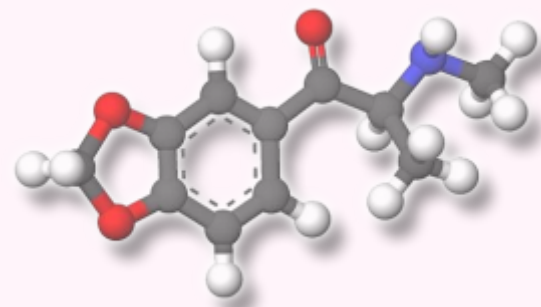




New Psychoactive Substances

How to keep up with the never ending need for reference materials.

International Forensics Symposium
July 2014 Washington, DC



- Law Enforcement
- Legislation
 - changing legislation
- Health



- Identification without reference materials

- Forensic methodology

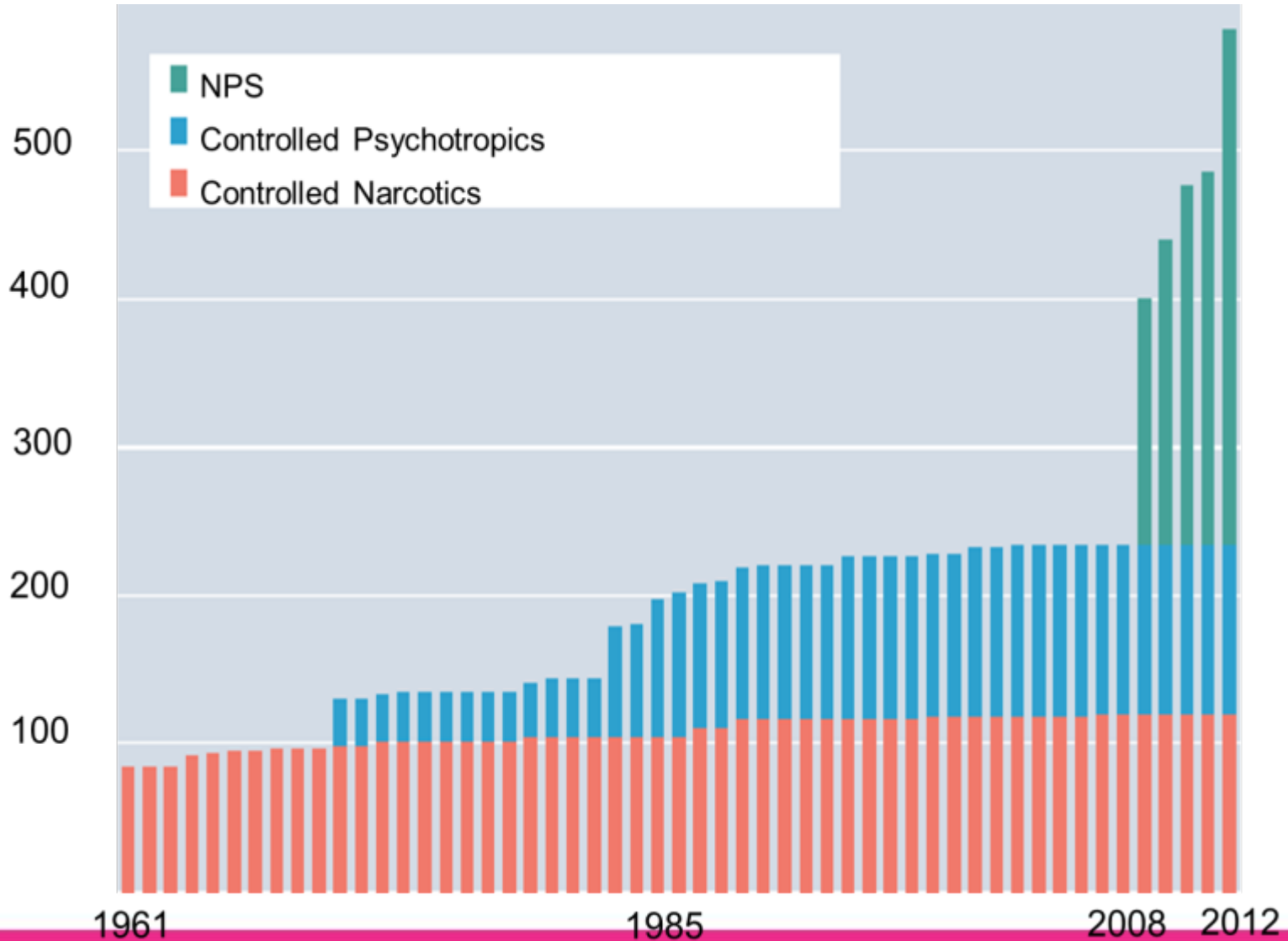
- Reference materials.



- You figured out what it is, now how to quantify it?

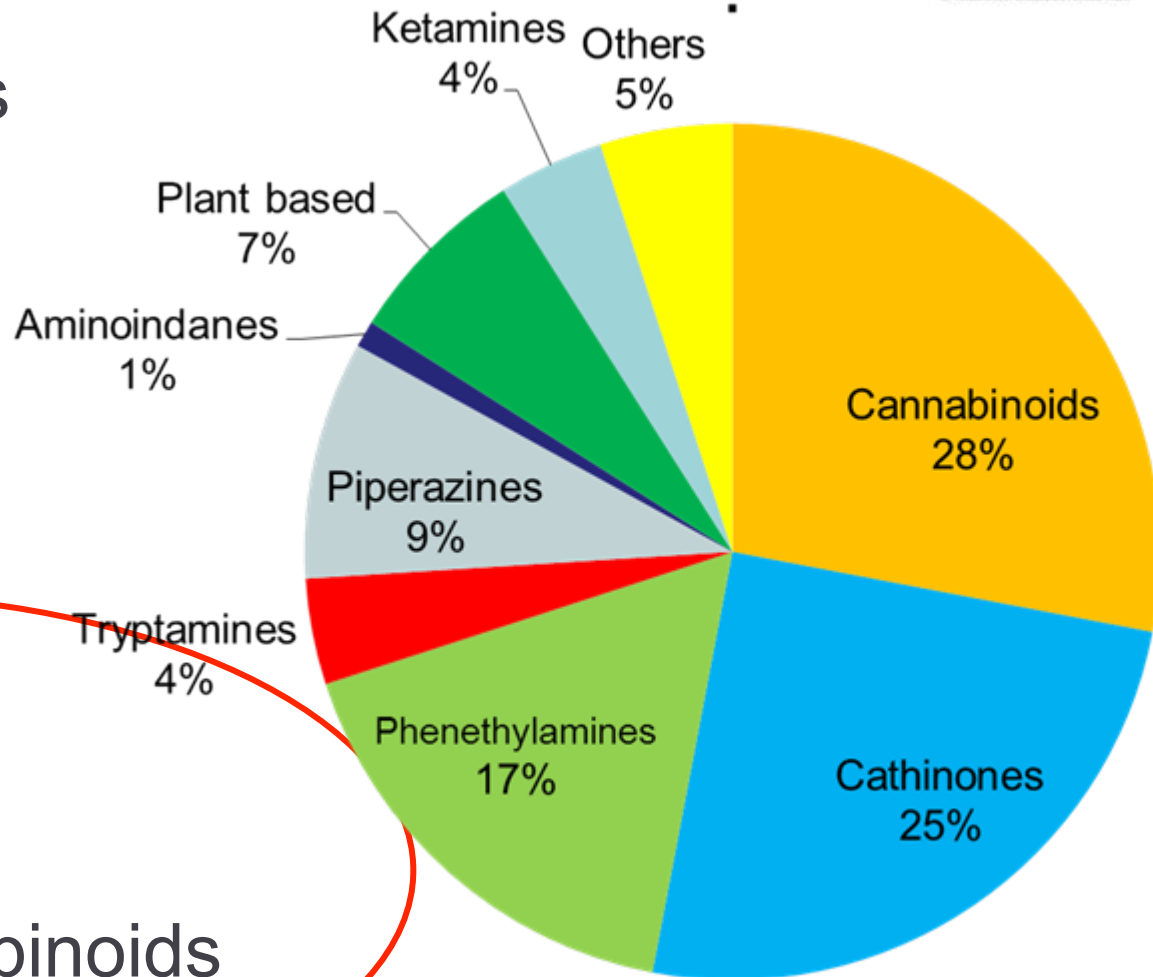
- Potential for error

Designer Drug Explosion

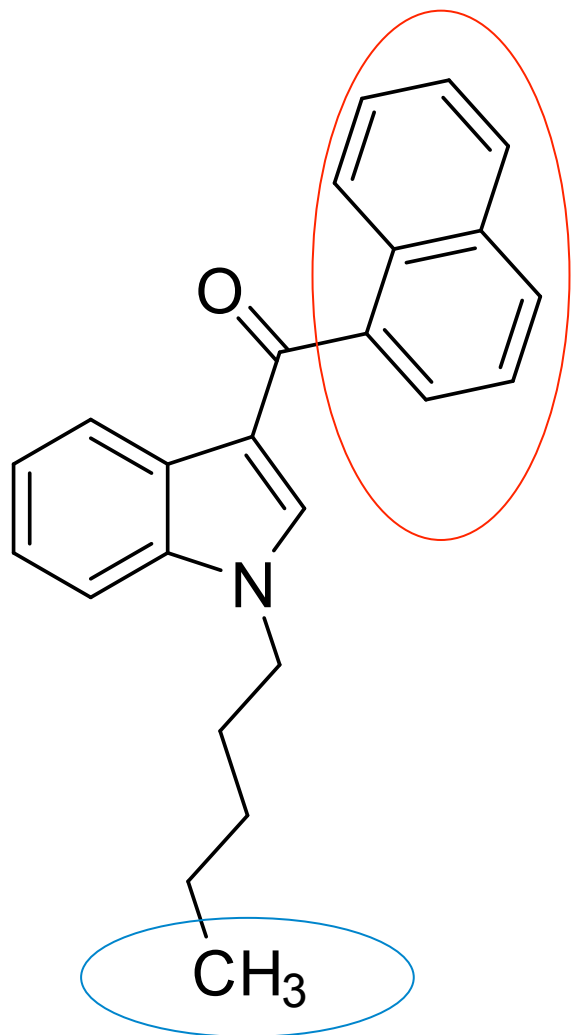


Types of Designers

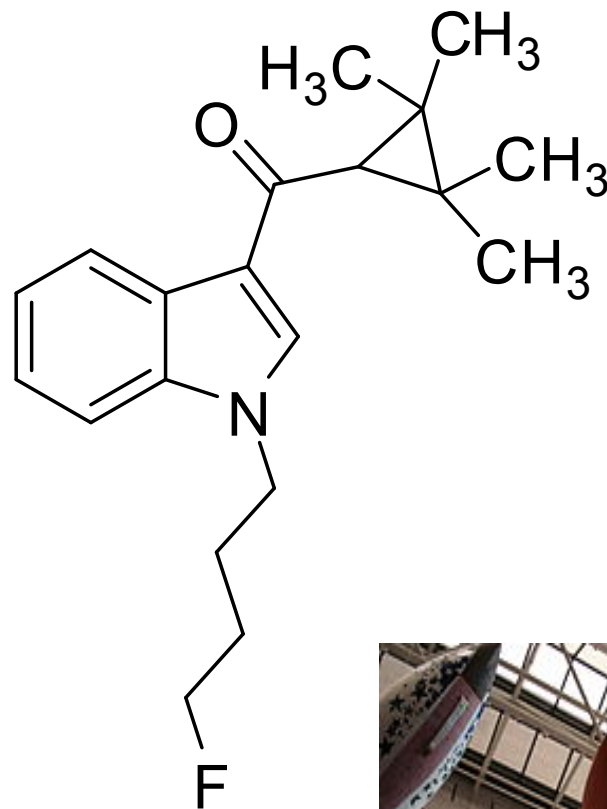
- Phenethylamines
- Piperazines
- Tryptamines
- Cathinones
- Synthetic Cannabinoids



Major Modifications

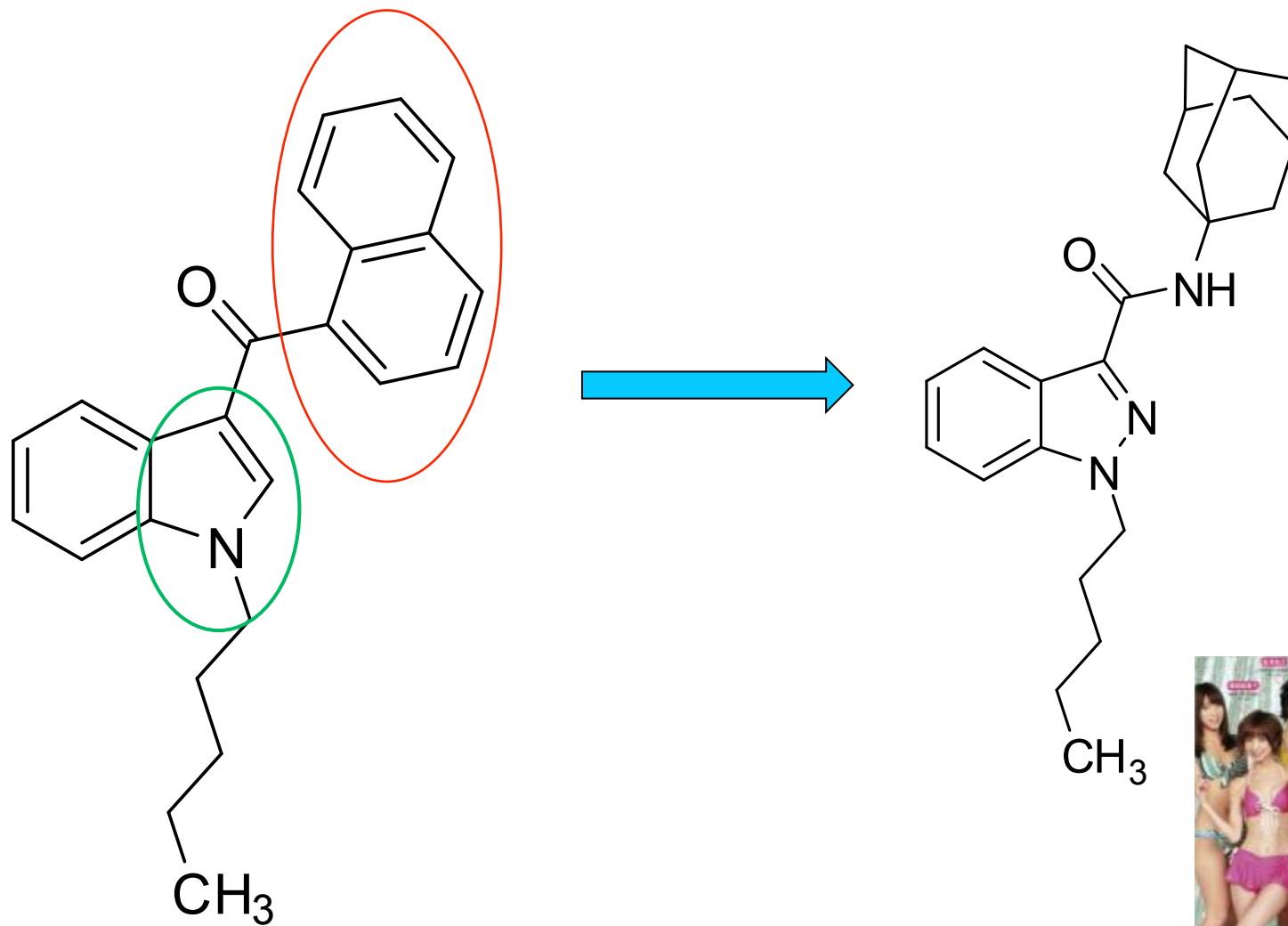


JWH-18

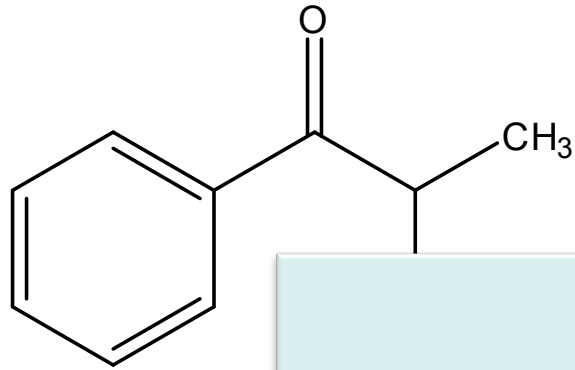


XLR-11

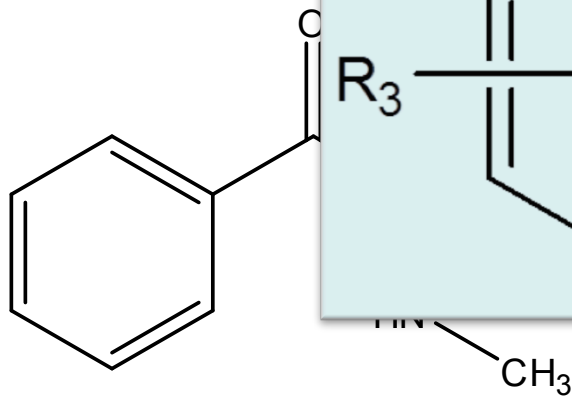
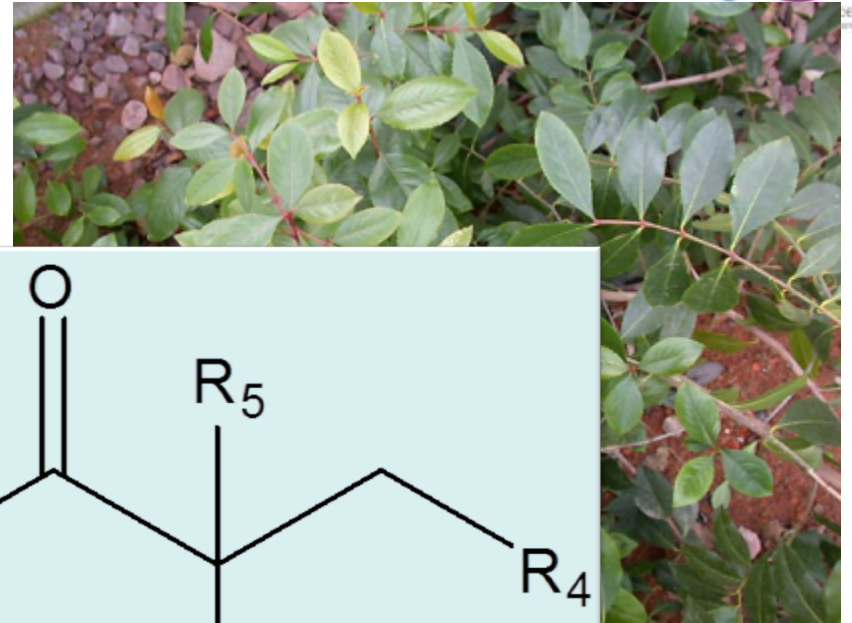
Major Modifications



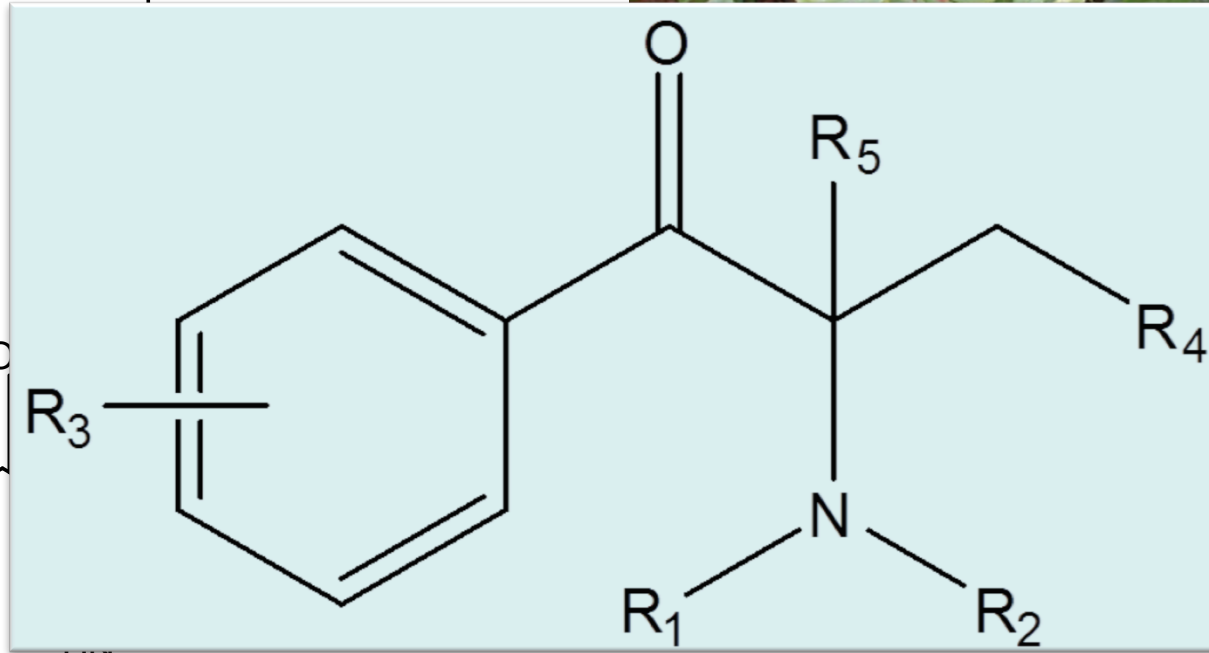
Cathinone



Cathinone

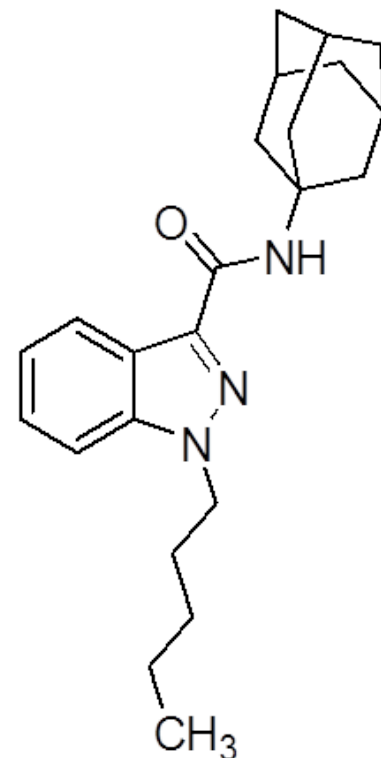
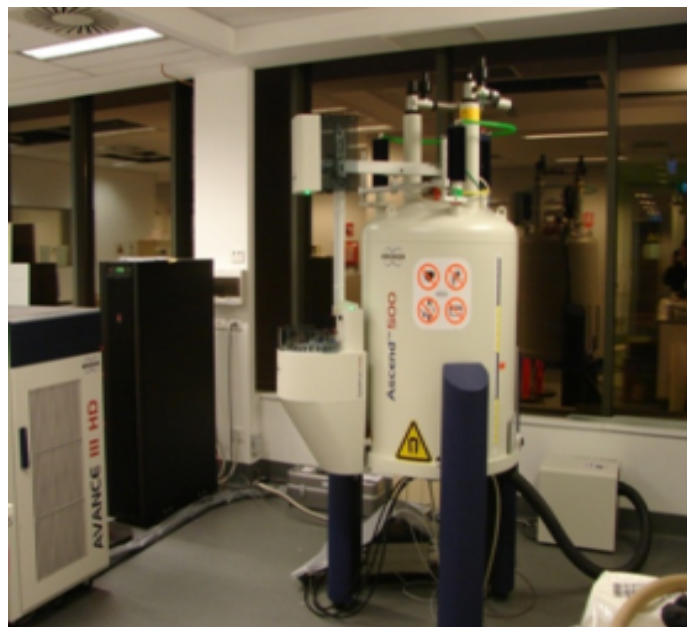


Methcathinone



Identification of new designer drugs

- ~ 1-2 new psychoactive substances produced each month



New “designer”

NMR Spectroscopy

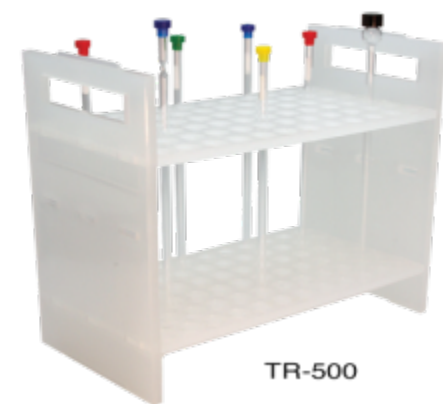
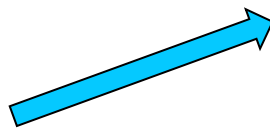
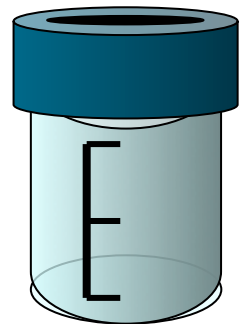
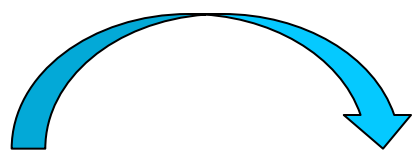
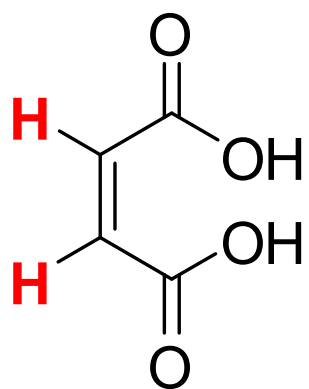
Final identity

- ID still requires primary method
 - 1D NMR (^1H , ^{13}C , ^{19}F , ^{15}N)
 - 2D NMR (COSY, HSQC, HMBC)
 - High Resolution Mass Spectroscopy
- Quantification
 - ^1H qNMR
 - Primary method
 - Compares protons with protons
 - Reference material not required.

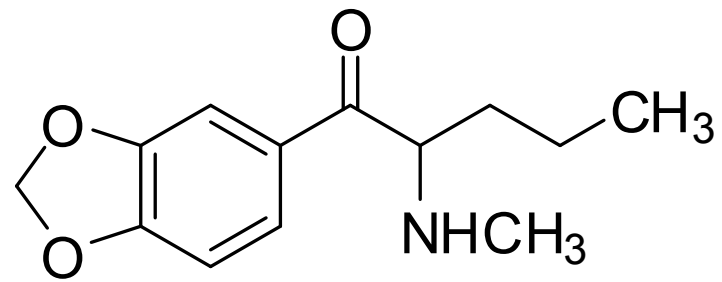
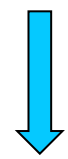


A Q-NMR Experiment

3.275 mg maleic acid (internal standard) delivered in D₂O



TR-500

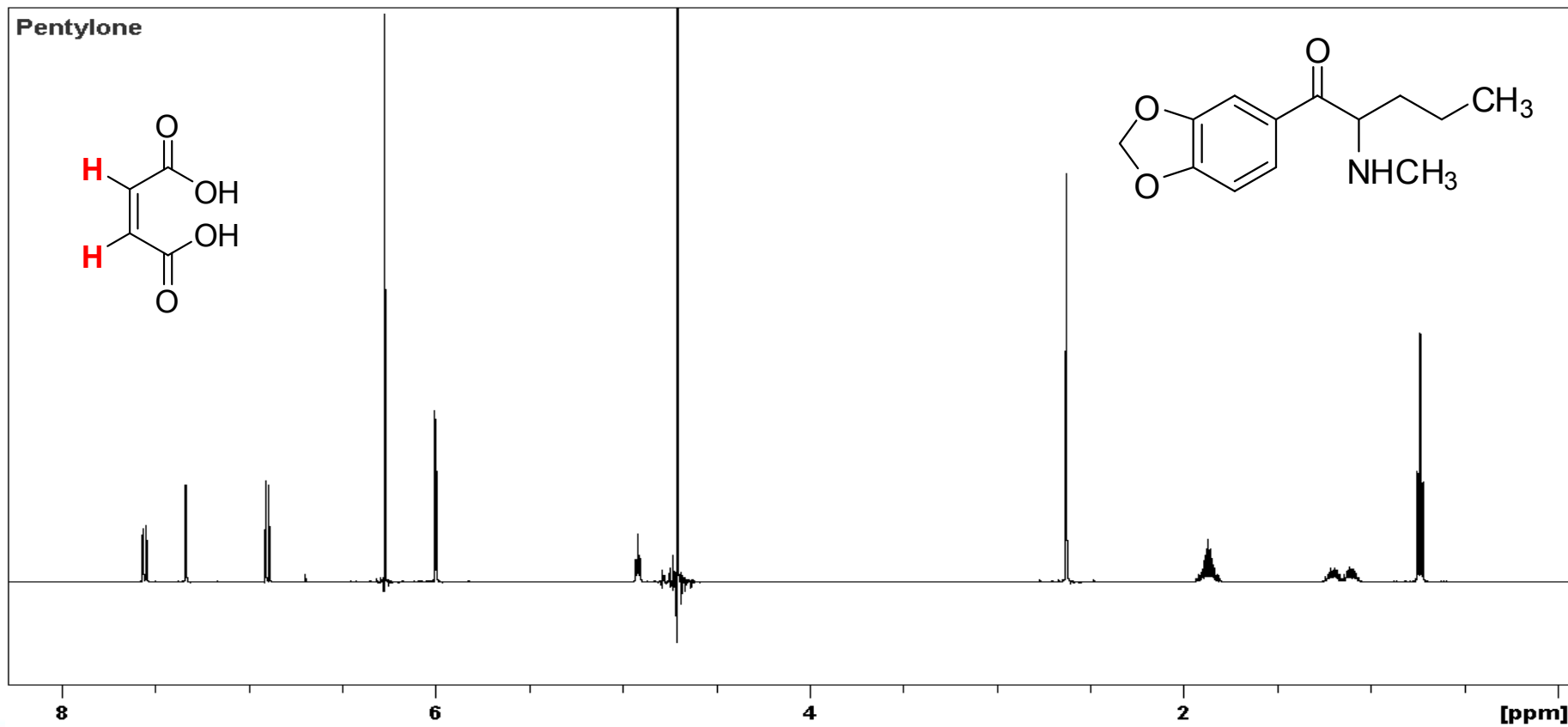


Pentylone certified reference standard (CRM D992): Assigned Purity of $99.8 \pm 1.5\%$



Q-NMR Result

99.5 (Std. Dev) 0.4 % (n=10)

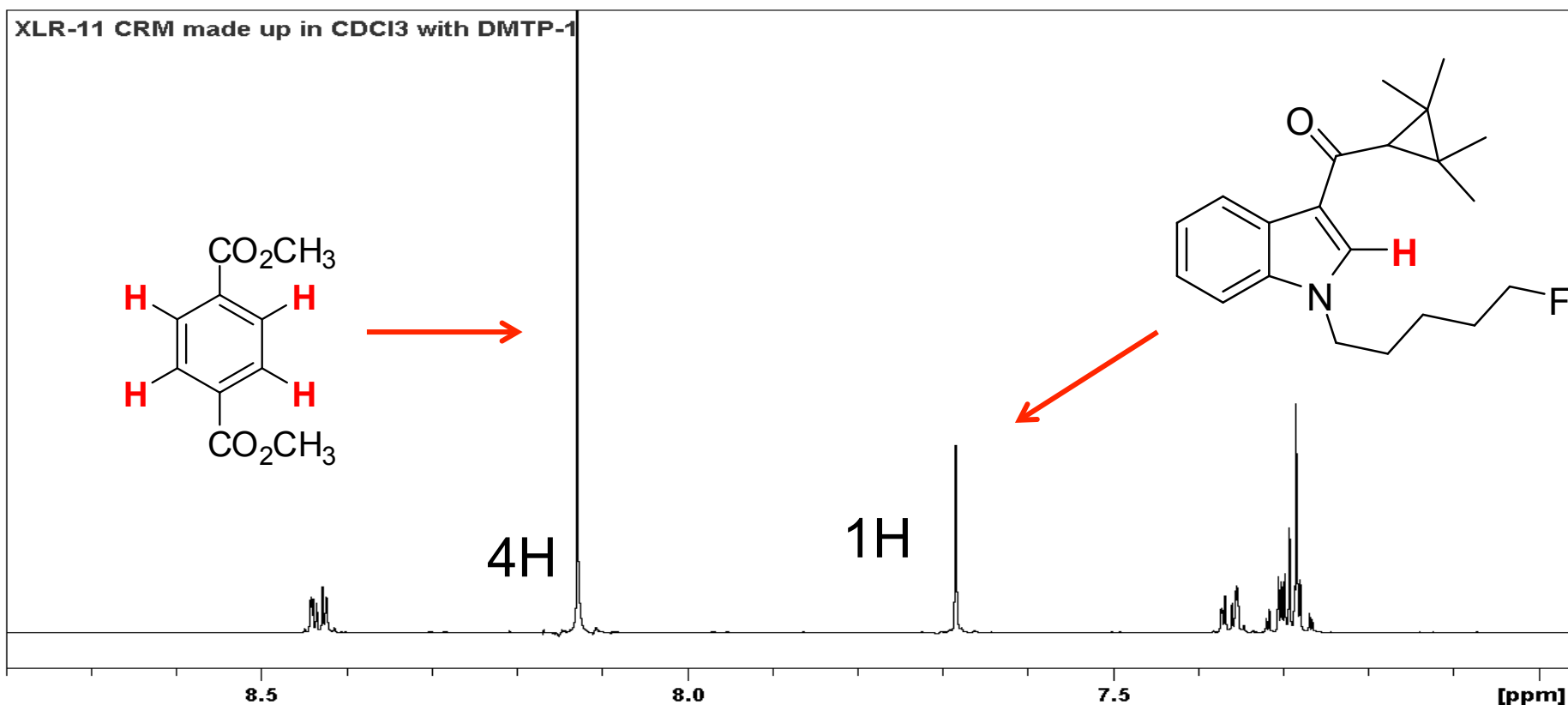


XLR-11 certified reference standard (CRM 13-D-17): Assigned Purity of $94.5 \pm 3.7\%$



Q-NMR Result

94.0 (Std. Dev) 0.8 % (n=10)

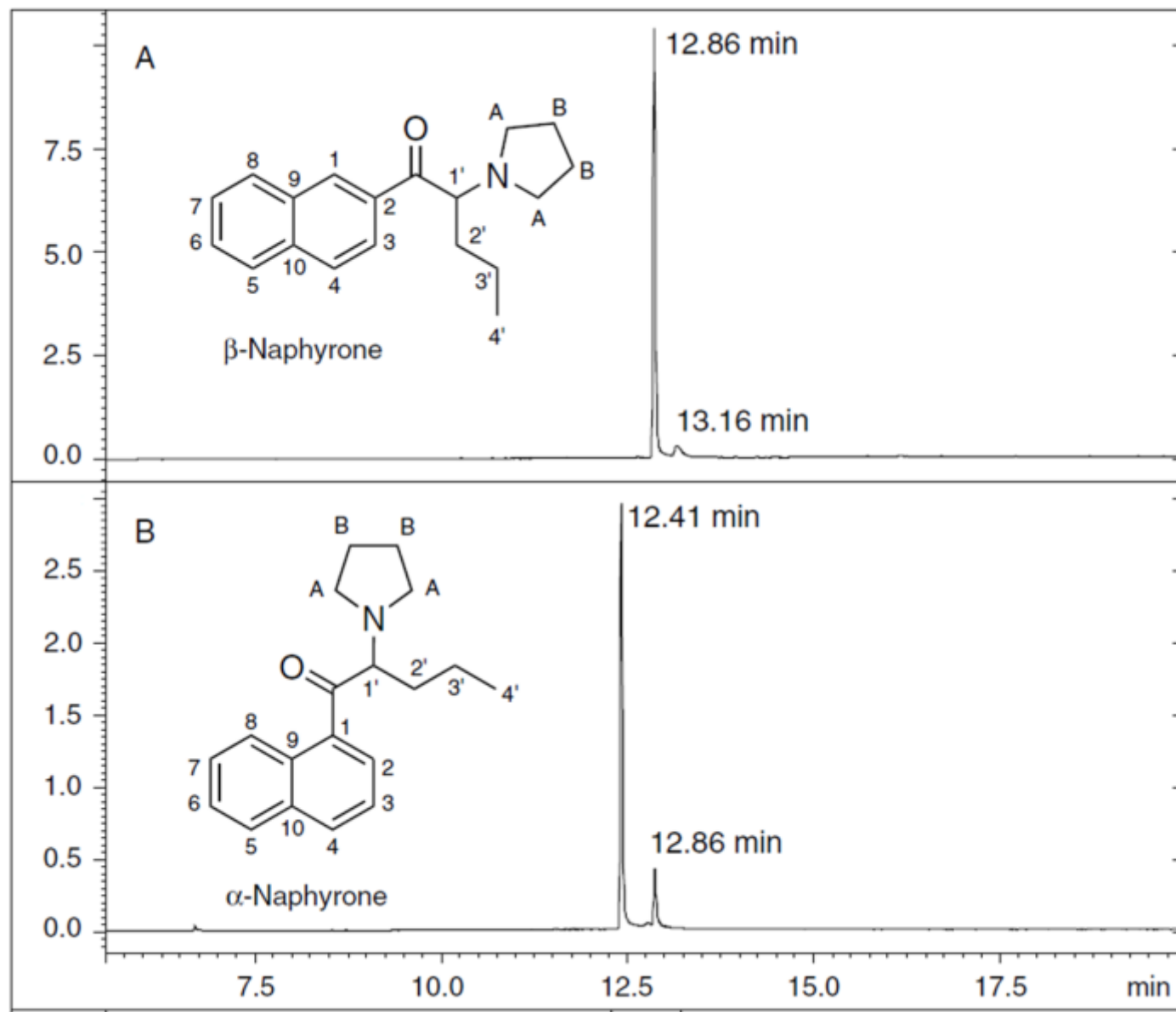


- Some have NMR or access through a University - most do not !
- Gas Chromatography- Mass Spectroscopy is the workhorse instrument
- Reliance on reference standards

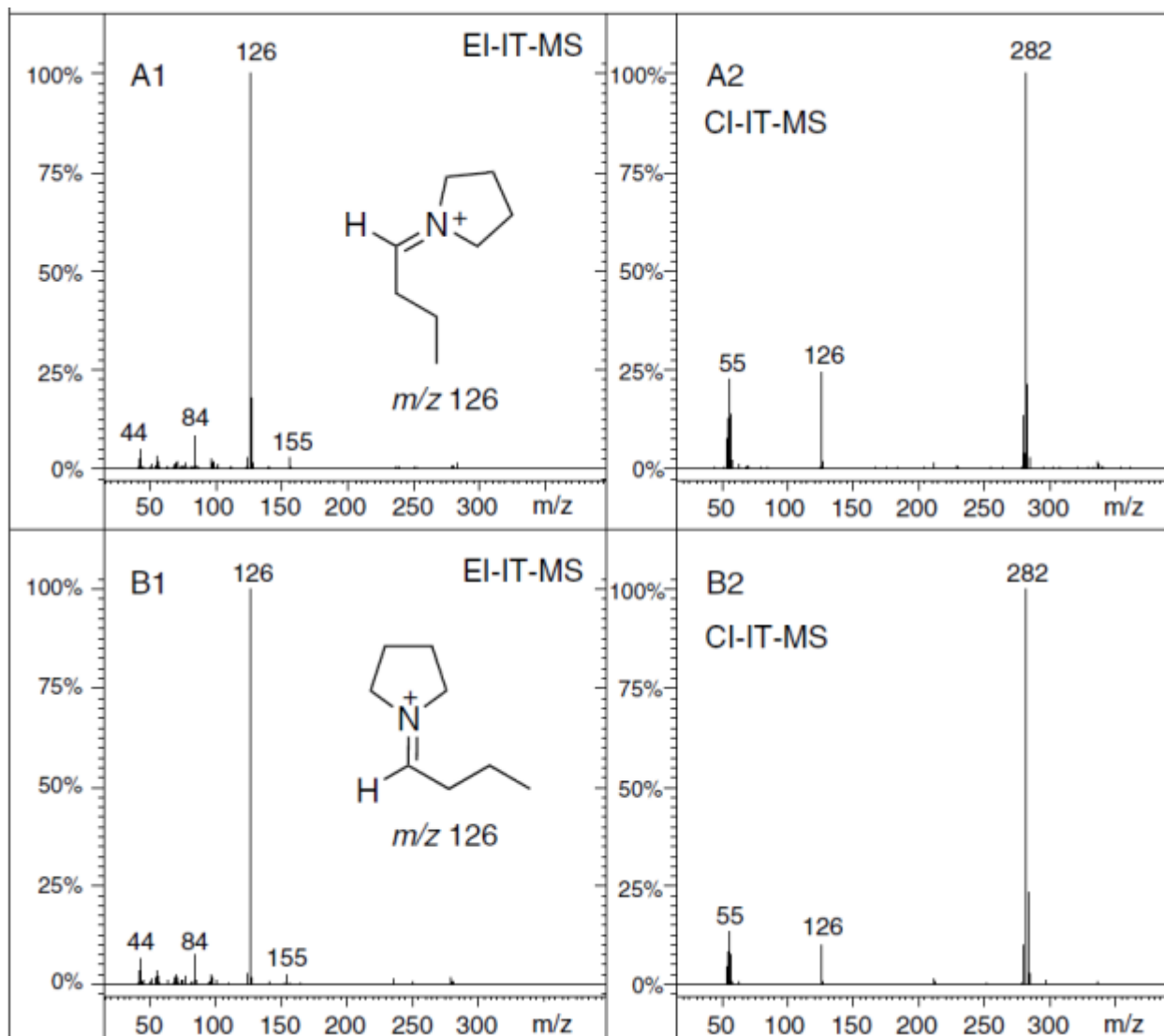
First Steps to Identify Drug



- SWG Drug Monographs
- SWG Drug Mass Spectral Library
- CLIC email trails

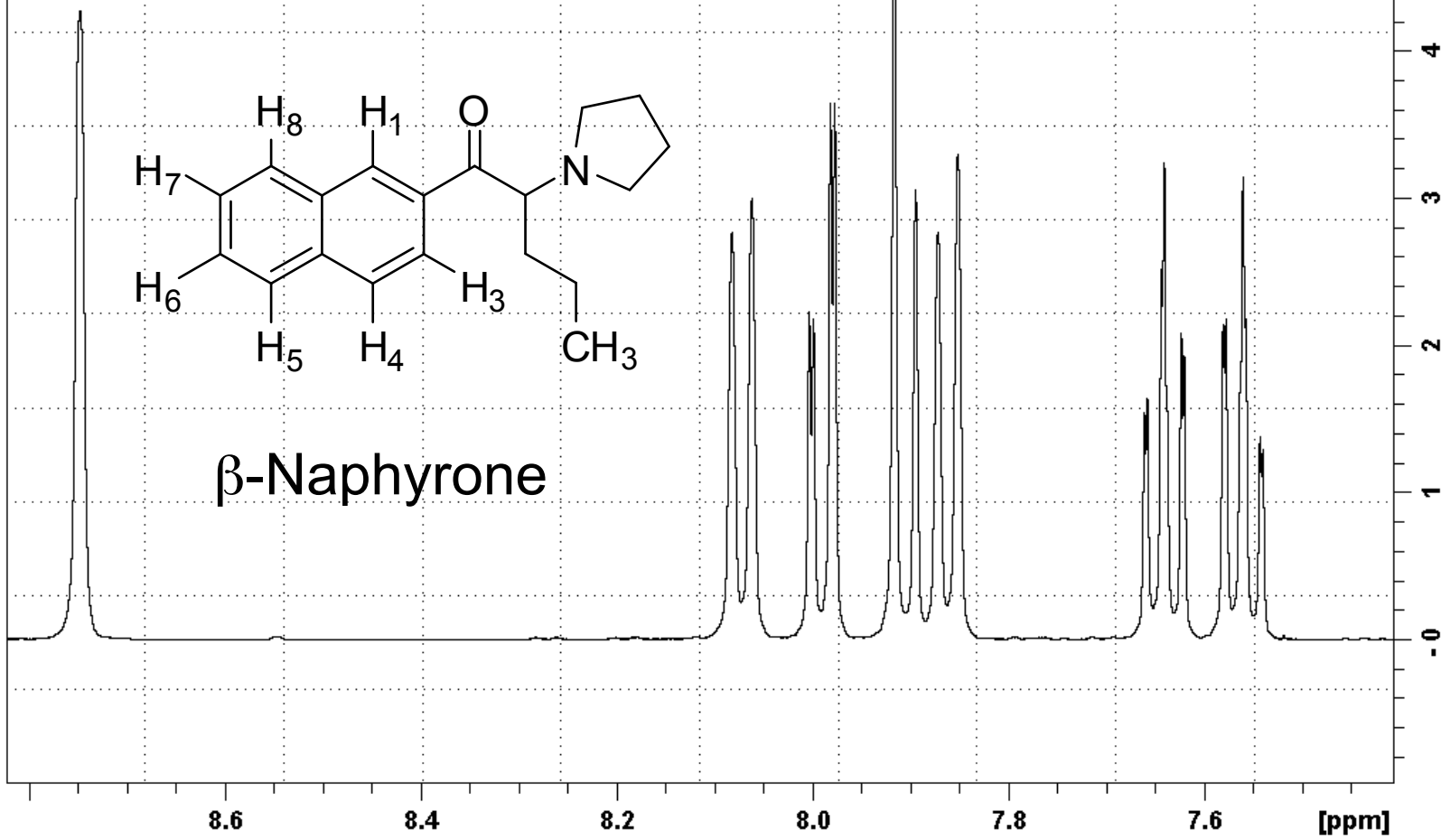


Brandt et al, *Drug Testing and Analysis*, 2010, 496-502



Brandt et al, *Drug Testing and Analysis*, 2010, 496-502

Analyst: Collins
NF103946 Unknown (20mg) in CDCl₃ (over K₂CO₃)
1H.NMR CDCl₃ D
20 October 2010

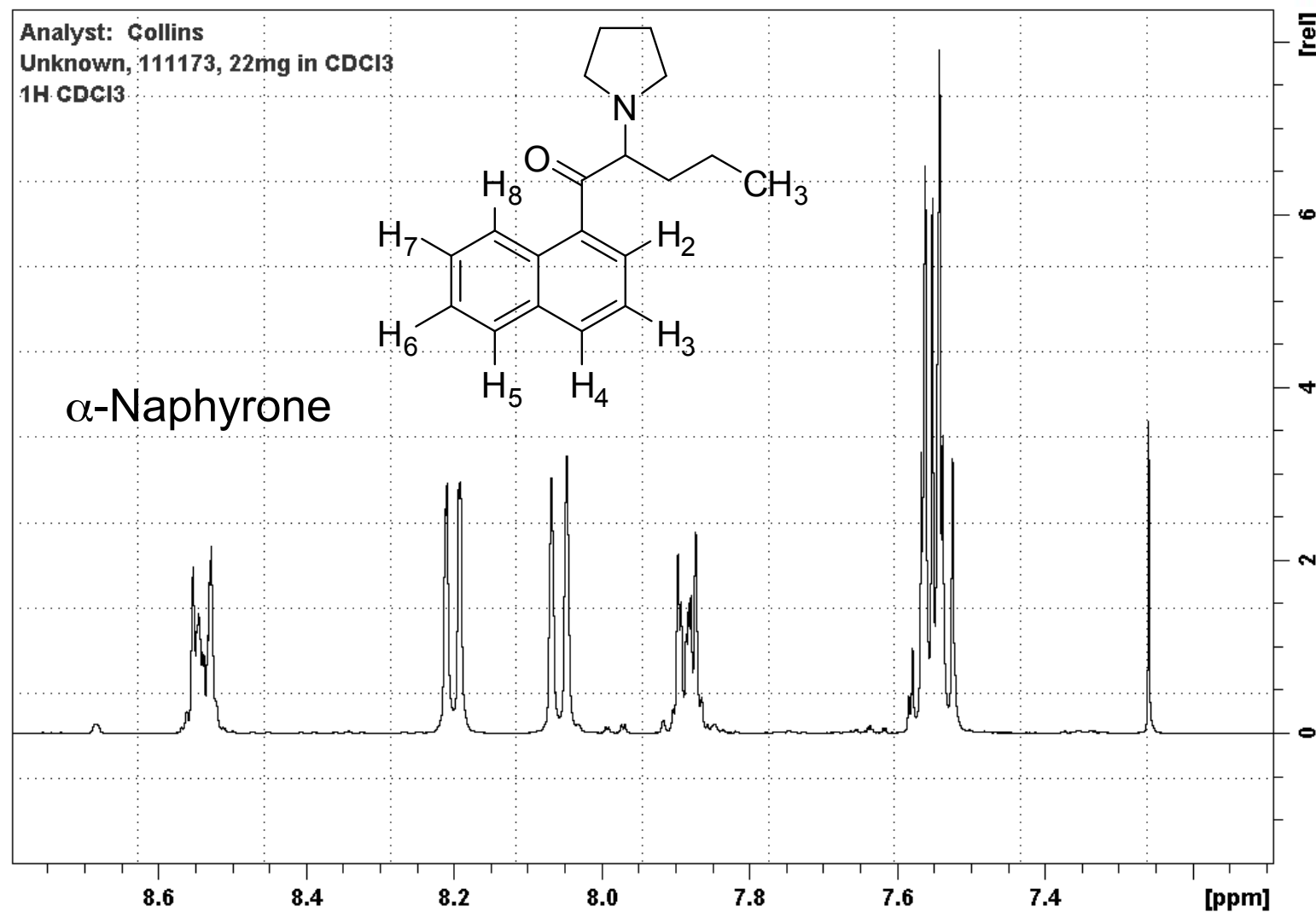
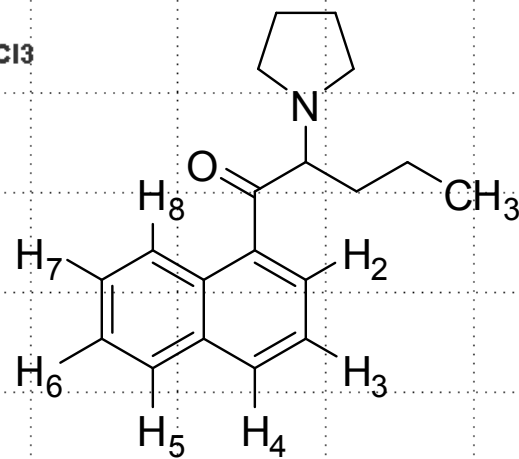


Analyst: Collins

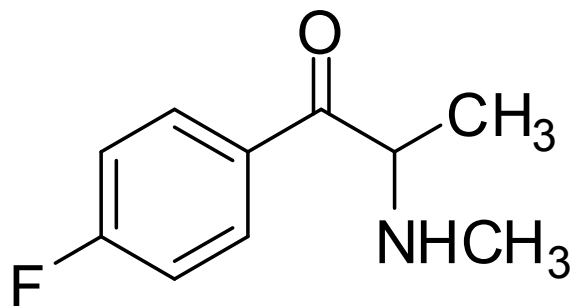
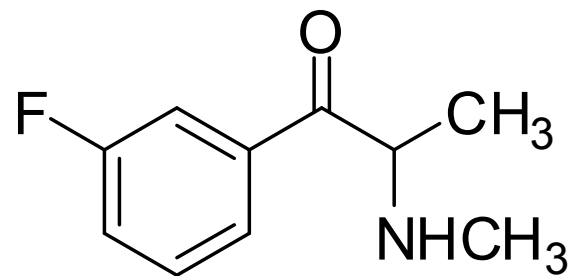
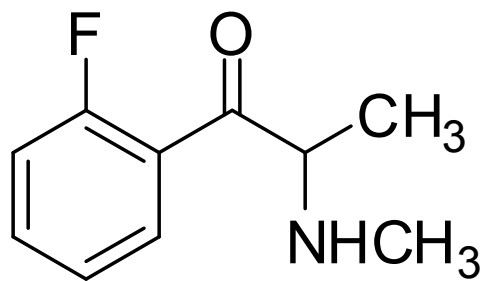
Unknown, 111173, 22mg in CDCl₃

¹H CDCl₃

α -Naphyrone



Regioisomers of Fluoromethcathinone



Intergovernmental Committee on Drugs

- Project Proposal: Increased Forensic Capability
- AFP provided ~\$700K for synthesis and certification of ~ 200 reference materials



AFDL and Chemical Reference Materials Laboratory

- Intelligence sharing between the two sections on the newest designer drugs
- Agreement between AFP and NMI for use of seizures of new drugs to prepare new reference materials



