Assessing The Quality and Reliability of the DEA Drug Identification Process

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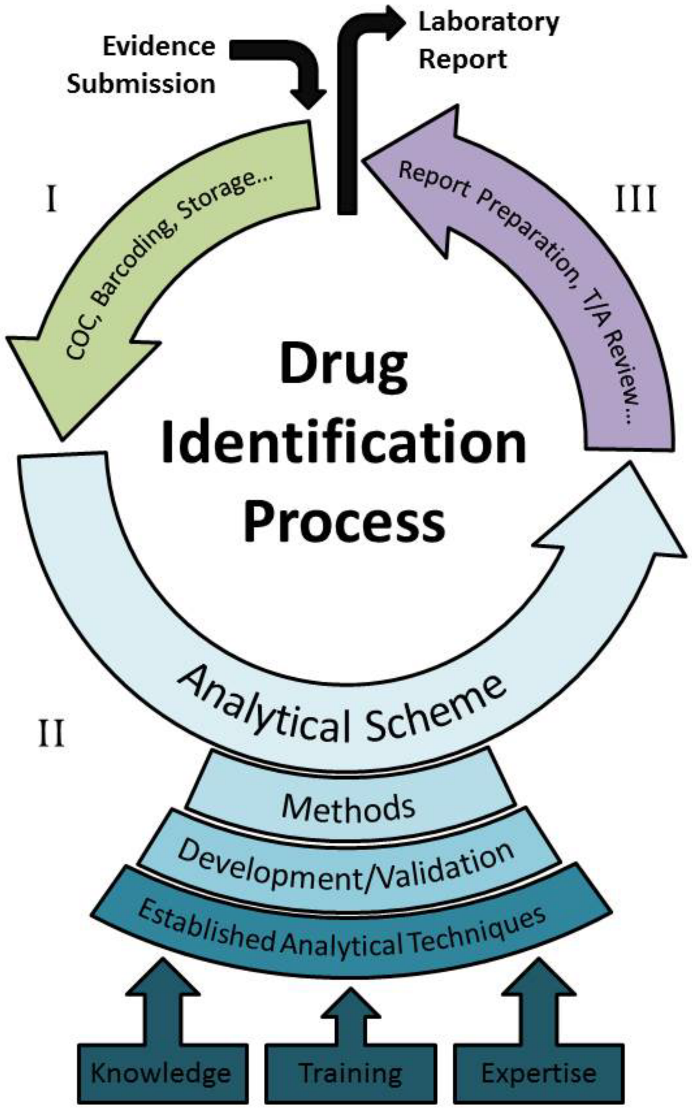
INTRODUCTION

- **Background:**
  - DEA laboratory system (8 labs; > 270 chemists)
  - Tens of thousands reports per year
  - Produce accurate and scientifically-supported results
- **Objective:**
  - Quantitative assessment of the reliability of the *overall* laboratory process
  - Quality of laboratory results
  - Confidence (or uncertainty) of reported identifications

DEA Drug Identification Process:



DEA Laboratory Analytical Scheme:

- **Requires analysts to test, at minimum:**
  - Two portions
  - Two different and independent techniques
  - Use negative controls
  - Use positive controls (traceable reference materials)
- **SWGDRUG Recommendations**
- **ASTM E2329**
  - *Standard Practice for Identification of Seized Drugs*

DEA Drug Identification Process:

- **Where can errors occur?**
- **Phase I**
  - Sample swapping, wrong barcoding, etc.
- **Phase II**
  - Analysis, sample swapping, contamination, etc.
- **Phase III**
  - Report preparation, dissemination, etc.

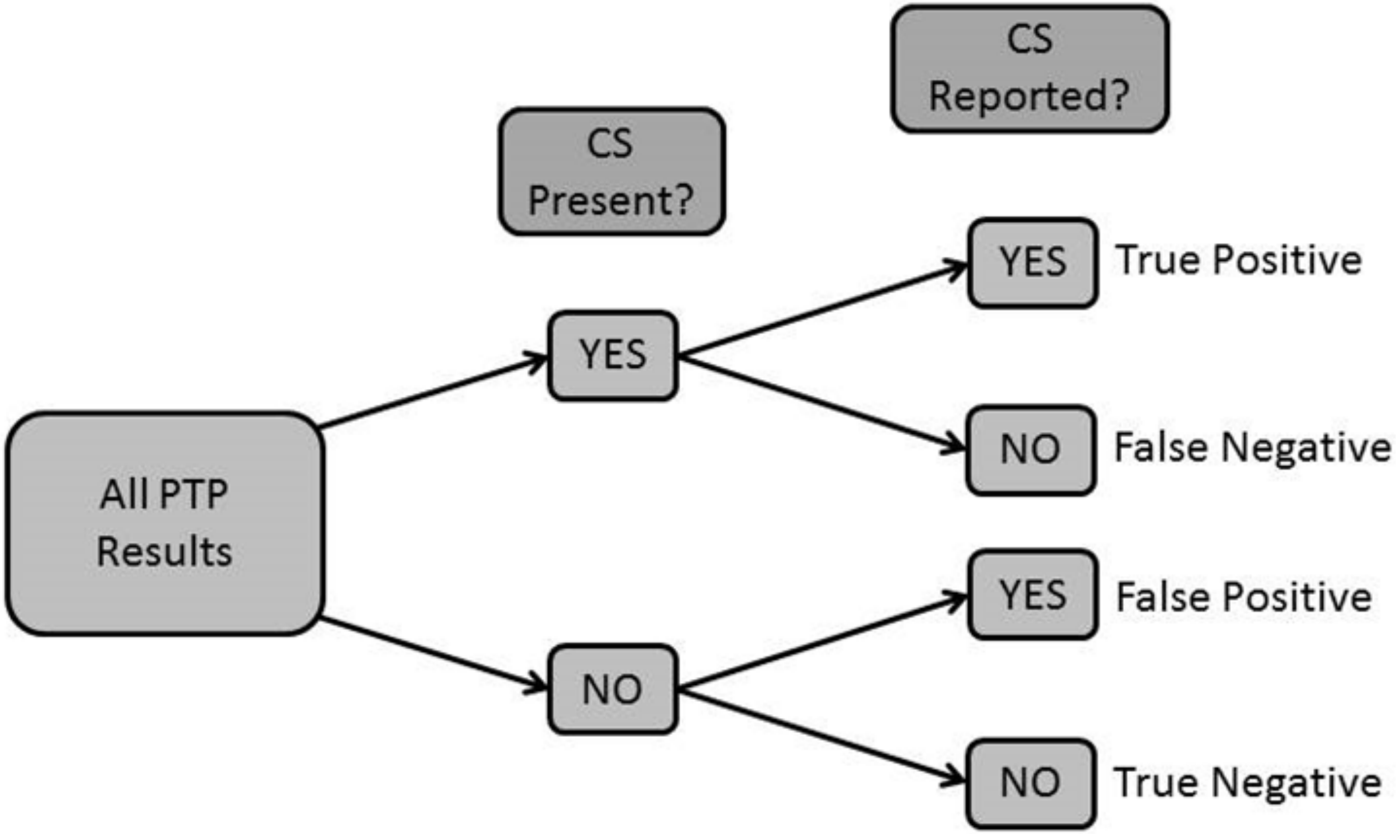
Uncertainty in Qualitative Analysis:

- **Limited studies**
- **Past emphasis on quantitative analysis:**
  - Measurement uncertainty
- **References:**
  - S.L.R. Ellison, *Accred. Qual. Assur.* 5 (2000) 346-348.
  - A. Pulido, I. Ruisanchez, R. Boque, F.X. Rius, *Trend Anal. Chem.* 22 (2003) 647-654.
  - B.L. Milman, *Trend Anal. Chem.* 24 (2005) 493-508.

DEA PTP Historical Data:

- **2005-2016**
- **4746 test results**
- **2392 inter-laboratory** (24-27 PT rounds/year)
- **2058 intra-laboratory**
- **216 external**
- **80 blind**

Classification of PT Results:



Calculating Response Rates:

$$TPR\ (\textbf{sensitivity}) = \frac{True\ Positives}{All\ Positives} = \frac{TP}{(TP + FN)}$$

$$TNR\ (\textbf{specificity}) = \frac{True\ Negatives}{All\ Negatives} = \frac{TN}{(TN + FP)}$$

$$FPR\ (\textbf{Type I error}) = \frac{False\ Positives}{All\ Negatives} = \frac{FP}{(TN + FP)} = 1 - specificity$$

$$FNR\ (\textbf{Type II error}) = \frac{False\ Negatives}{All\ Positives} = \frac{FN}{(TP + FN)} = 1 - sensitivity$$

Results Matrix:

		CS Reported				
		YES	NO	Total:		
CS Present	YES	**4285**	**4**	4289	**0.99907**	**TPR** (sensitivity)
	NO	**4**	**453**	457	**0.00875**	**FPR** (type I error)
	Total:	4289	457	4746		
		0.00093	**0.99125**			
		FNR (type II error)	**TNR** (specificity)			

ABOUT THE FALSE RESULTS:

- **4 False Positives:**
  - Sample swapping
  - Low-level secondary CS reported w/o fulfilling QA and documentation requirements
  - 2 incorrect CS reported (LIMS)

Synthetic cathinones

- **4 False Negatives:**
  - Sample swapping
  - Low concentration of target CS
  - 2 cases of low-level secondary CS

PRECISION AND ACCURACY:

$$\textit{Precision} = \frac{\text{True Positives}}{\text{All Positives Results}} = \frac{TP}{(TP + FP)}$$

$$= \frac{4285}{(4285 + 4)} = 99.90\%$$

$$\textit{Accuracy} = \frac{\text{All True Results}}{\text{All Results}} = \frac{TP + TN}{(TP + FP + TN + FN)}$$

$$= \frac{(4285 + 453)}{(4746)} = 99.83\%$$

PT / Response Rates Results:

High ***sensitivity***	**99.90%**
High ***specificity***	**99.12%**
Low ***type I*** error rate	**0.87%**
Low ***type II*** error rate	**0.093%**
High ***precision***	**99.90%**
High ***accuracy***	**99.83%**

Error Rates (type I and type II error rates)

USING BAYESIAN INFERENCE:

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)}$$

Confidence

$$P(CS|+) = \frac{P(+|CS) \cdot P(CS)}{P(+)}$$

$$P(nCS|+) = \frac{P(+|nCS) \cdot P(nCS)}{P(+)}$$

Uncertainty

S.L.R. Ellison, S. Gregory, W.A. Hardcastle, *Analyst* 123 (1998) 1155-1161.

Confidence in the Positive ID:

True Positive Rate

Prior probabilities

$$P(CS|+) = \frac{P(+|CS)\cdot P(CS)}{P(+|CS)\cdot P(CS) + P(+|nCS)\cdot P(nCS)}$$

Posterior probability

False Positive Rate

- *Probability CS <u>is</u> present, given a reported result*
- *Confidence in the positive identification result*

Uncertainty in the Positive ID:

False Positive Rate

Prior probabilities

$$P(nCS|+) = \frac{P(+|nCS) \cdot P(nCS)}{P(+|nCS) \cdot P(nCS) + P(+|CS) \cdot P(CS)}$$

True Positive Rate

Posterior probability

- ► *Probability CS is <u>not</u> present, given a reported result*
- ► *Uncertainty in the positive identification result*

Estimating Prior Probabilities:

- **Population information**
  - *Which population?*
- **Historical data**
- **Prior knowledge**
- **Seizure circumstances**
- **Reasonable and supported assumptions**

$P(CS)$ → low
$P(nCS)$ → high

ESTIMATING PRIOR PROBABILITIES:

- **No Information:**
  - $P(CS) = P(nCS) = 0.50$

- **Prior Information:**
  - Statistics on laboratory submissions
  - Field testing results
  - Undercover purchase
  - Smuggling operations (clan lab, POE)
  - Identifying wrappings, markings, etc.

No Population Information:

- **$P(CS) = P(nCS) = 0.50$**

Confidence =

$$P(CS|+) = \frac{P(+|CS) \cdot \cancel{P(CS)}}{P(+|CS) \cdot \cancel{P(CS)} + P(+|nCS) \cdot \cancel{P(nCS)}}$$

$$P(CS|+) = \frac{(0.99907)}{(0.99907) + (0.00875)} = 0.9913 = 99.13\%$$

No Population Information:

- $P(CS) = P(nCS) = 0.50$

Uncertainty =

$$P(nCS|+) = \frac{P(+|nCS) \cdot P(\cancel{nCS})}{P(+|nCS) \cdot P(\cancel{nCS}) + P(+|CS) \cdot P(\cancel{CS})}$$

$$P(nCS|+) = \frac{(0.00875)}{(0.00875) + (0.99907)} = 0.0086 = 0.86\%$$

Estimating Prior Probabilities:

- **No Information:**
  - $P(CS) = P(nCS) = 0.50$
- **Prior Information:**
  - Statistics on laboratory submissions
  - Field testing results
  - Undercover purchase
  - Smuggling operations (clan lab, POE)
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DEA Submissions & Reports:

Year	Total	Laboratory Results		CS (%)	NCS (%)
		CS	NCS		
1994	37,115	32,779	4,336	88.32	11.68
1995	38,668	34,645	4,023	89.60	10.40
1996	43,662	38,836	4,826	88.95	11.05
1997	49,156	43,965	5,191	89.44	10.56
1998	55,946	49,919	6,027	89.23	10.77
1999	60,093	53,869	6,224	89.64	10.36
2000	64,608	57,840	6,768	89.52	10.48
2001	66,235	59,776	6,459	90.25	9.75
2002	64,504	58,065	6,439	90.02	9.98
2003	59,793	54,148	5,645	90.56	9.44
2004	56,709	50,973	5,736	89.89	10.11
Total	**596,489**	**534,815**	**61,674**	**88.20-90.96**	**9.04-11.80**
				(95% Confidence Interval)	

POPULATION: DEA LAB SUBMISSIONS

- **$P(CS) = 0.90$**
- **$P(nCS) = 0.10$**

$$Confidence = P(CS|+) = \frac{P(+|CS) \cdot P(CS)}{P(+|CS) \cdot P(CS) + P(+|nCS) \cdot P(nCS)}$$

$$P(CS|+) = \frac{(0.99907)(0.90)}{(0.99907)(0.90) + (0.00875)(0.10)}$$

$$P(CS|+) = 0.99902 = 99.90\%$$

POPULATION: DEA LAB SUBMISSIONS

- $P(CS) = 0.90$
- $P(nCS) = 0.10$

$$Uncertainty = P(nCS|+) = \frac{P(+|nCS) \cdot P(nCS)}{P(+|nCS) \cdot P(nCS) + P(+|CS) \cdot P(CS)}$$

$$P(nCS|+) = \frac{(0.00875)(0.10)}{(0.00875)(0.10) + (0.99907)(0.90)}$$

$$P(nCS|+) = 0.00097 = 0.097\%$$

Confidence/Uncertainty:

P(CS)	*P(nCS)*	*Confidence (%)*	*Uncertainty (%)*
0.001	0.999	10.25	89.74
0.01	0.99	53.55	46.44
0.05	0.95	85.73	14.27
0.10	0.90	92.69	7.30
0.25	0.75	97.43	2.56
0.5	**0.5**	**99.13**	**0.86**
0.75	0.25	99.70	0.29
0.90	**0.10**	**99.90**	**0.097**
0.95	0.05	99.95	0.046
0.99	0.01	99.99	0.009
0.999	0.001	99.99	0.001

LIMITATIONS:

- **Using PTP data:**
  - Not a ‘true’ representation of routine submissions?
  - Analyst “knows” it is a test
- **‘True’ sample identity not known**
- **No framework currently available**
  - PTP data could be only data available to laboratories
- **Prior probabilities (base rates) on the population**
- **Communicating approach to lay persons**

CONCLUSIONS:

- PTP data provides means for assessing reliability of ***overall laboratory drug identification process***.
- **DEA laboratory ID process:**
  - High sensitivity and specificity
  - Low type I and type II error rates
  - High accuracy and precision
- **Bayesian & population assessment:**
  - High confidence & low uncertainty
- **Valuable assessment:**
  - Improving laboratory testing & QA procedures

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QUESTIONS?

- **Thank You!**

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