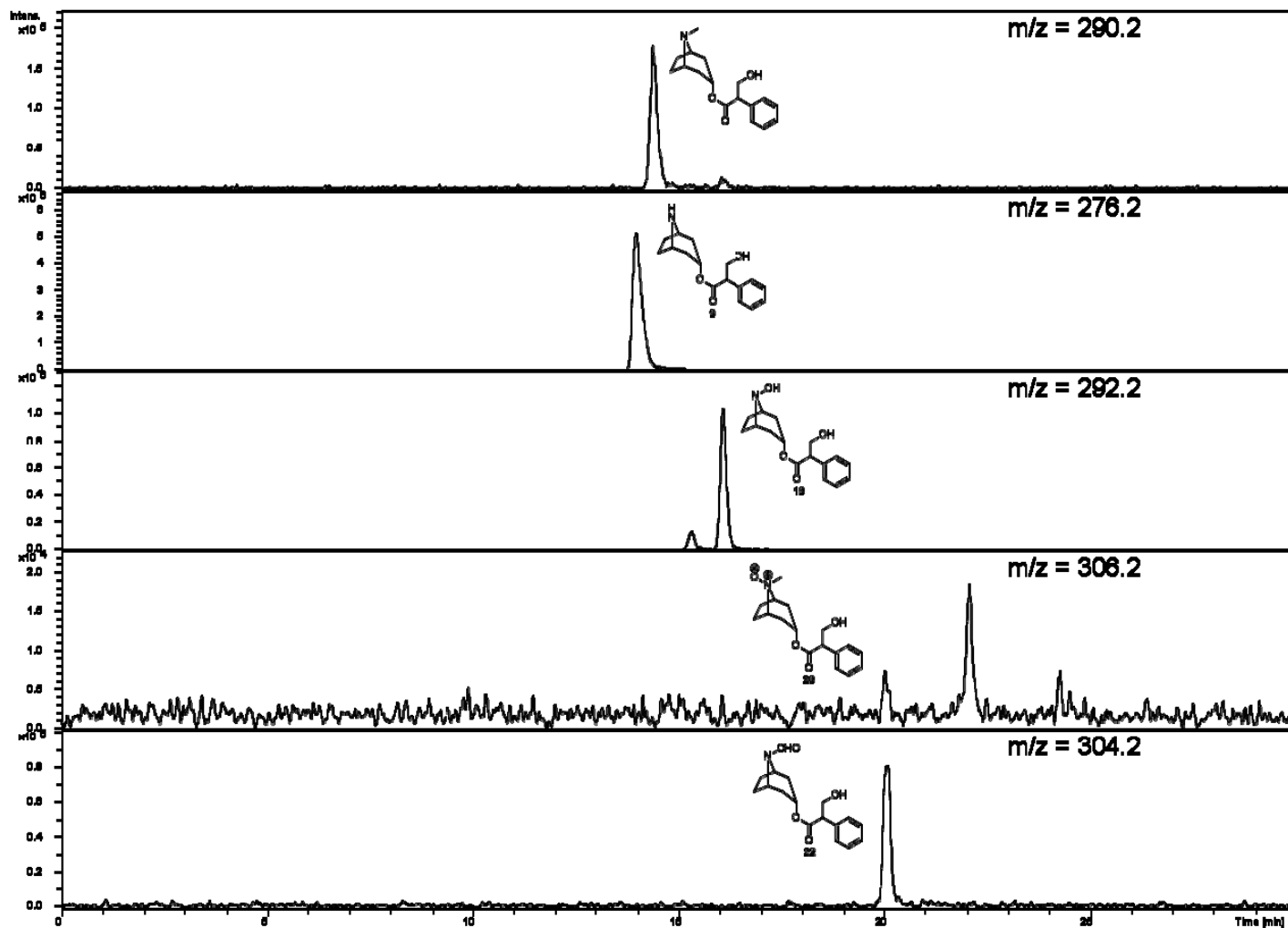


a) 0.9 mol% 18, 3.45 mmol atropine, 172 mmol H₂O₂, 30 mL ethanol, 1 h



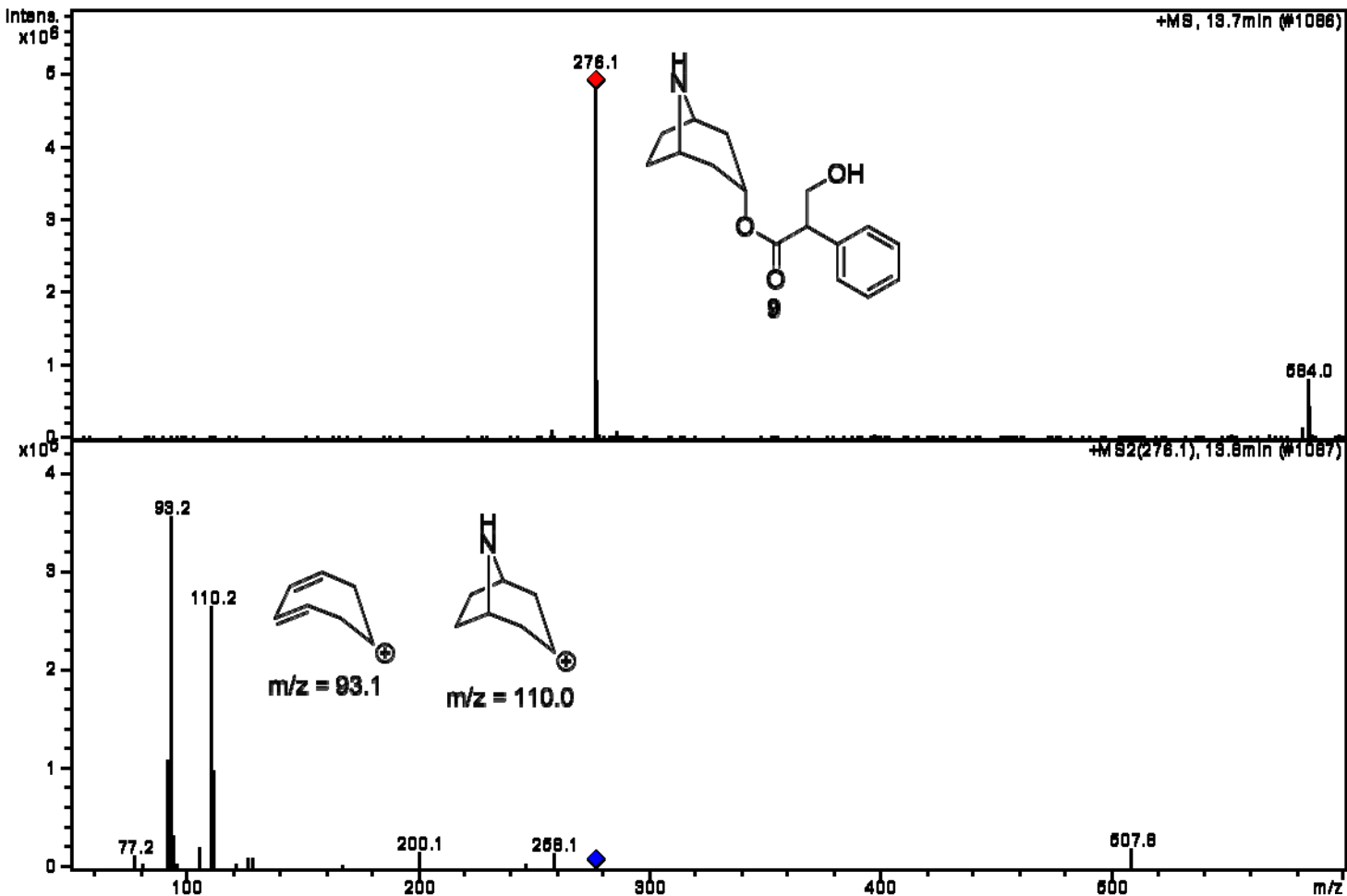
a) 0.45 mol% **18**, 115 mM atropine in acetone, 100 eq. H_2O_2 , 1 h

LC-MS of noratropine (9) product mixture^a

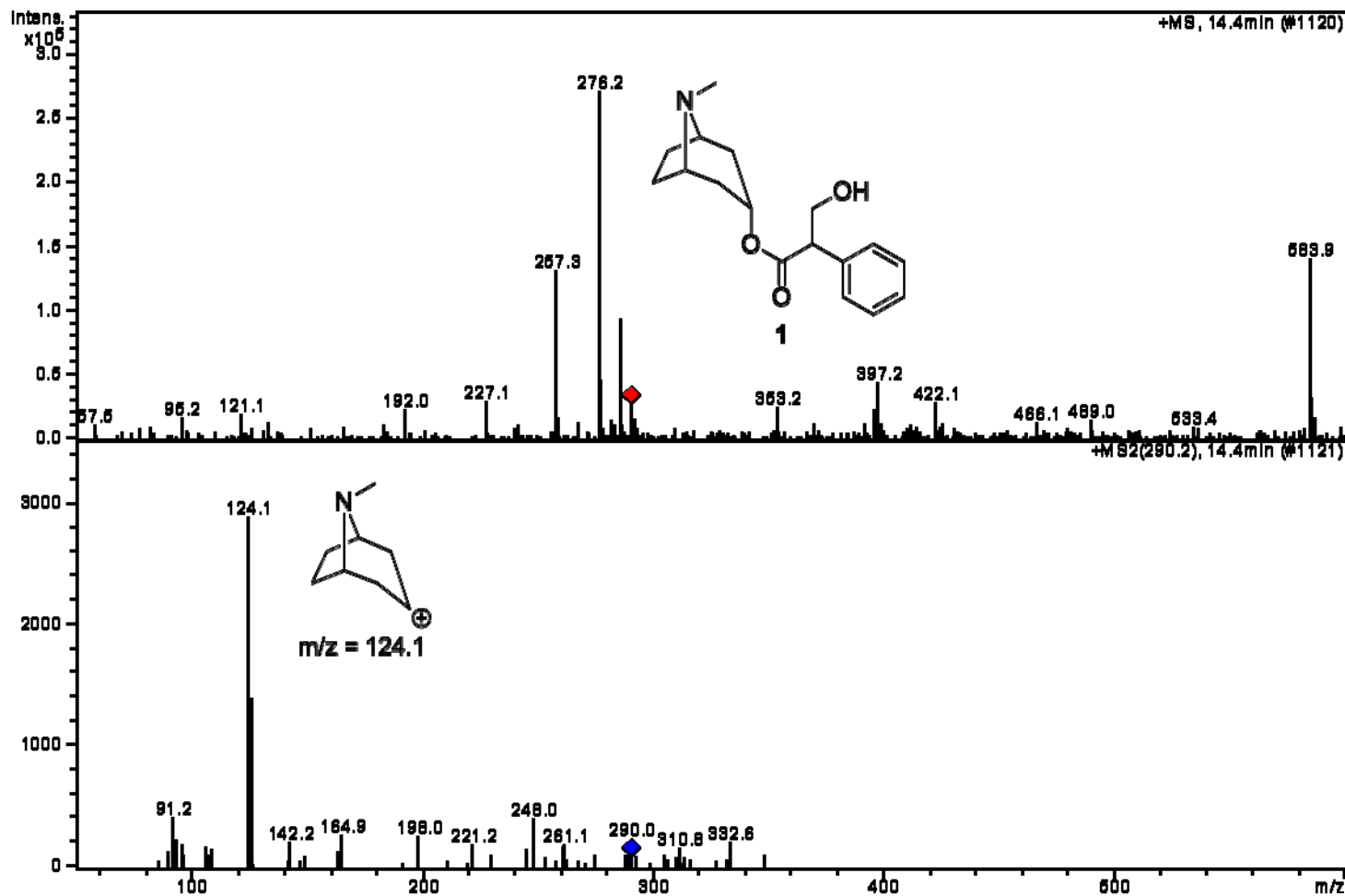


a) 0.45 mol% 18, 115 mM atropine in acetone, 100 eq. H₂O₂, 1 h

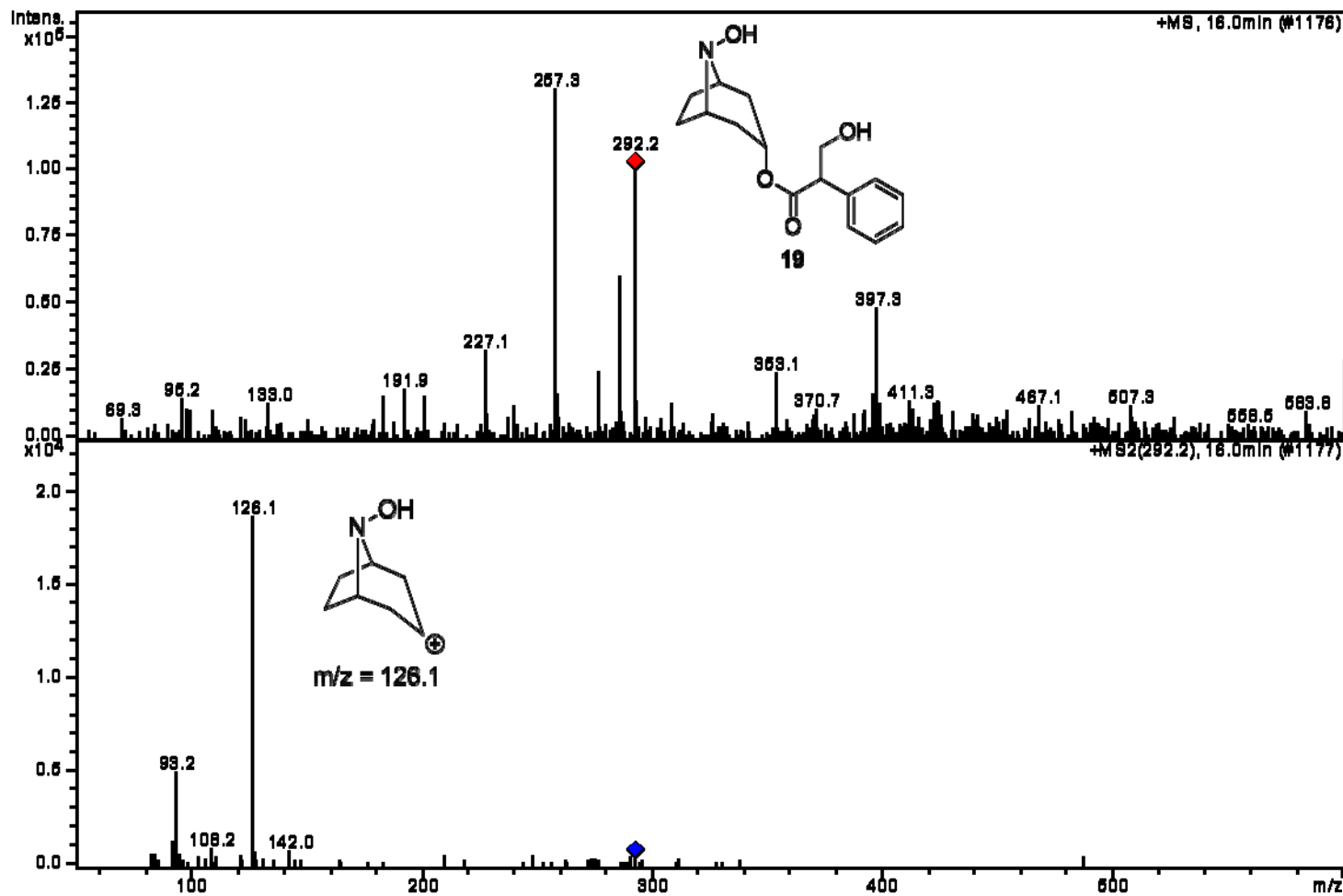
MS/MS fragmentation of noratropine (9)



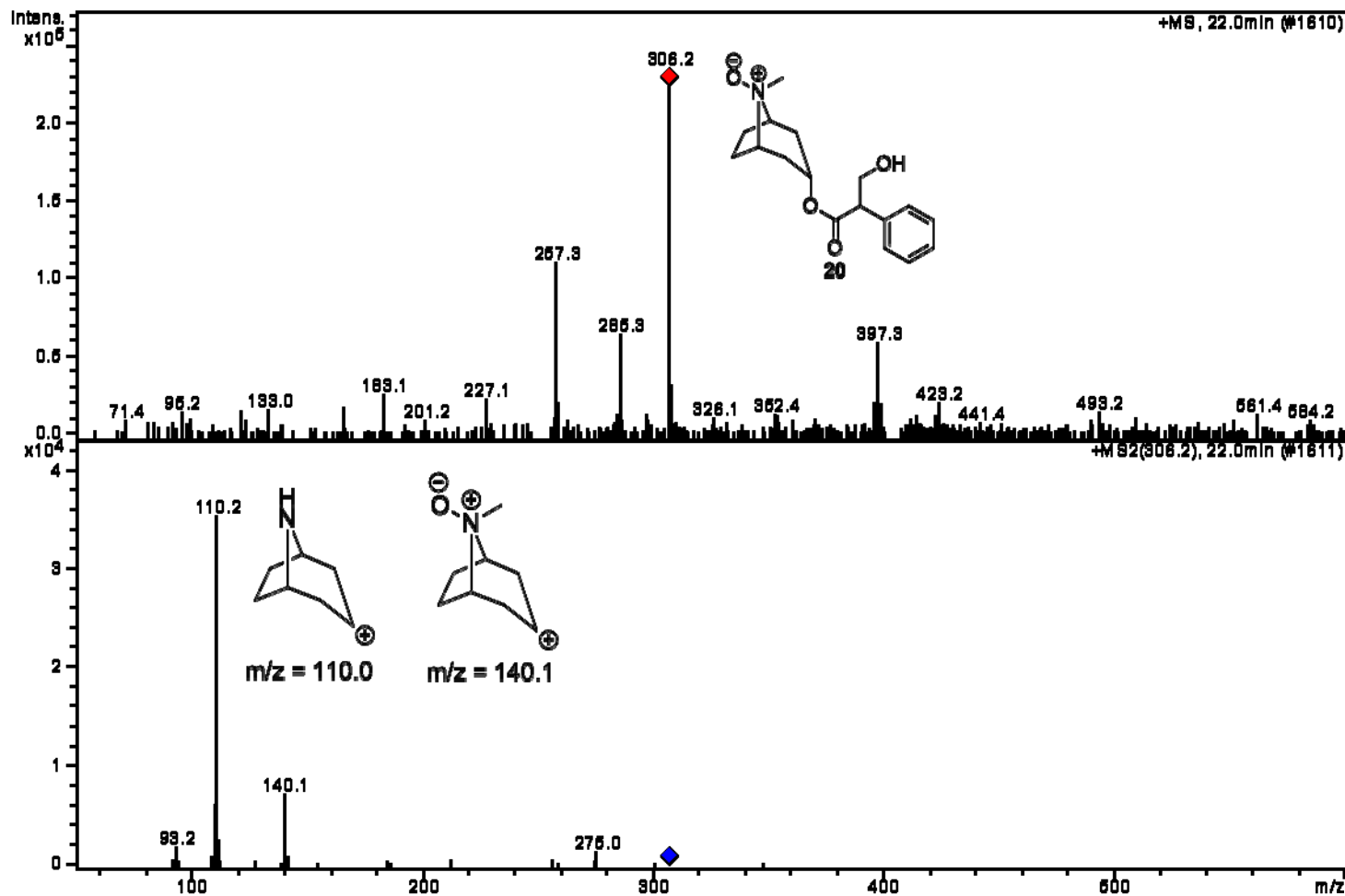
MS/MS fragmentation of atropine (1)



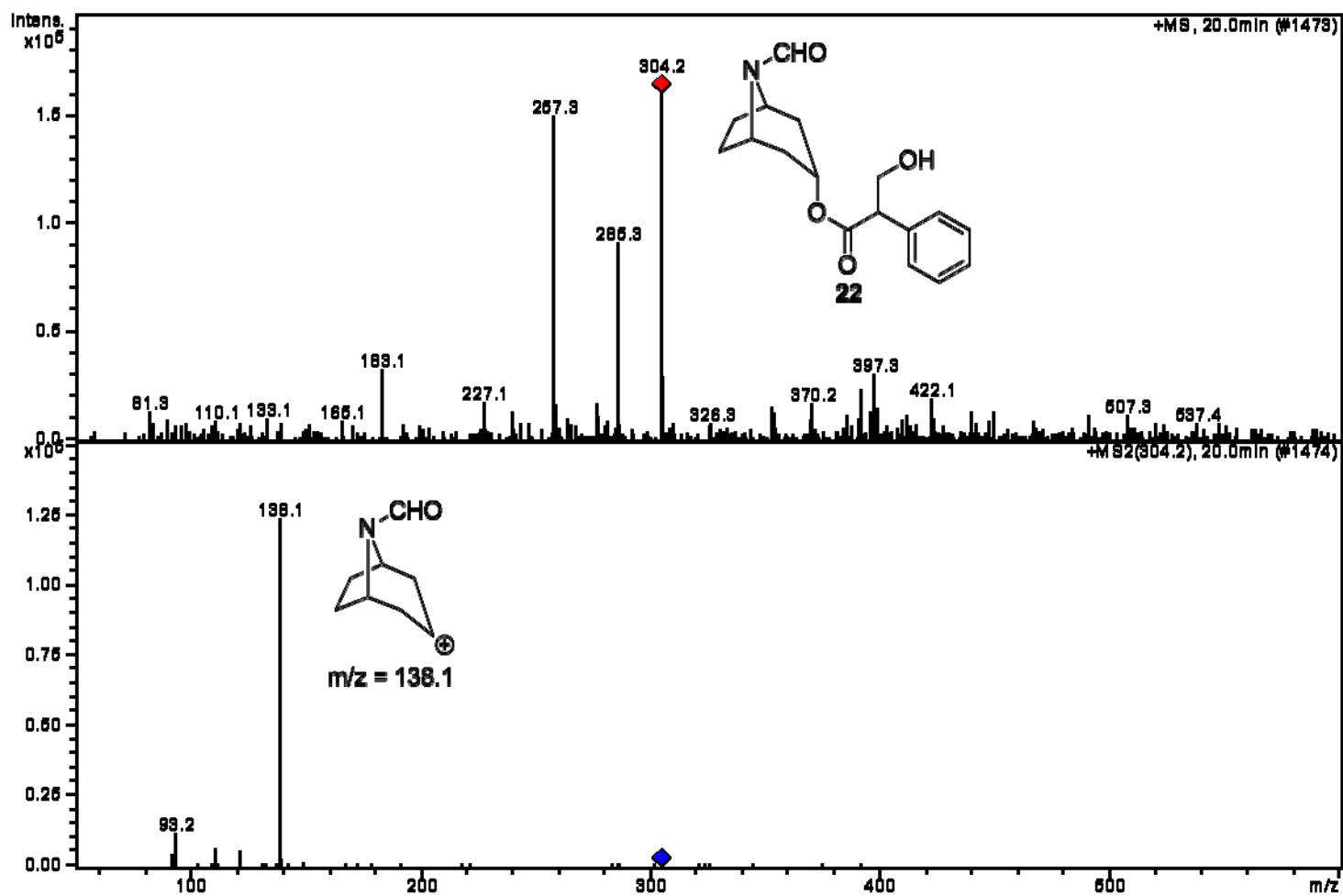
MS/MS fragmentation of *N*-hydroxy-noratropine (19)

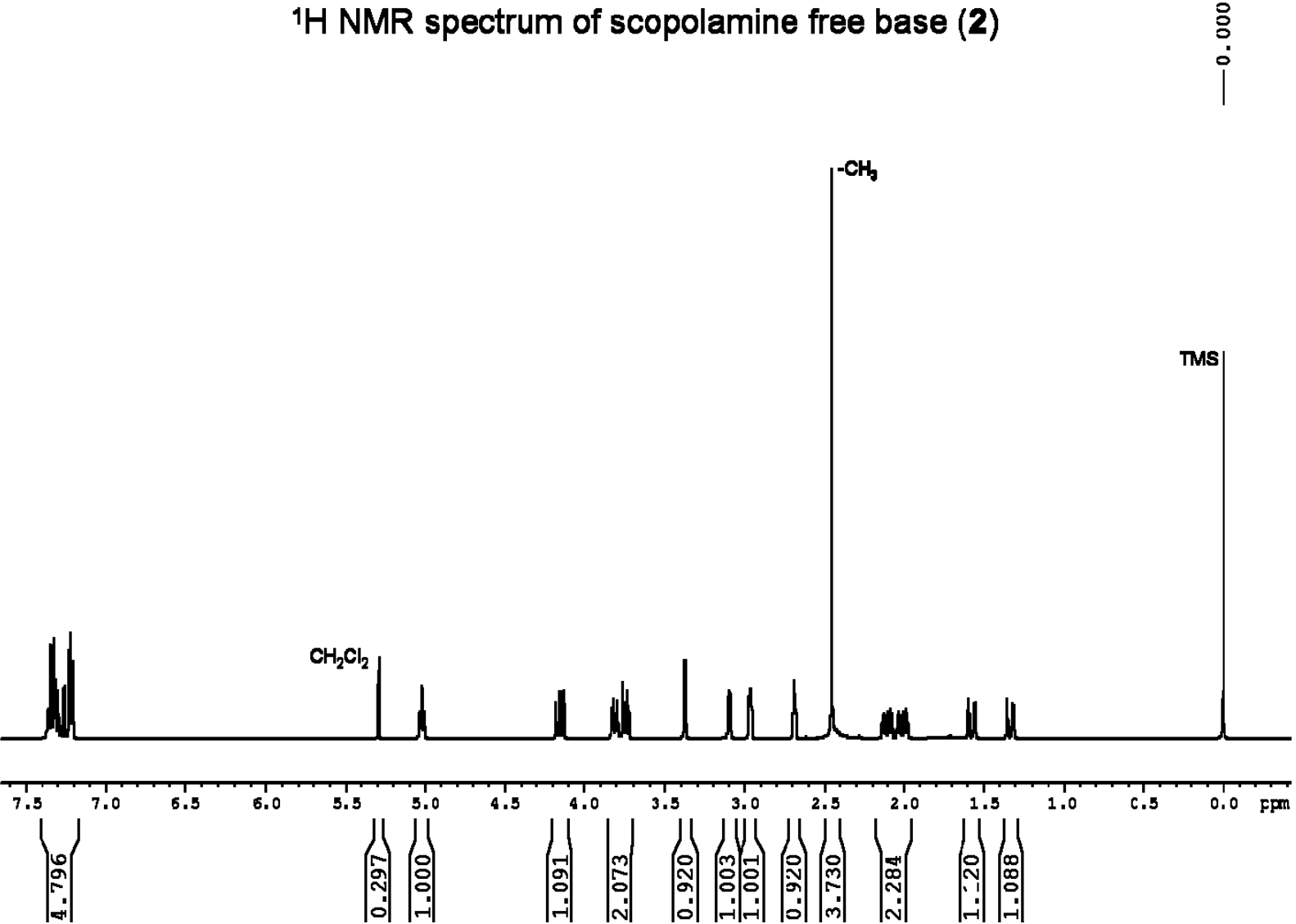


MS/MS fragmentation of atropine N-oxide (20)

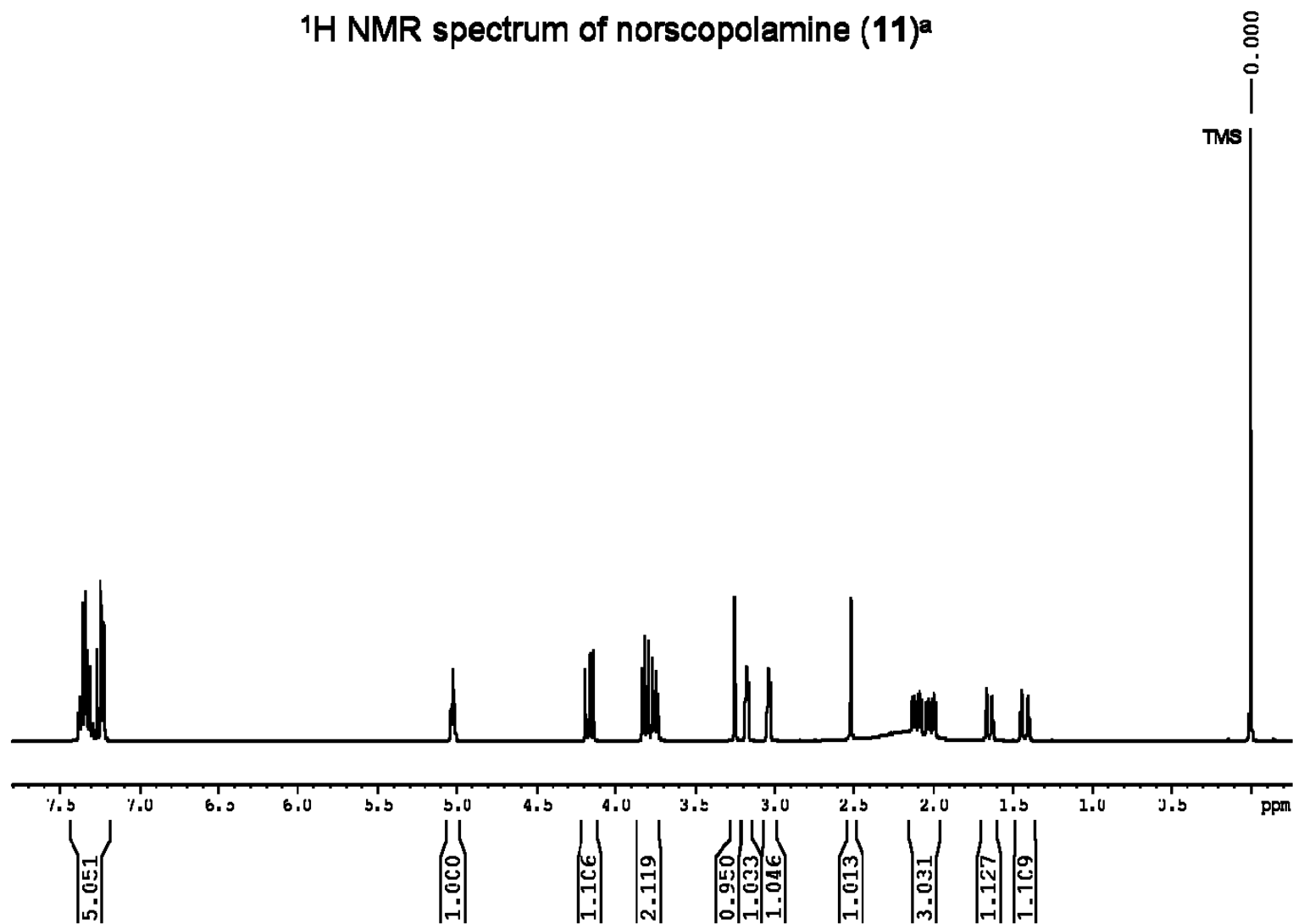


MS/MS fragmentation of *N*-formyl-noratropine (**22**)

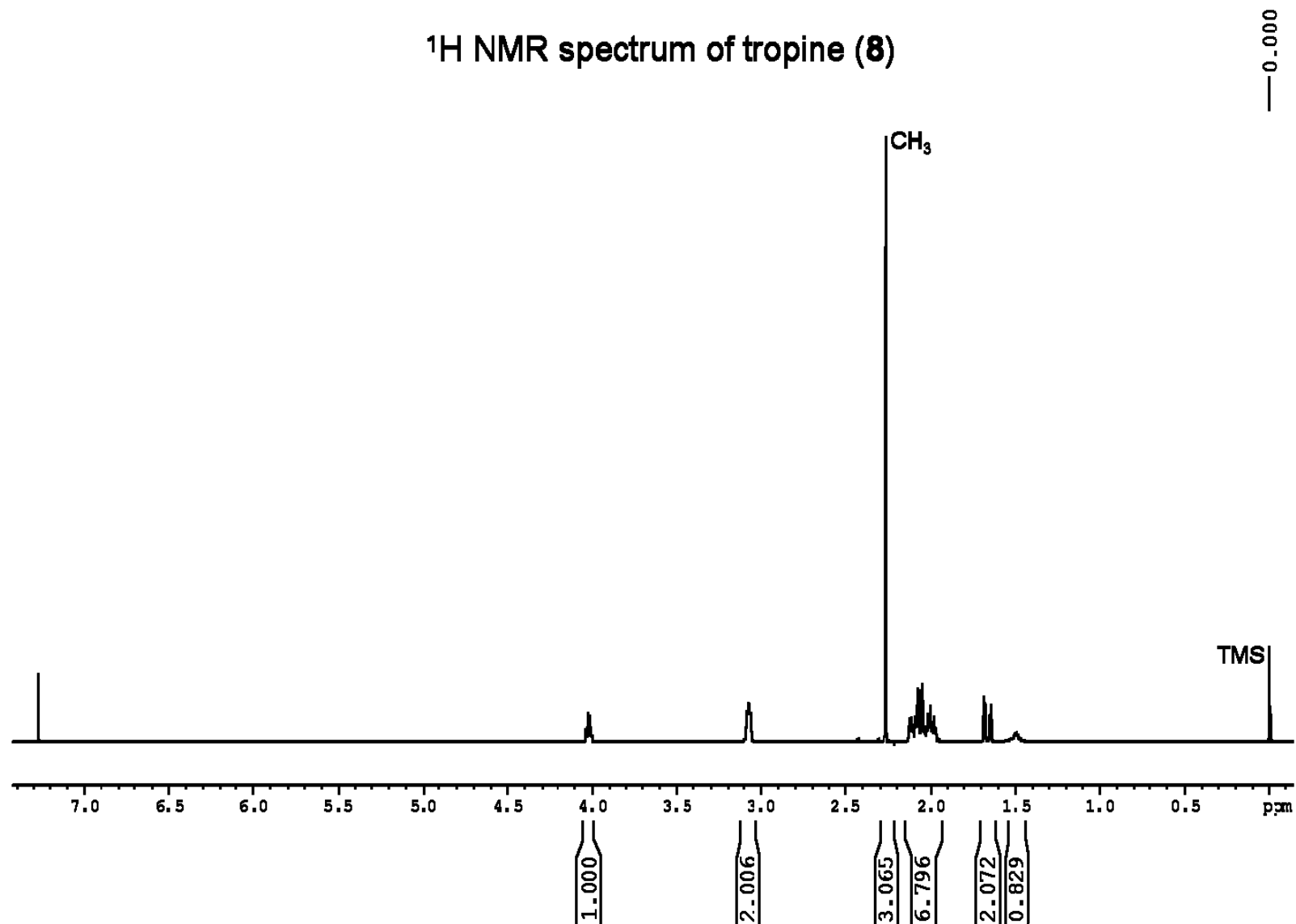




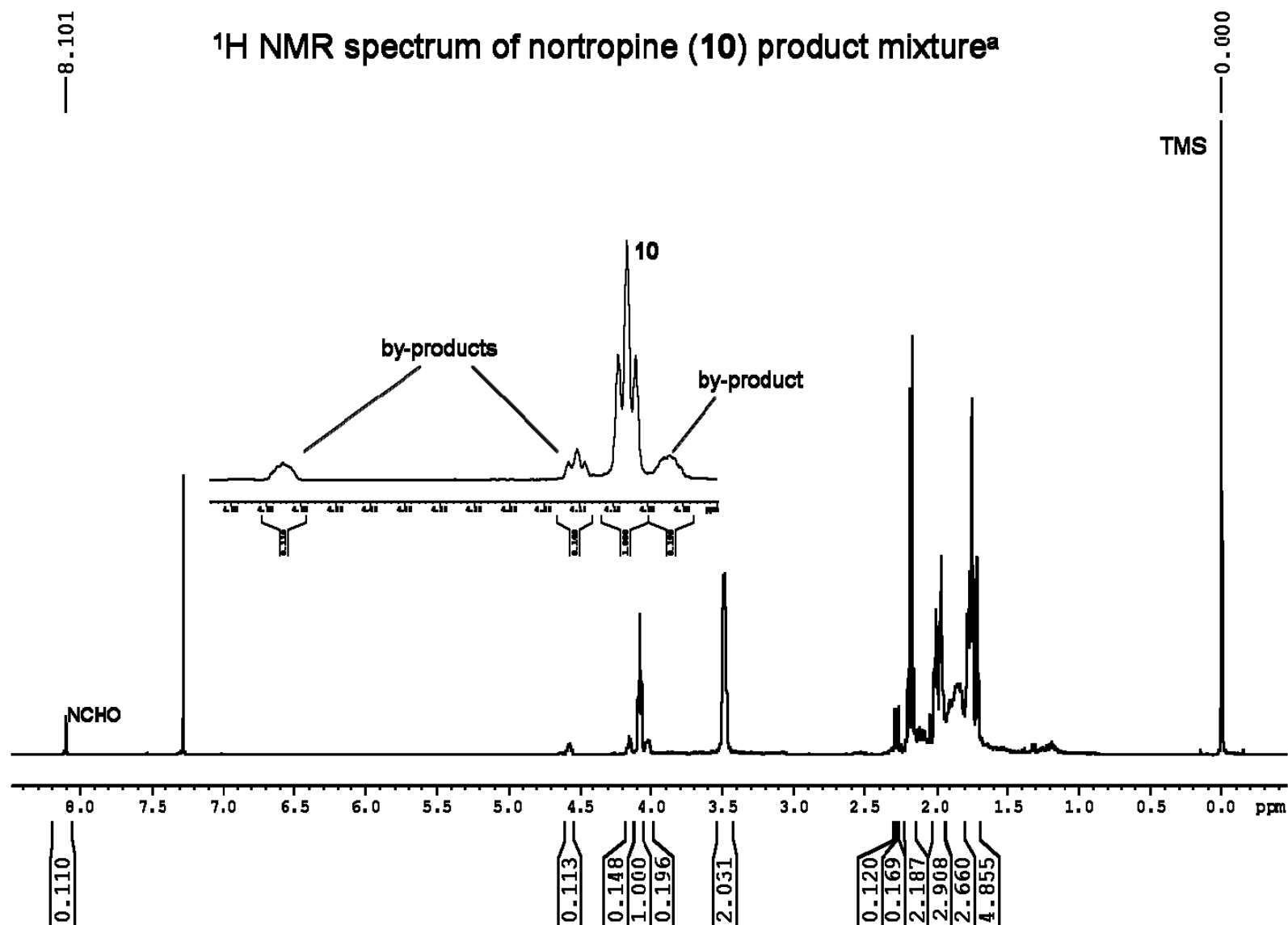
¹H NMR spectrum of norscopolamine (11)^a



a) 0.9 mol% 18, 3.30 mmol scopolamine, 165 mmol H₂O₂, 30 mL ethanol, 1 h

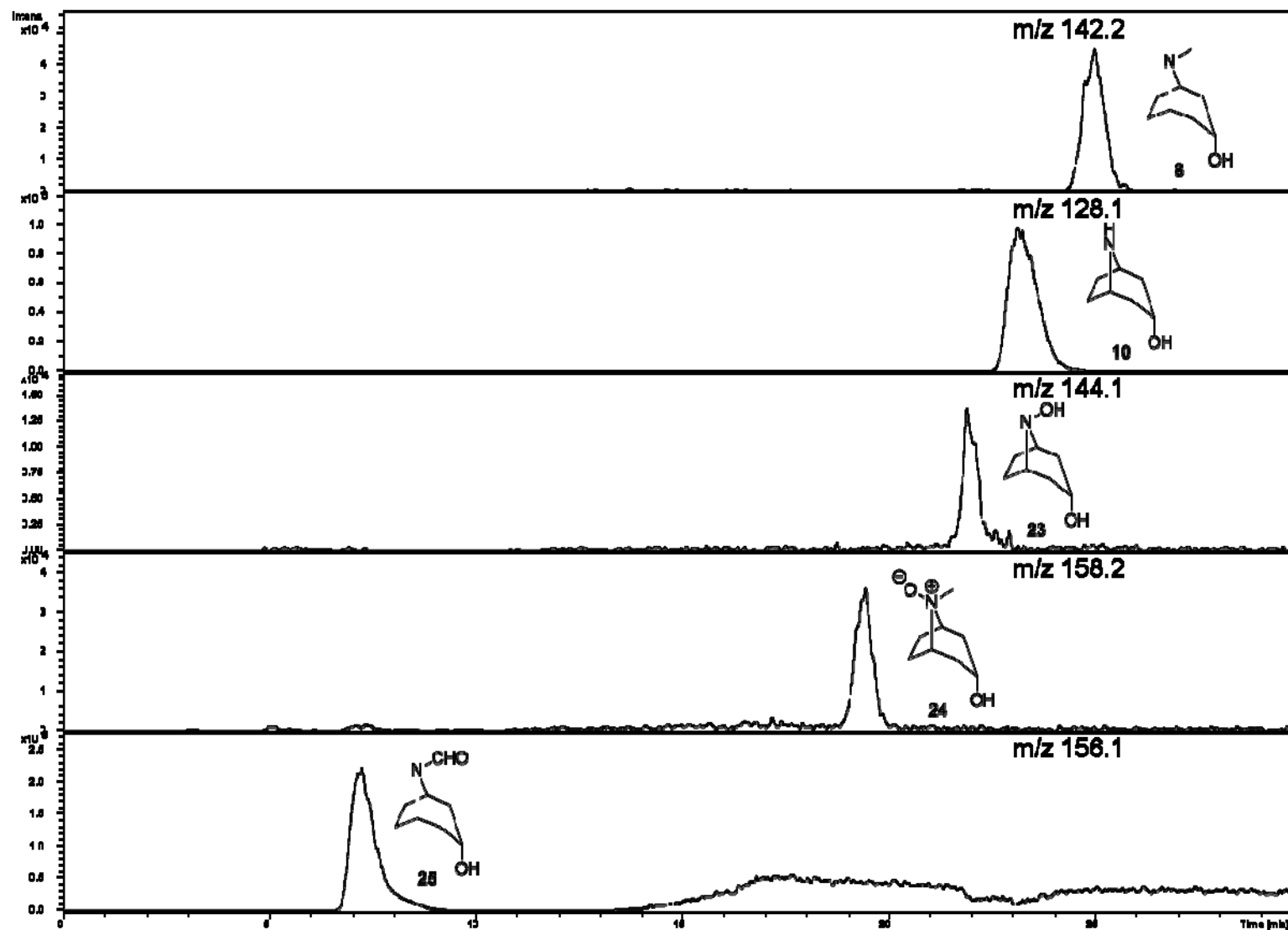


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LC-MS of nortropine (10) product mixture^a



^a) 0.71 mmol tropine, 35 mmol H₂O₂, 0.9 mol% 18, 6 mL EtOH, 1 h