
Design, Synthesis, and Biological Evaluation of Phenol Bioisosteric Analogues of 3-Hydroxymorphinan

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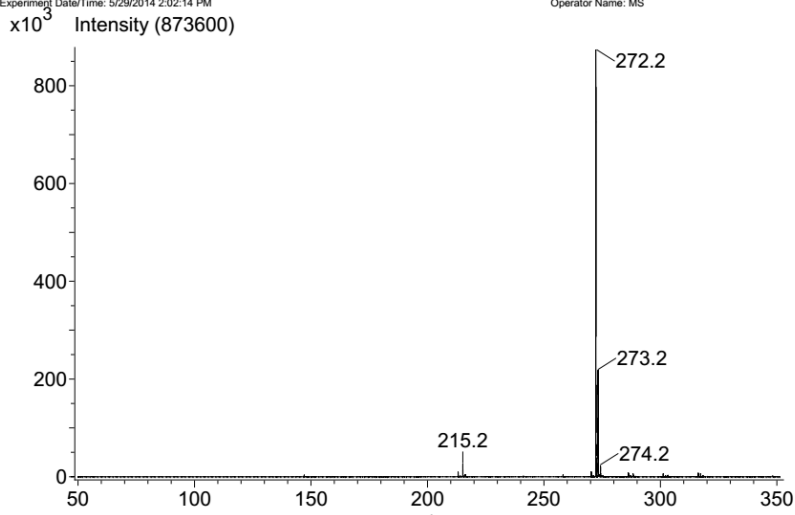
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MS and NMR spectra of synthesized imidazolone-morphinan and intermediates

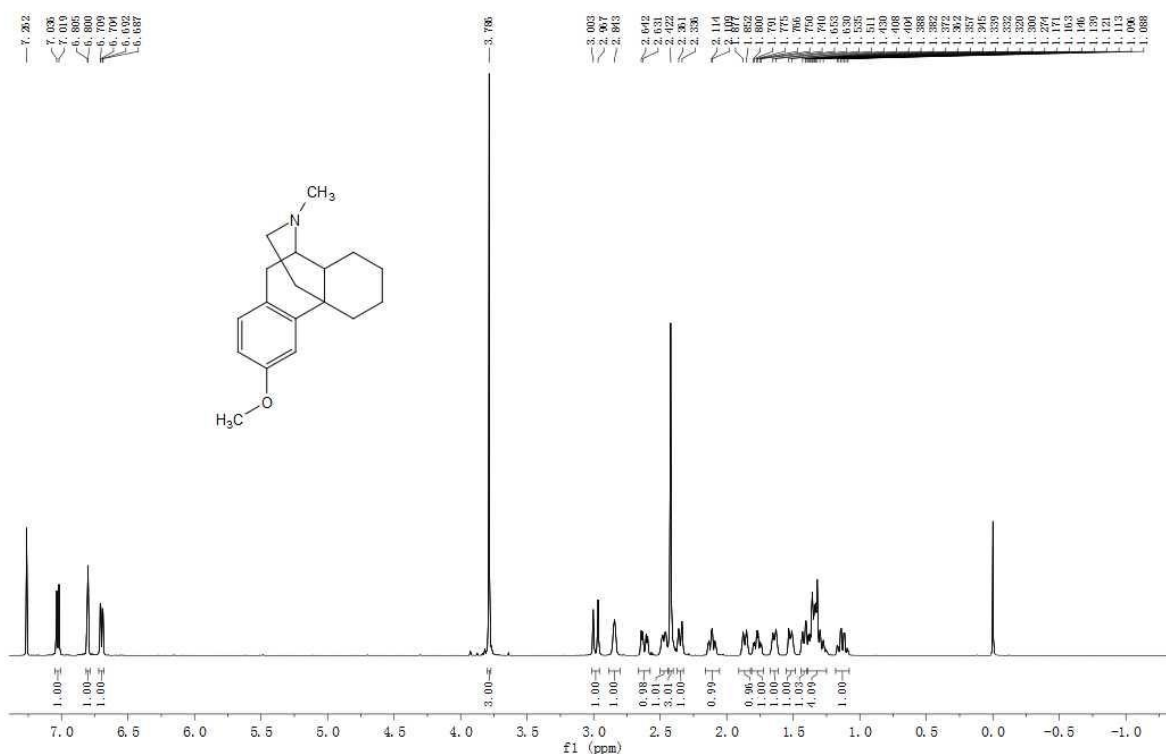
JEOL AccuTOF CS (JMS T100CS)

National Research Center for Analysis of Drugs and Metabolites

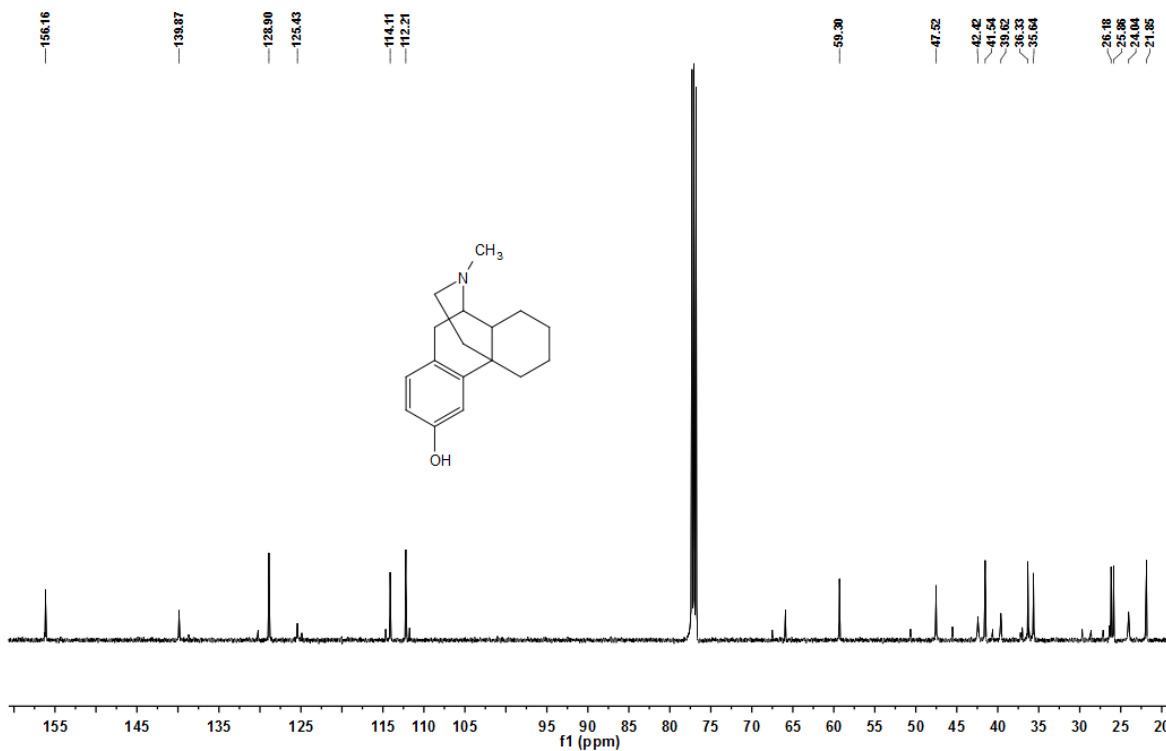
Acq. Data Name: HM-140526
Internal Sample Id:
Ionization Mode: ESI+
MS Calibration Name: TFANA_ESI+-1000
Reduction History: Subtract[Correct Base(5.0%);Average(MS[1] 0.3090..0.4000);D:\TESTDATA\TEST2013\20140529-BK8.1.0;Average(MS[1] 0.2810..0.3170)-1.0*Average(MS[...
Experiment Date/Time: 5/29/2014 2:02:14 PM
Orifice1 Volt Sweep: 60V
Acquired m/z Range: 50.0..1000.0
Spec. Record Interval: 1.0[s]
Ring Lens Volt: 20[V]
Time of Maximum: 0.510[min]
Operator Name: MS



BRUKER AV-III-500 1H-NMR HM-140526 IN CDCL3

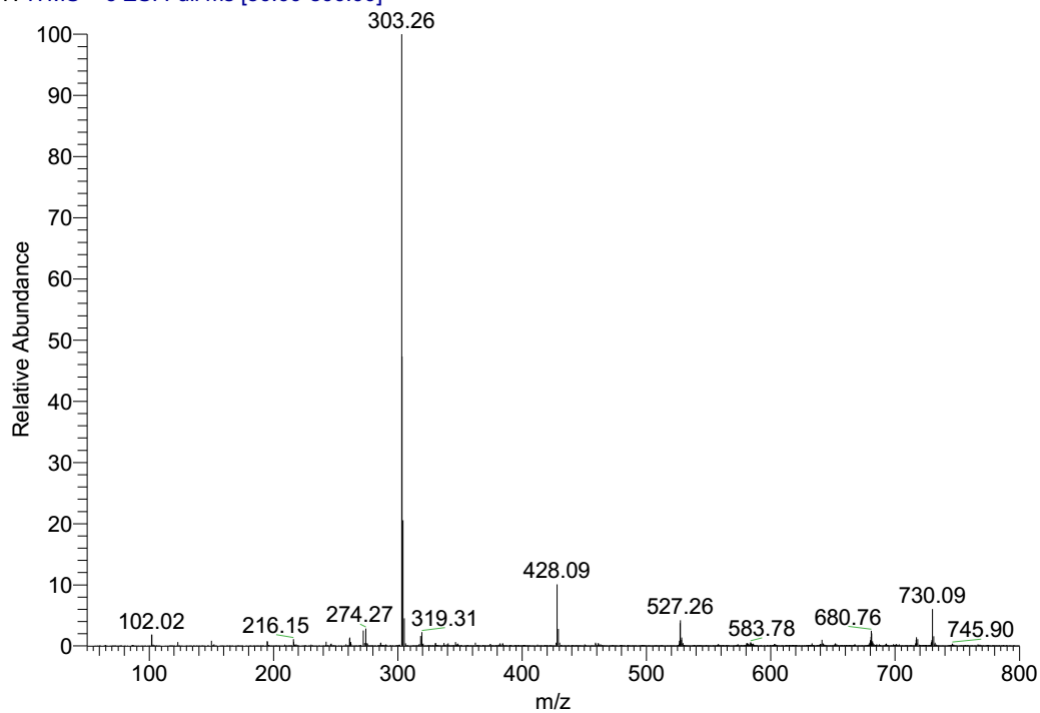


BRUKER AV-III-500 20181222-HM-140531-1 13C-NMR CDCI3



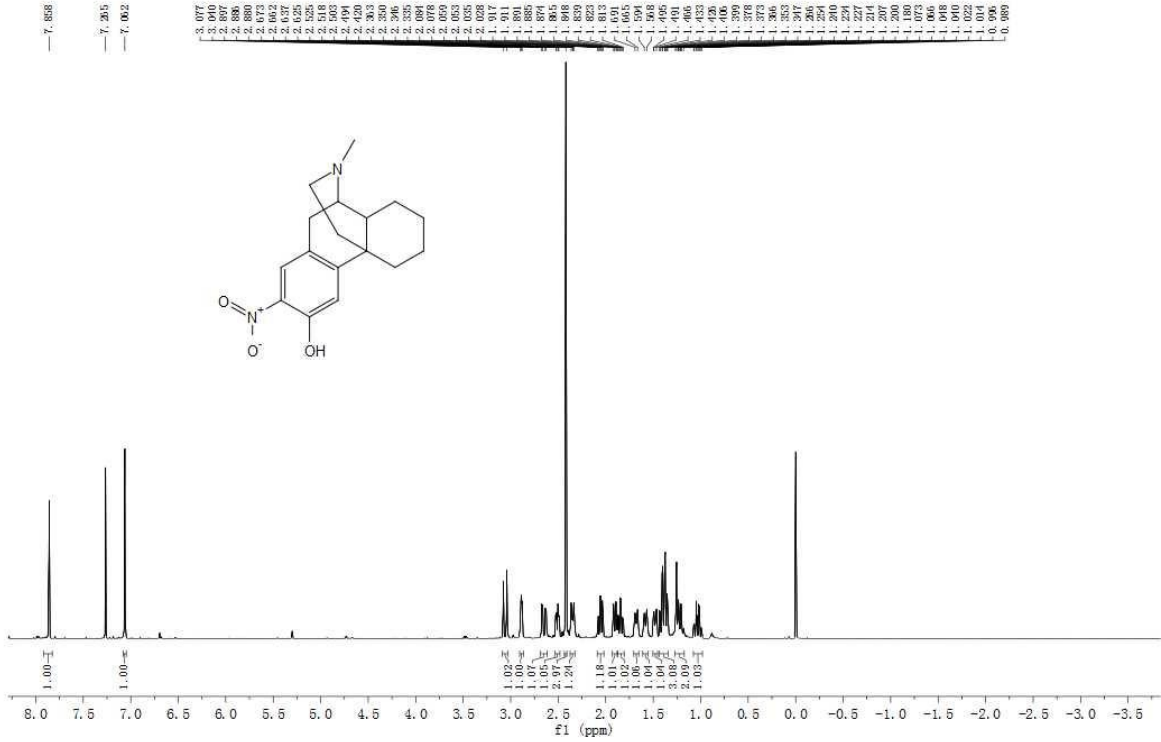
¹³C NMR spectra of compound dextrorphan (2)

HM-140603-3 #256-264 RT: 0.56-0.58 AV: 9 SB: 195 0.32-0.49 , 0.70-0.95 NL: 3.44E6
T: ITMS + c ESI Full ms [50.00-800.00]



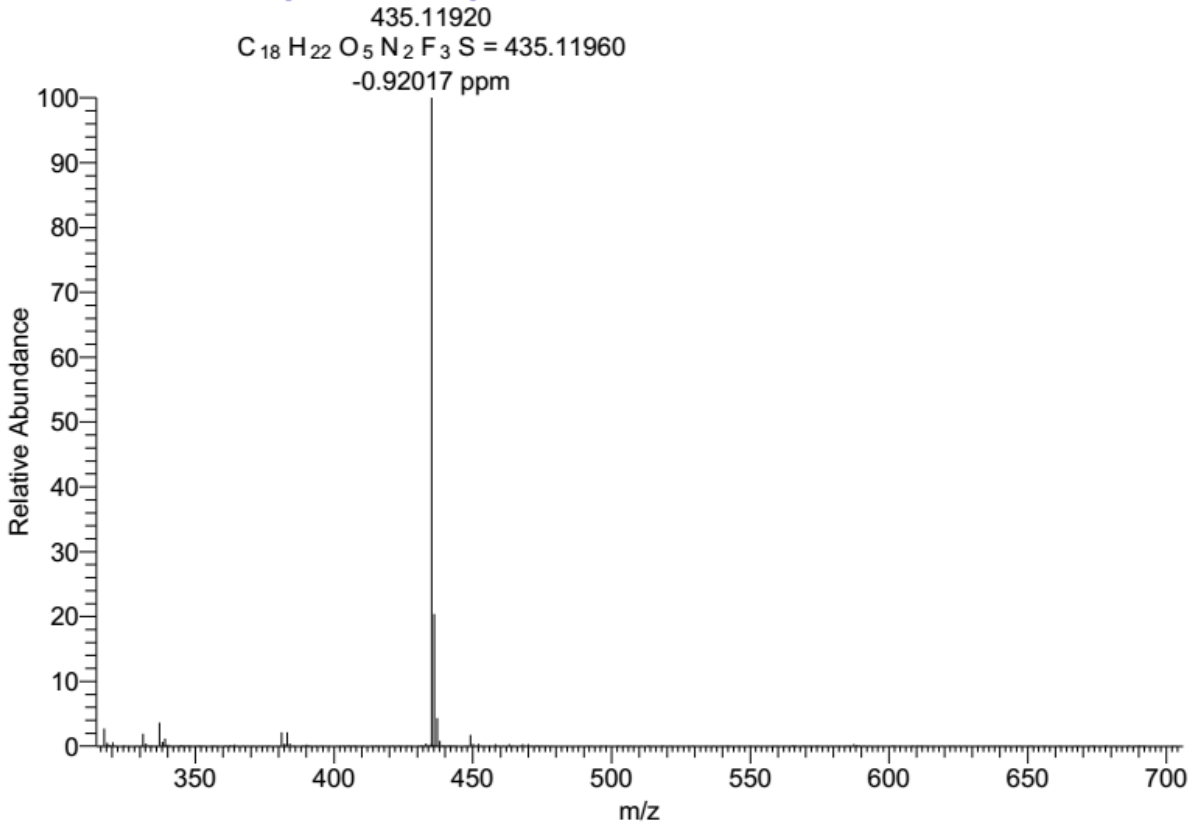
MS spectra of compound 2-nitro-3-hydroxyl-N-methylmorphinan (3)

BRUKER AV-III-500 1H-NMR HM-140603-3 IN CDCL3



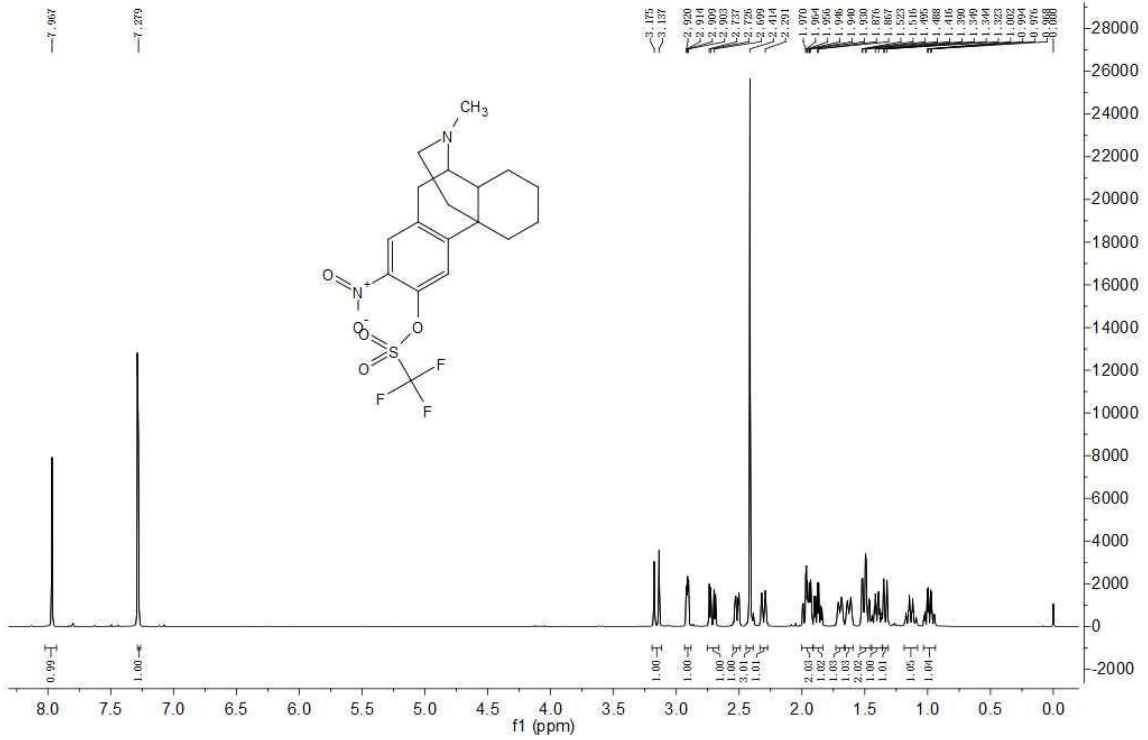
¹H NMR spectra of compound 2-nitro-3-hydroxyl-N-methylmorphinan (3)

HM-141110-2 -2 #53-62 RT: 0.71-0.80 AV: 10 NL: 4.50E8
T: FTMS + c ESI Full ms [150.00-1000.00]



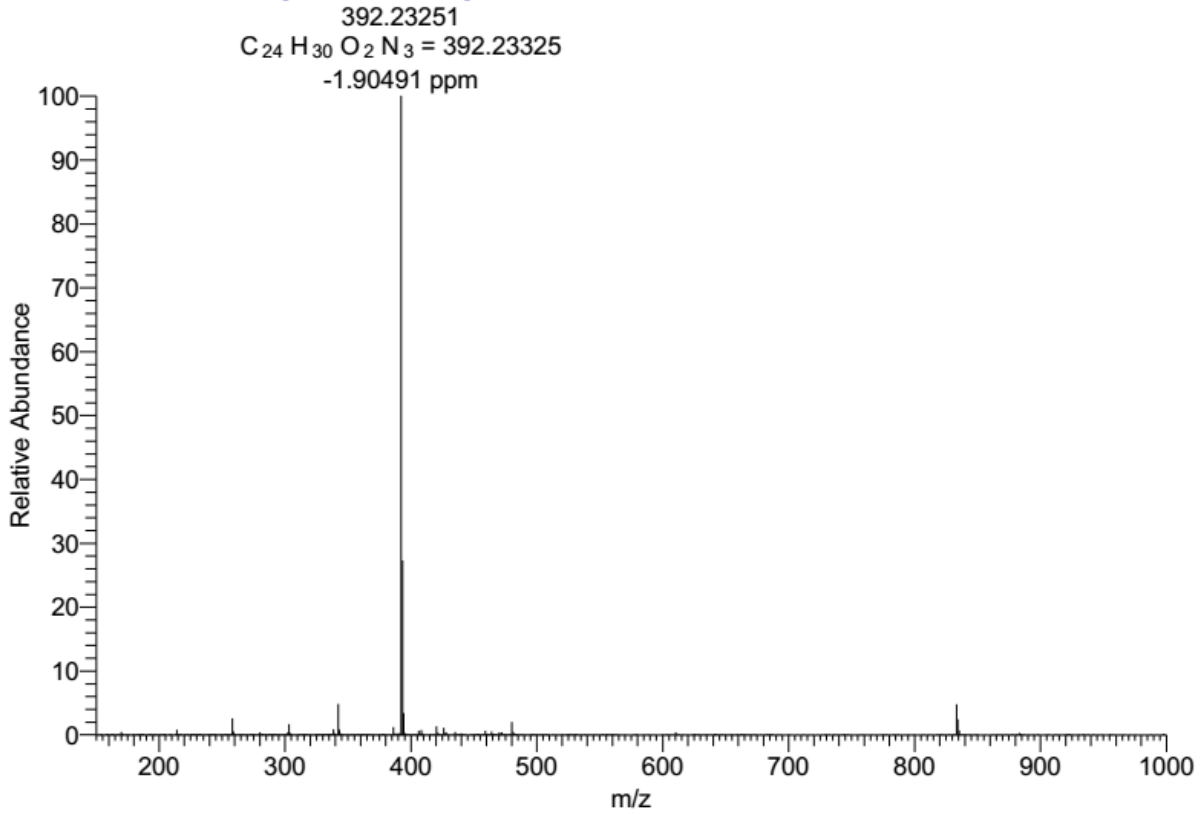
HRMS spectra of compound 2-Nitro-N-methyl-3-trifluoromethanesulfonatmorphinan ester (4)

BRUKER AV-III-500 1H-NMR HM-141110 IN CDCL3



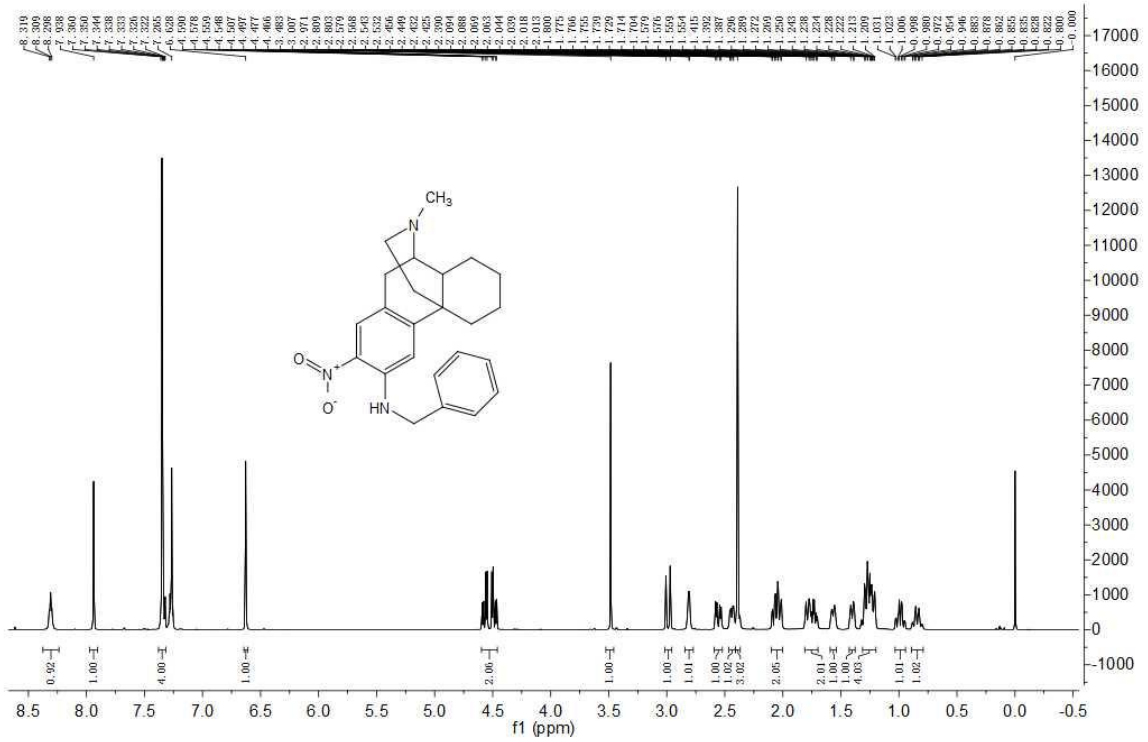
¹H NMR spectra of compound 2-Nitro-N-methyl-3-(trifluoromethanesulfonyloxy)morphinan ester (4)

HM-141119_-2 #57-62 RT: 0.83-0.89 AV: 6 NL: 1.80E8
T: FTMS + c ESI Full ms [150.00-1000.00]



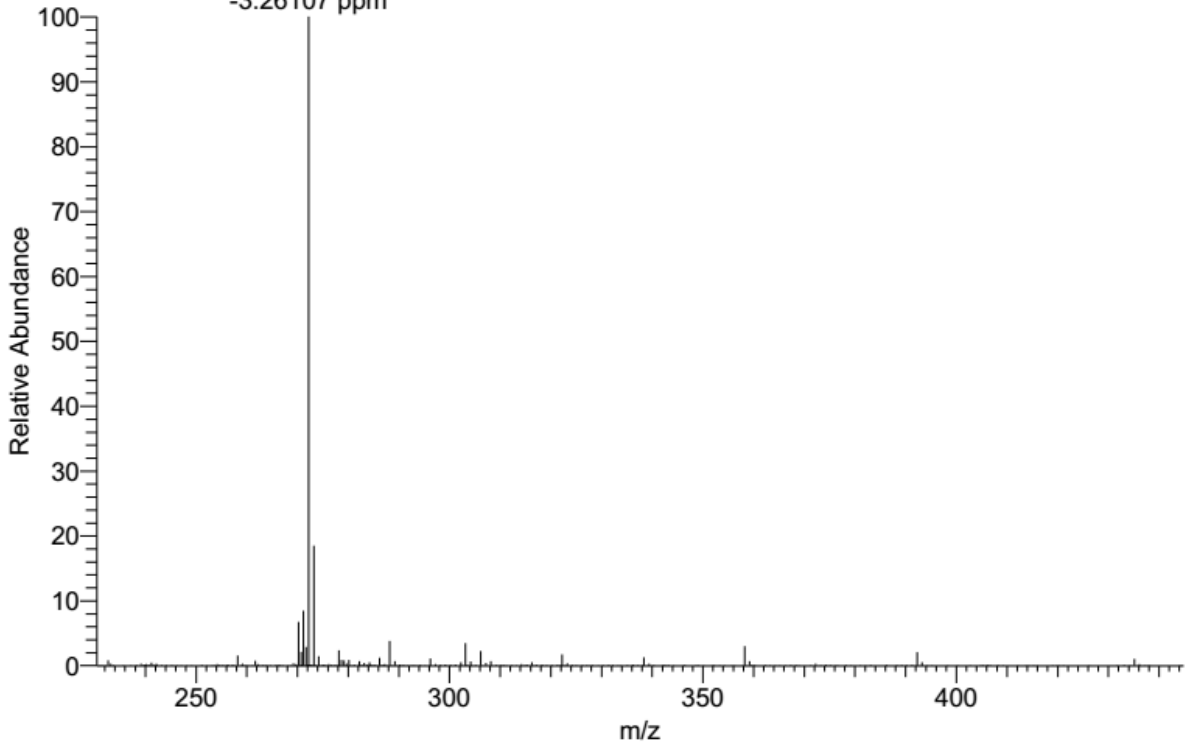
HRMS spectra of compound 2-nitro-3-benzylamino-N-methylmorphinan (5)

BRUKER AV-III-500 1H-NMR HM-141119 IN CDCL3

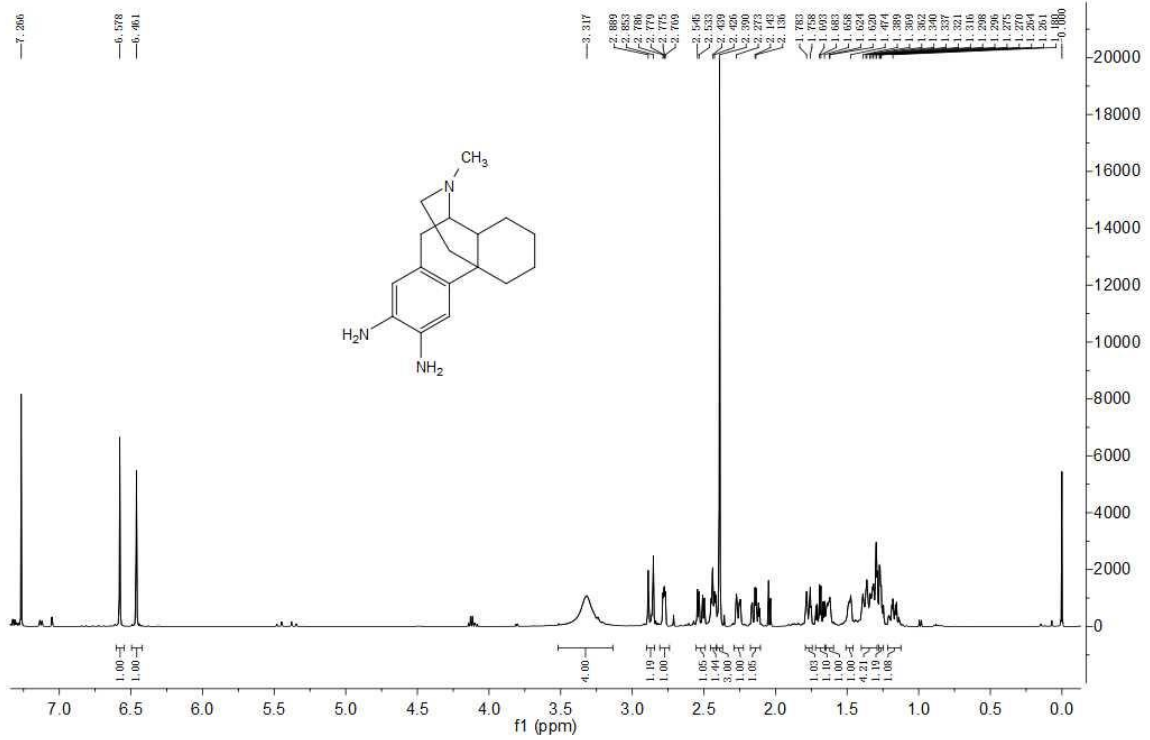


HM-141208_-2 #217-220 RT: 2.66-2.68 AV: 4 NL: 7.48E7
T: FTMS + c ESI Full ms [150.00-1000.00]

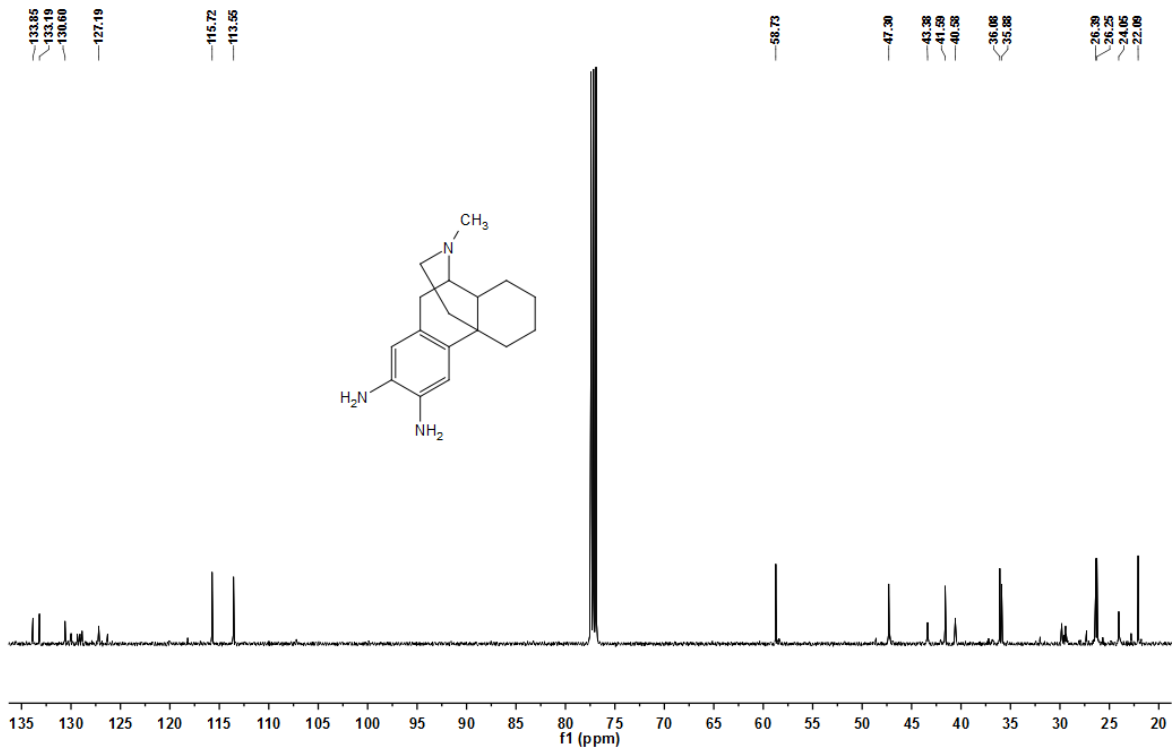
272.21124
C₁₇H₂₆N₃ = 272.21212
-3.26107 ppm



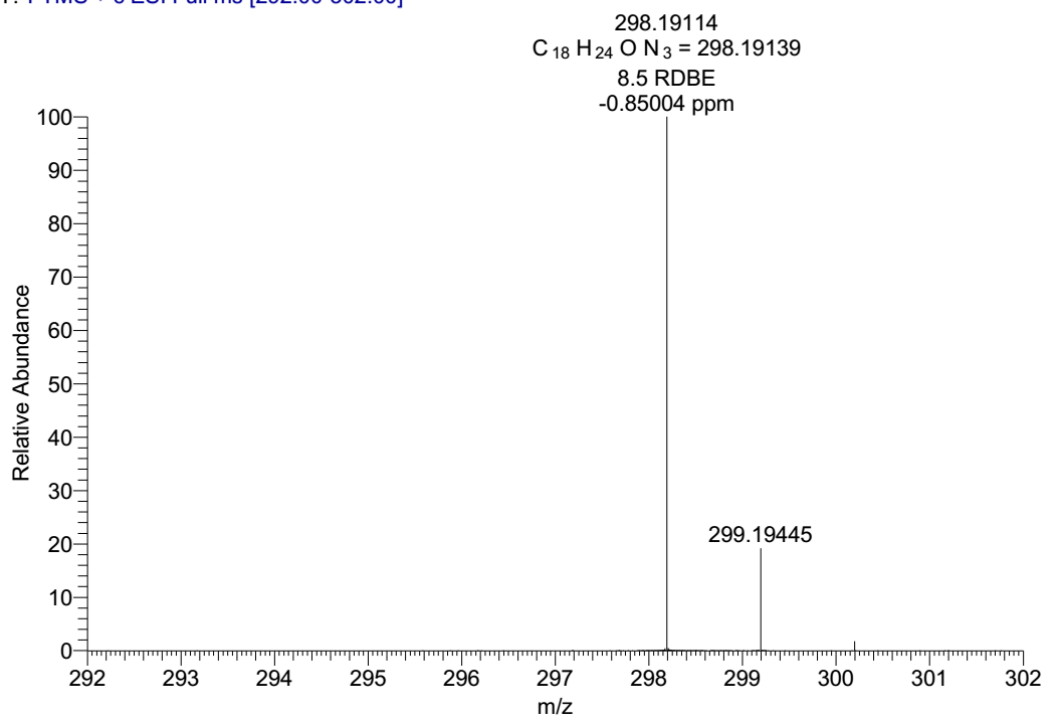
BRUKER AV-III-500 1H-NMR HM-141208 IN CDCL3



20181226-HM-141208 13C-NMR CDCl3

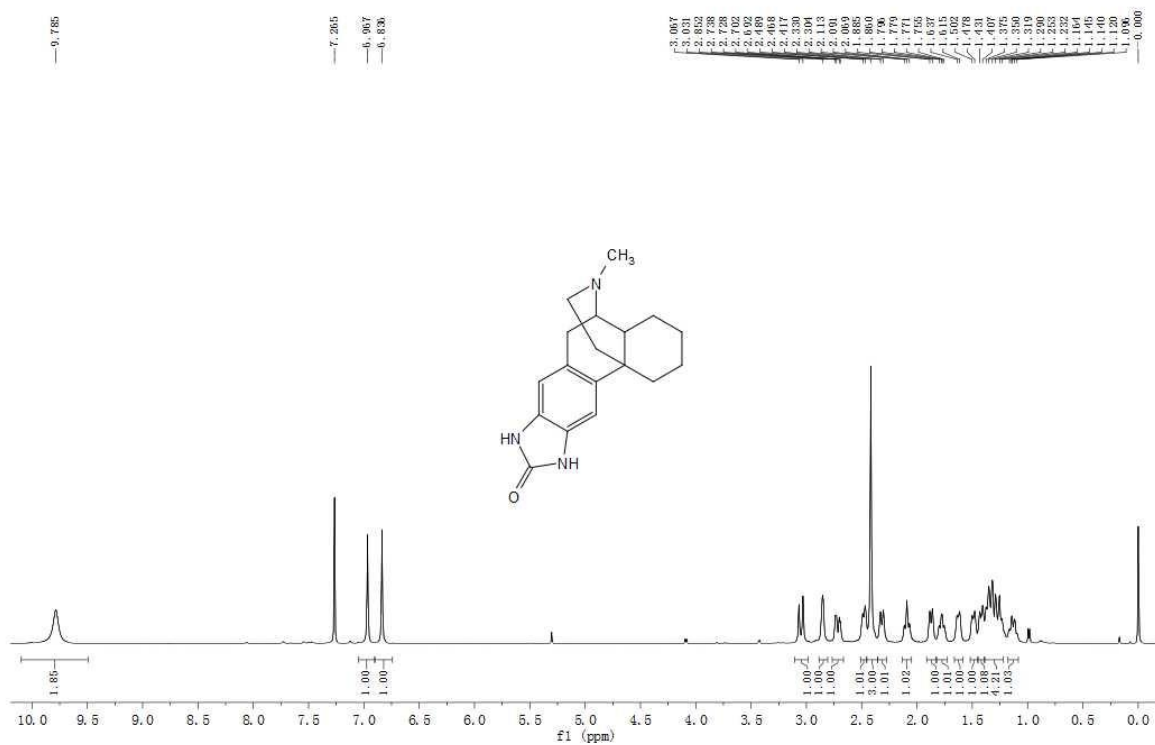


HM-141210 #48-54 RT: 0.56-0.63 AV: 7 SB: 21 0.37-0.48 , 0.73-0.85 NL: 4.44E7
T: FTMS + c ESI Full ms [292.00-302.00]



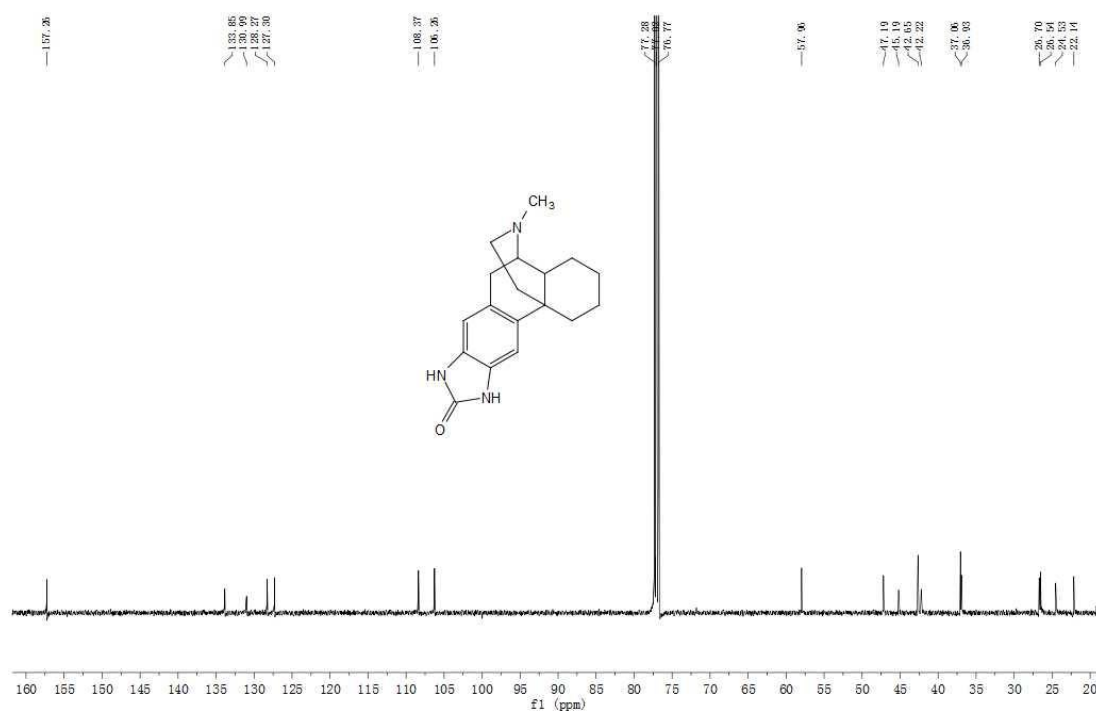
HRMS spectra of compound imidazolone-N-methylmorphinan (7)

BRUKER AV-III-500 1H-NMR HM-141210 IN CDCL3



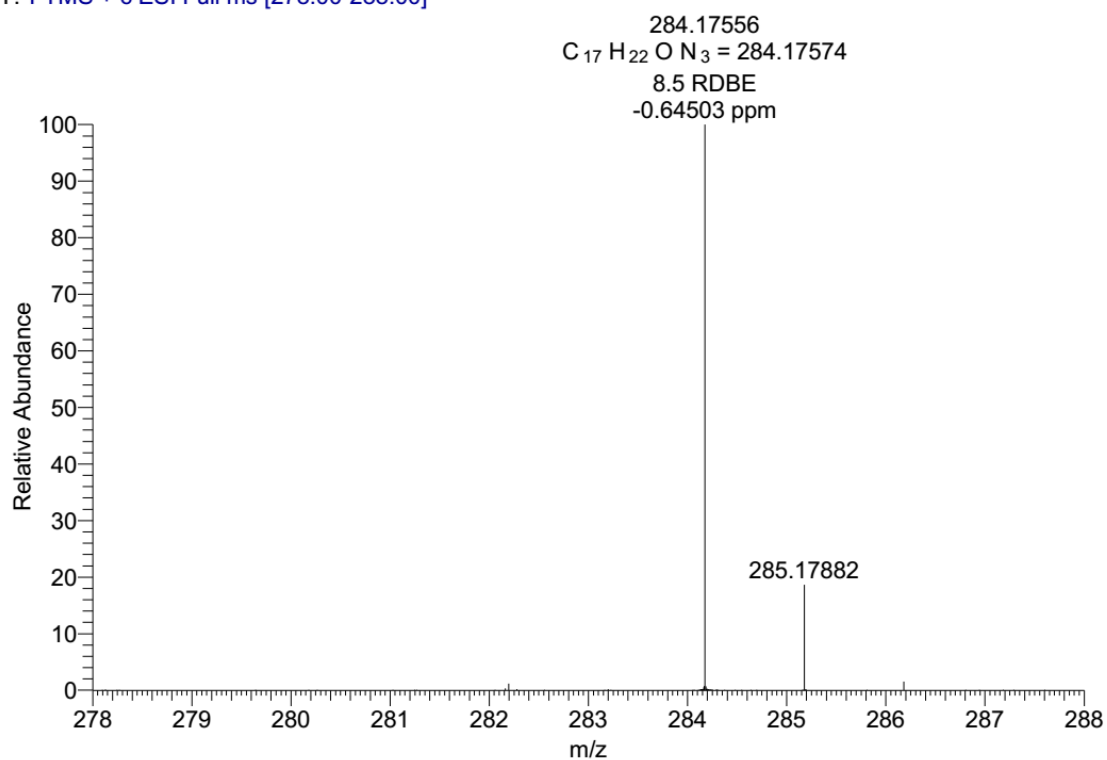
¹H NMR spectra of compound imidazolone-N-methylmorphinan (7)

BRUKER AV-III-500 13C-NMR HM-141210 IN CDCL3



¹³C NMR spectra of compound imidazolone-N-methylmorphinan (7)

HM-150115 #73-77 RT: 0.87-0.92 AV: 5 SB: 30 0.46-0.63, 1.13-1.30 NL: 1.24E7
T: FTMS + c ESI Full ms [278.00-288.00]



HRMS spectra of compound imidazolone-morphinan (8)

