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Test purchase, synthesis and characterization of 2-methoxydiphenidine (MXP) and differentiation from its *meta*- and *para*-substituted isomers

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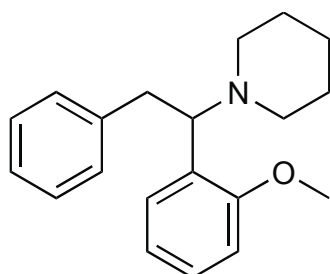
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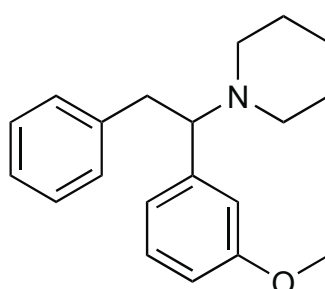
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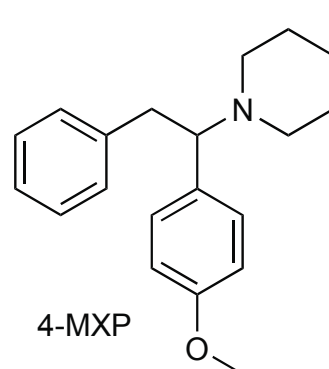
*Correspondence to: Simon D. Brandt, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, UK. E-Mail: s.brandt@ljmu.ac.uk



2-MXP
(2-MeO-diphenidine)



3-MXP



4-MXP

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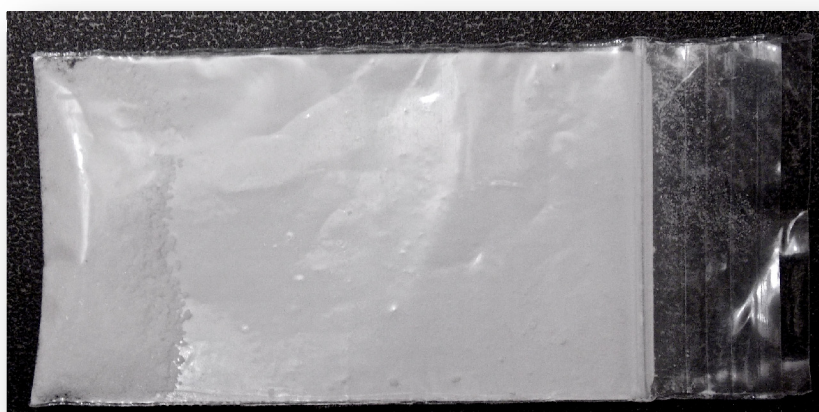
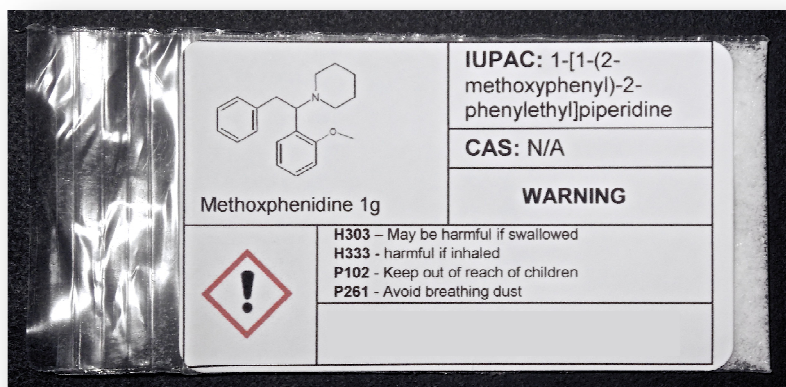
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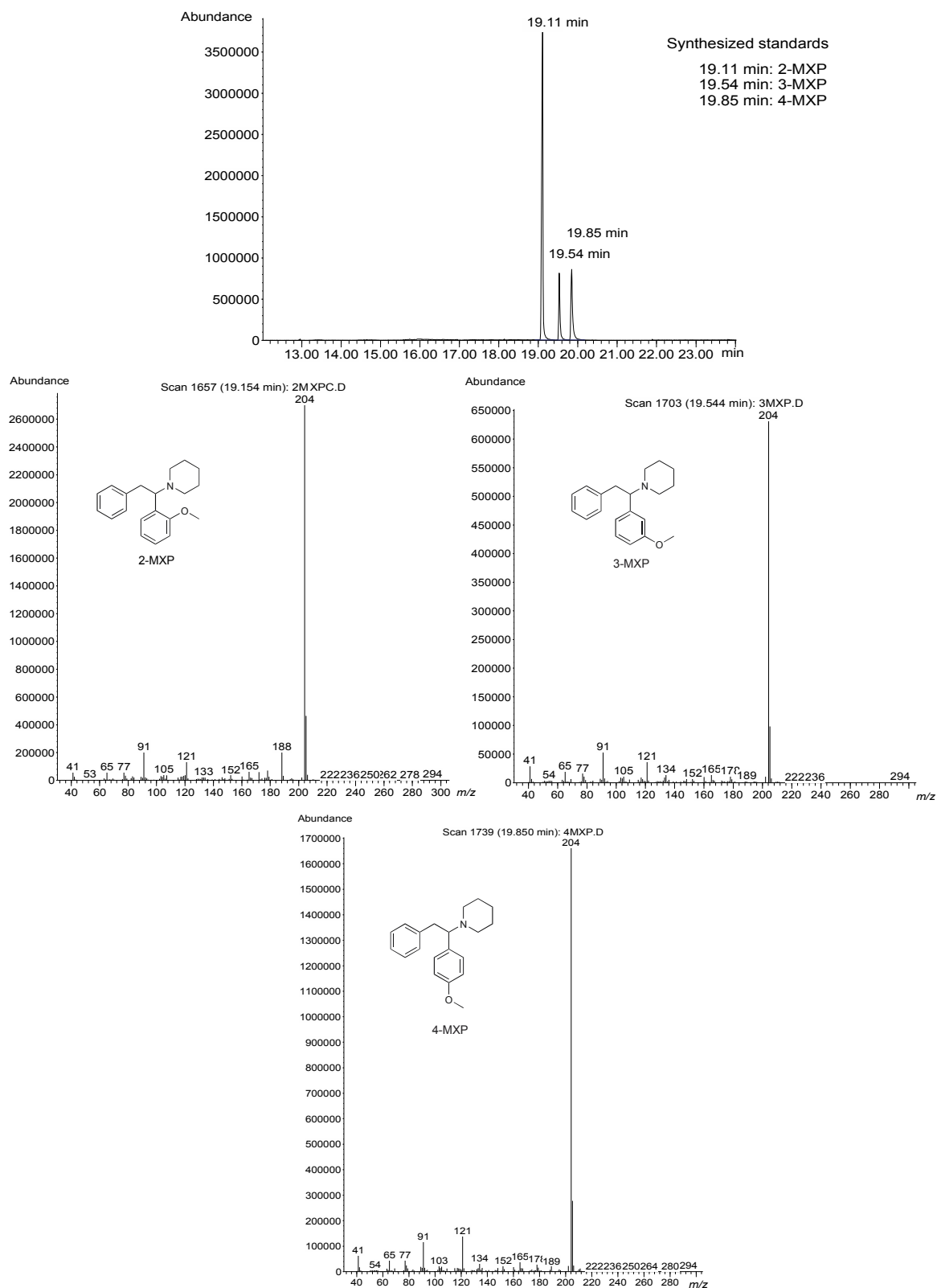
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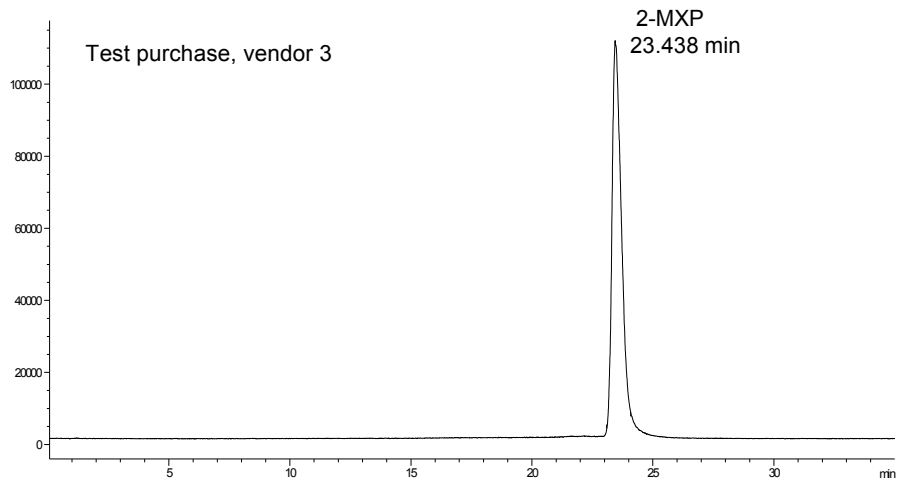
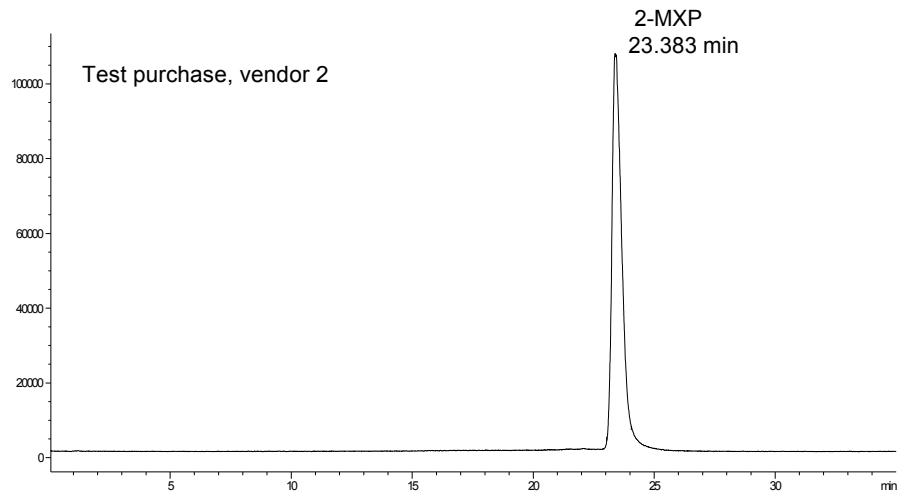
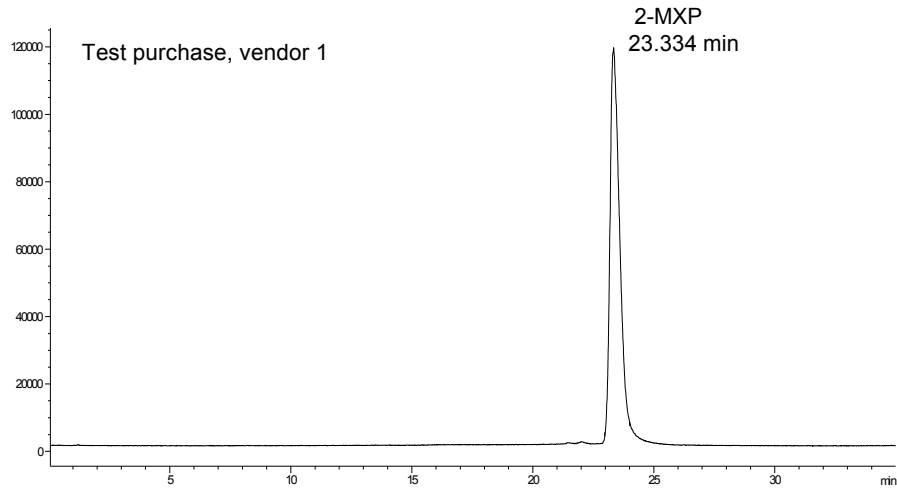
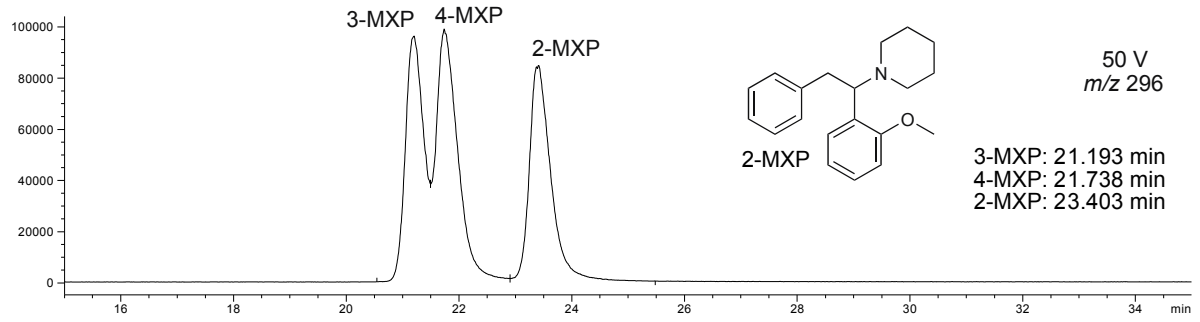
Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data



GC-EI-quadrupole mass spectra obtained from all three synthesized MXP isomers

Agilent 6980 GC coupled to an Agilent 5973 MSD (HP-5ms column, 30 m x 0.25 mm x 0.25 μ m). Helium carrier gas at a constant flow of 1 mL/min in splitless mode. Injection port and transfer line set at 250 $^{\circ}$ C and 280 $^{\circ}$ C. Oven temperature: 40 $^{\circ}$ C held for 1 min, ramped at 12 $^{\circ}$ C/min to 280 $^{\circ}$ C, held for 5 minutes, then ramped again at 20 $^{\circ}$ C/min to 300 $^{\circ}$ C and held for 3 min. The total run time was 30 min.

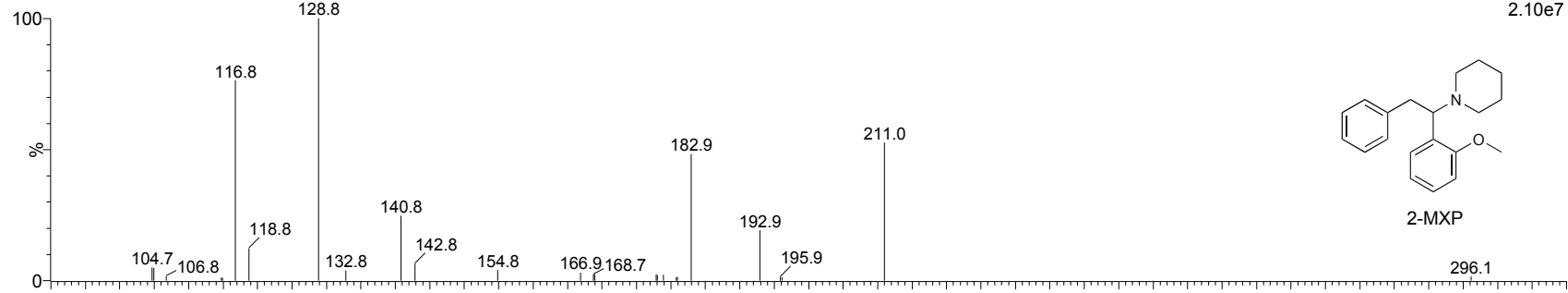
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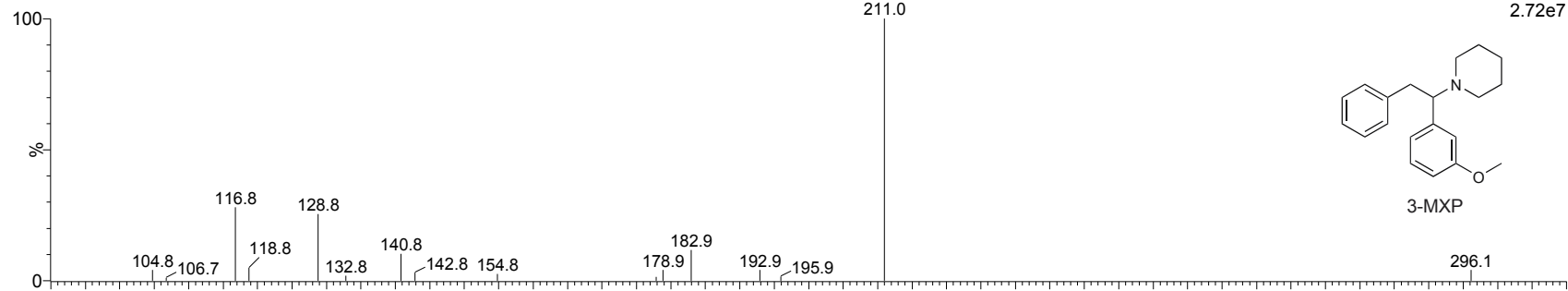
HPLC-SIM-MS traces of powdered 2-MXP sample s vs. synthesized standards

Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data

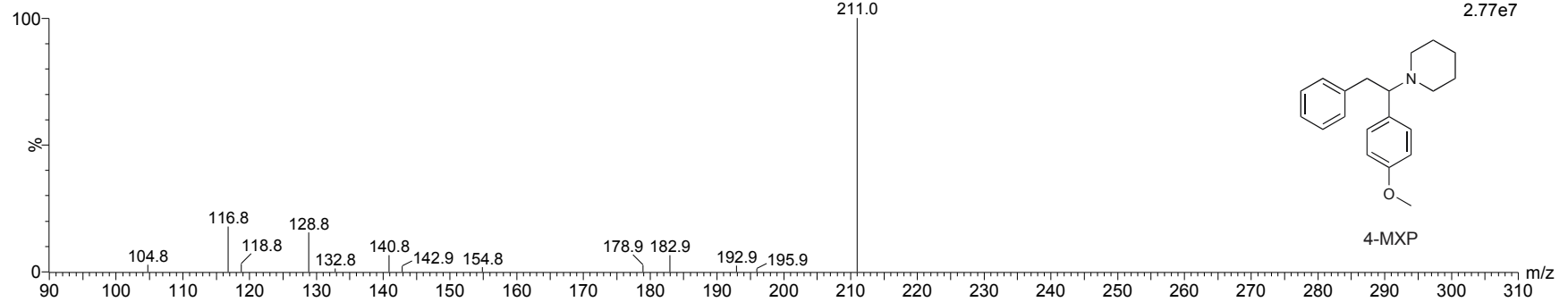
2-MXP MRM R 68 (0.686) Cn (Cen,2, 80.00, Ht); Cm (1:197)



3-MXP MRM R 133 (1.342) Cn (Cen,2, 80.00, Ht); Sm (SG, 2x1.00); Cm (1:197)

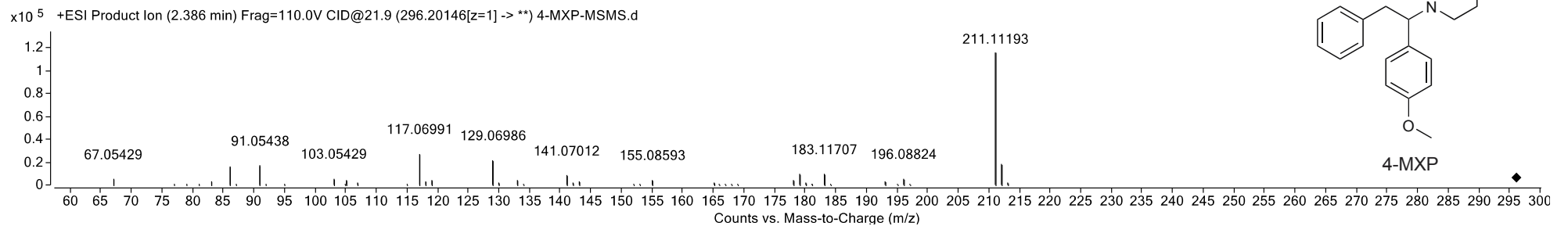
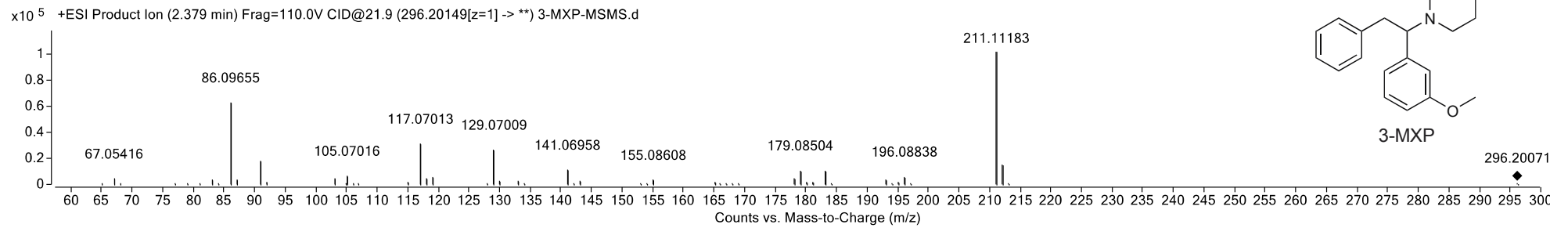
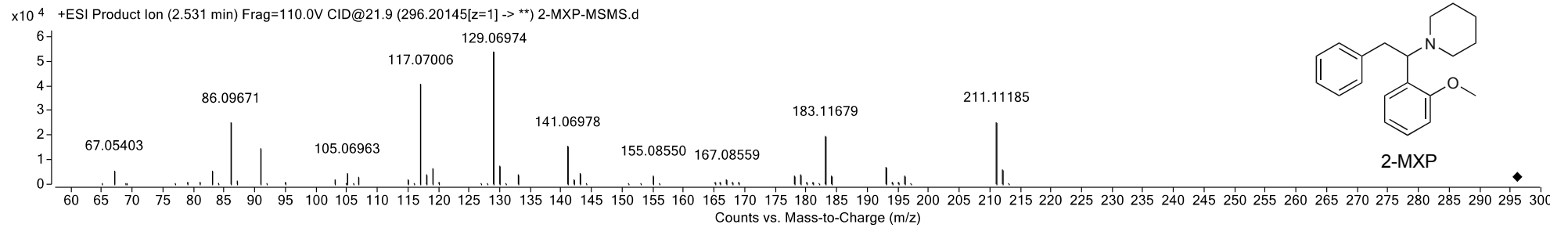


4-MXP MRM R 137 (1.382) Cn (Cen,2, 80.00, Ht); Sm (SG, 2x1.00); Cm (2:198)

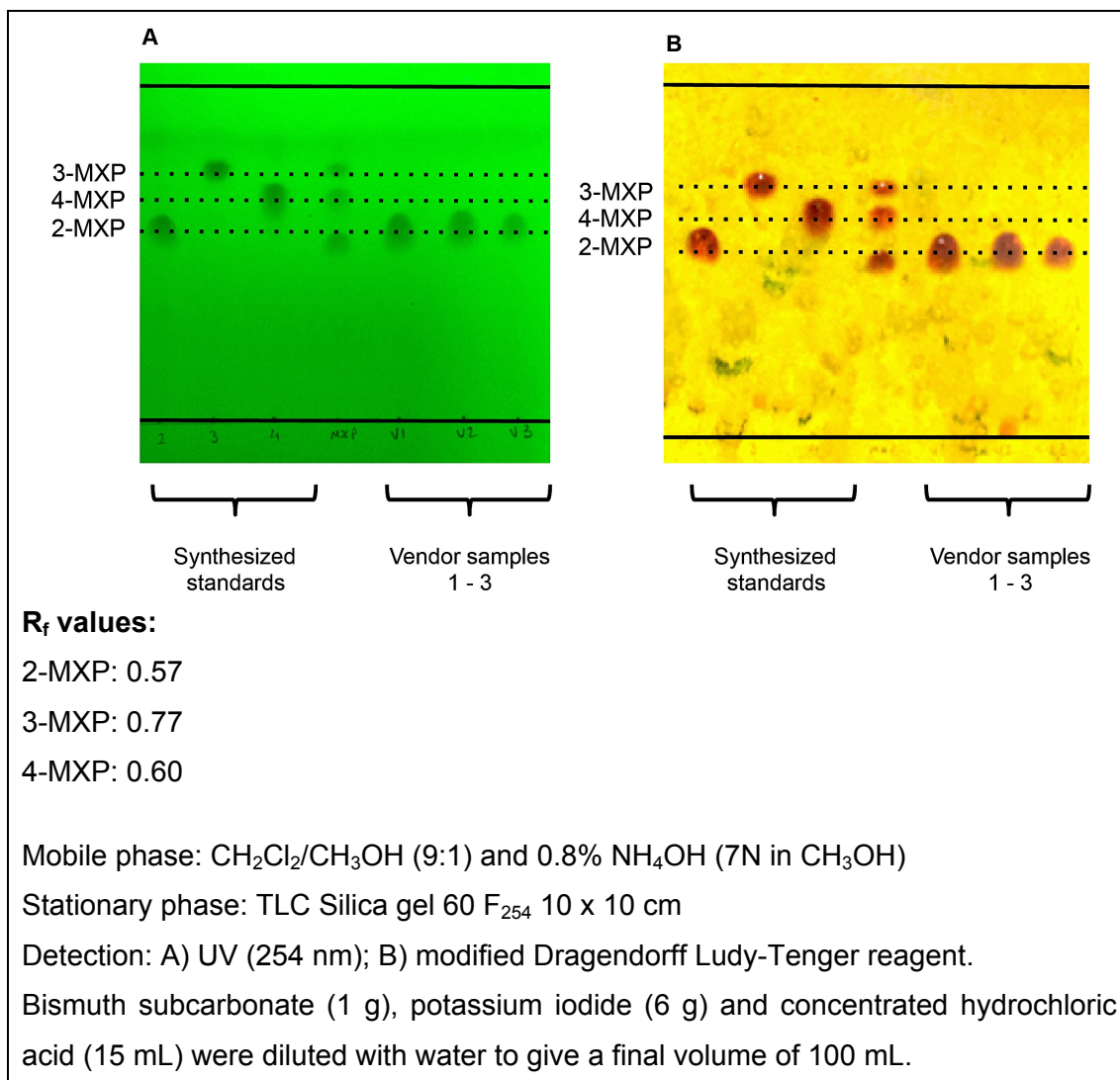


ESI-QqQ-MS/MS of synthesized MXP isomers

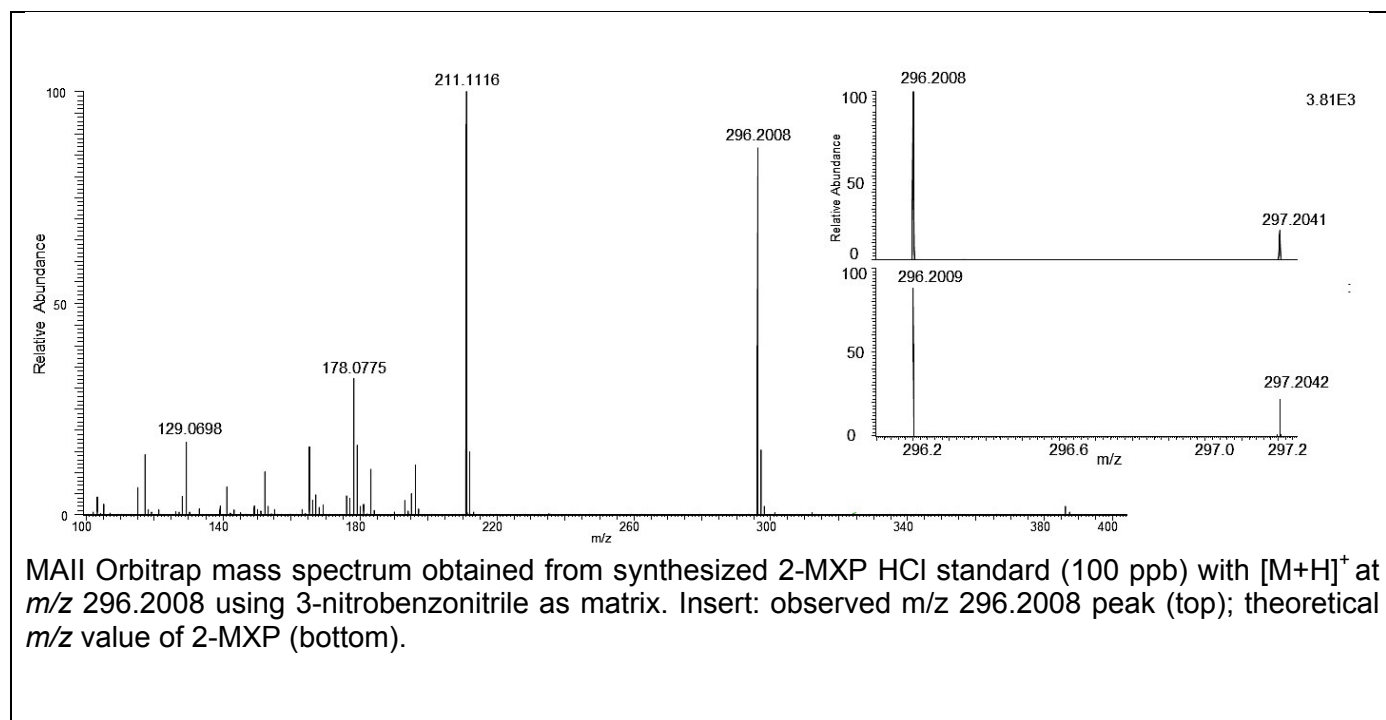
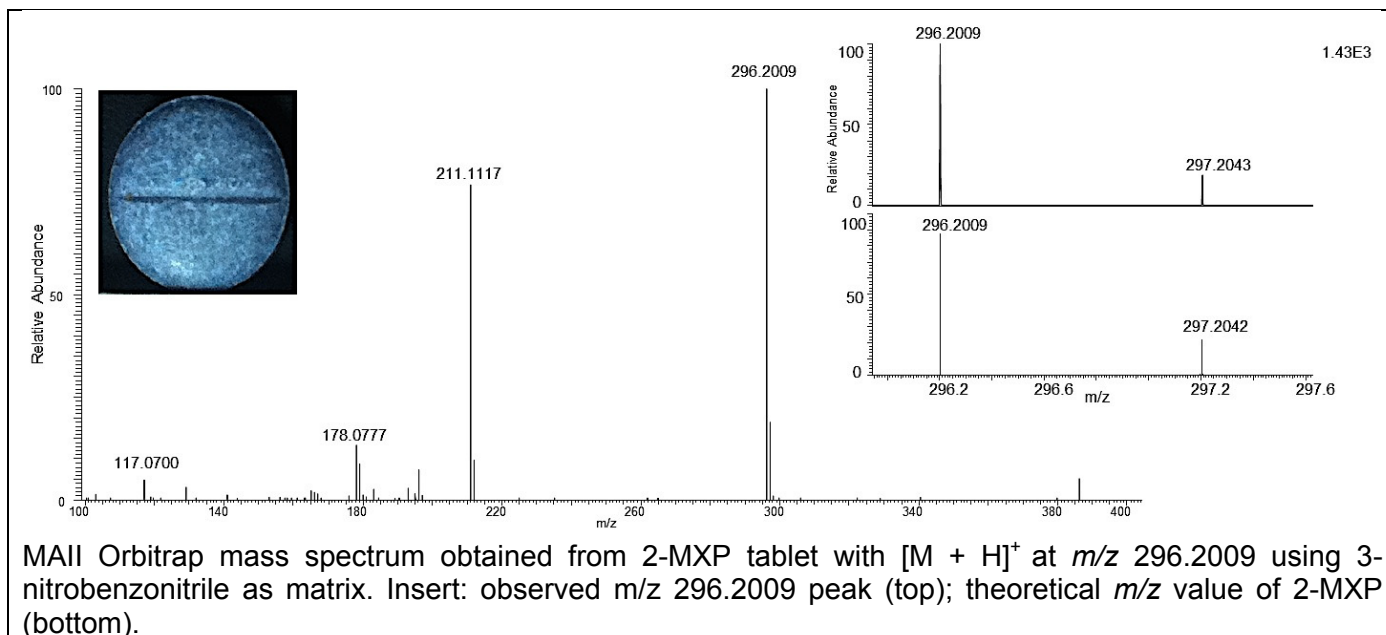
Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data



UHPLC-ESI-QTOF-MS/MS of synthesized MXP isomers

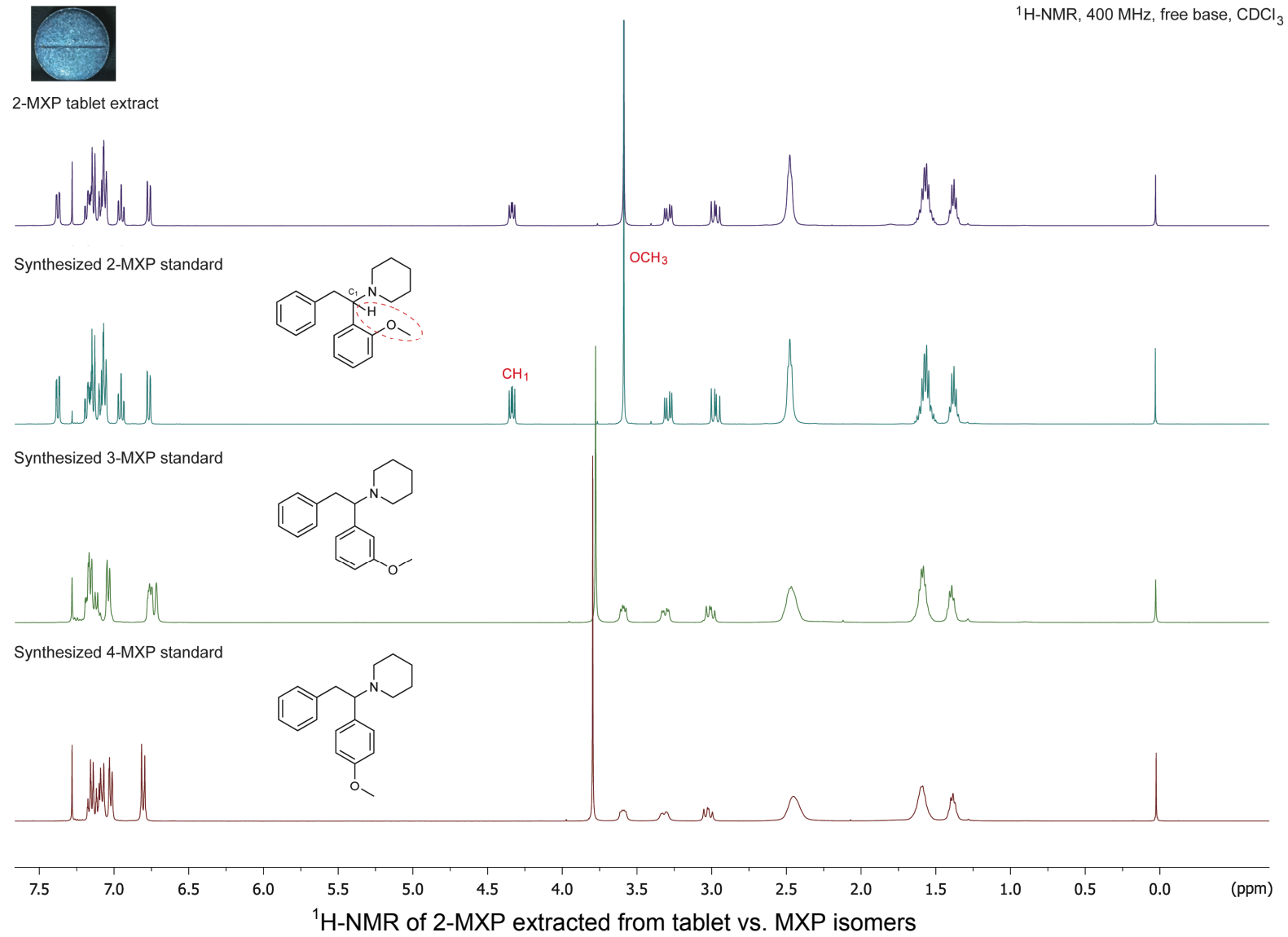


TLC analysis of powdered 2-MXP samples vs. synthesized standards

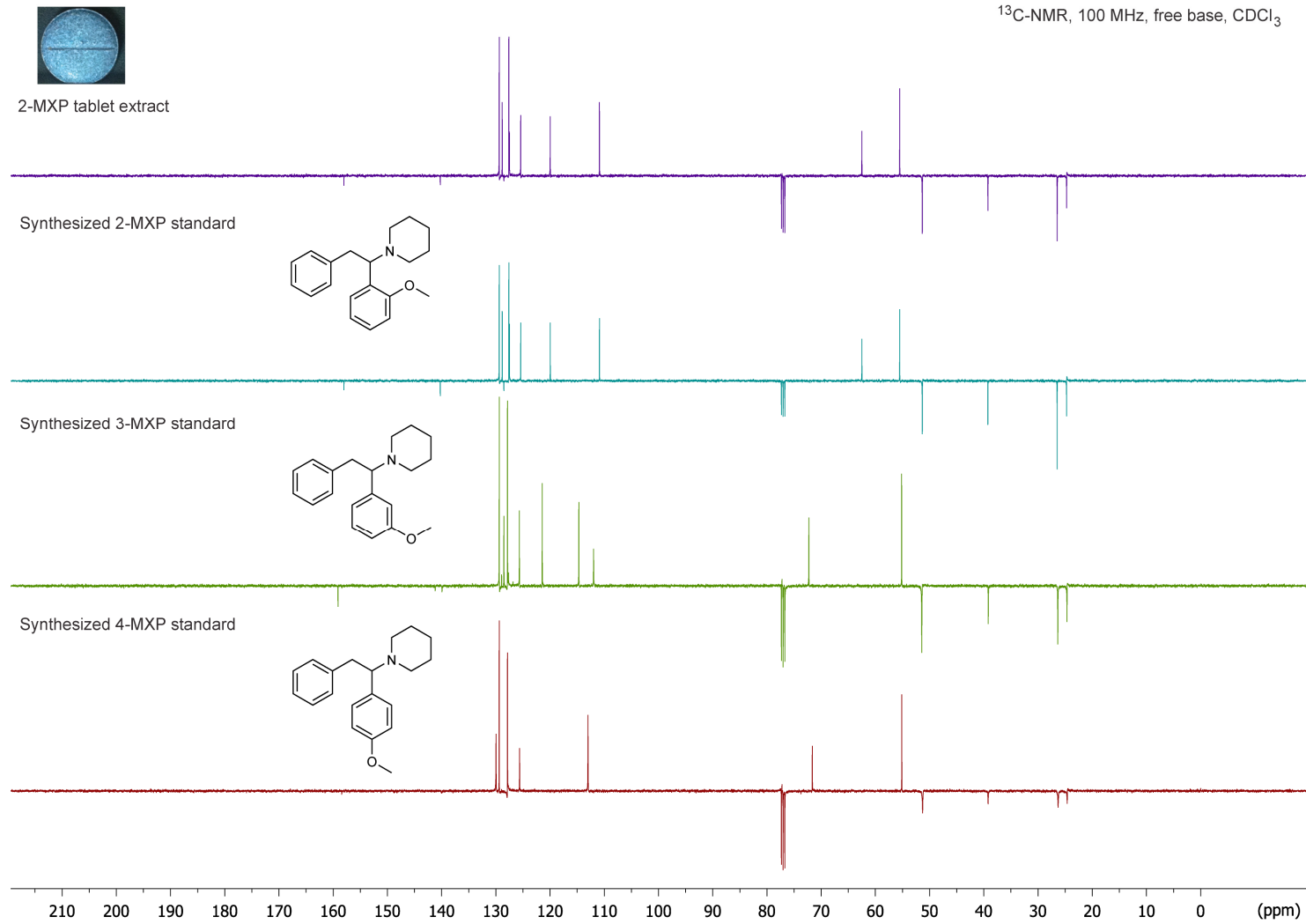


Matrix assisted inlet ionization mass spectra of 2-MXP tablet vs. 2-MXP standard

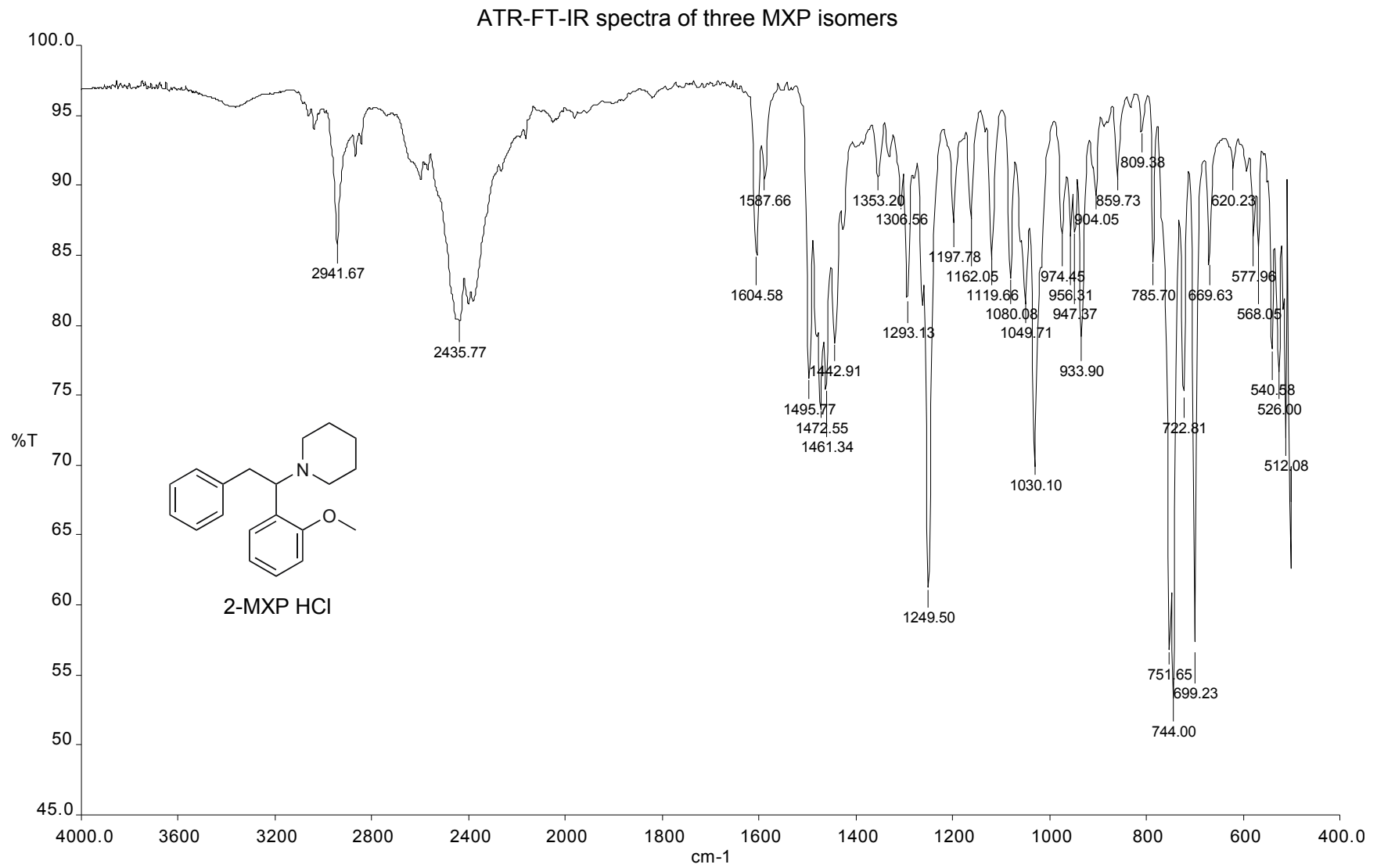
Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data



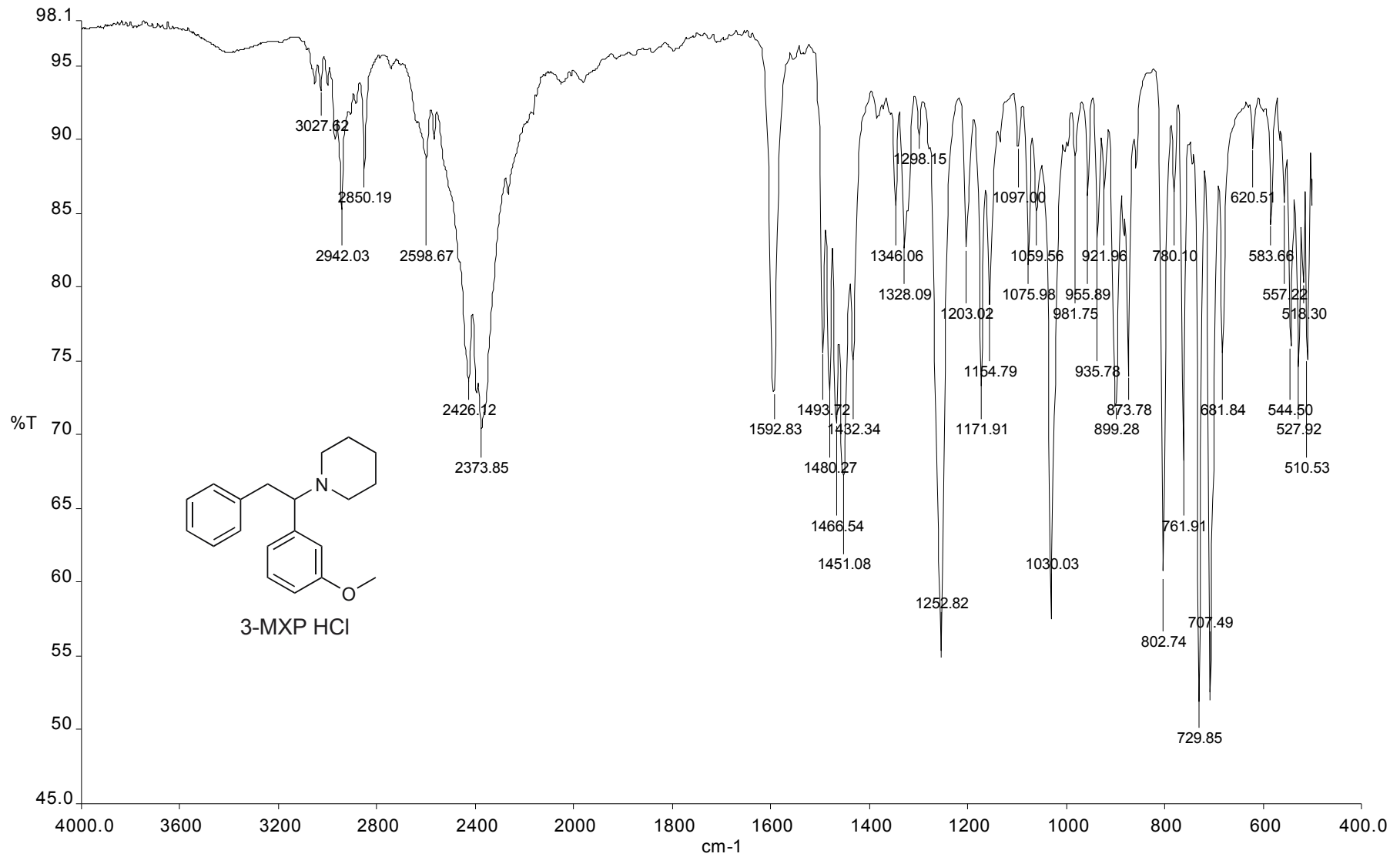
Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data



¹³C-NMR of 2-MXP extracted from tablet vs. MXP isomers



Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data



Drug Testing and Analysis – McLaughlin *et al.* – Supplementary data

