A data-reduction algorithm for broad-spectrum LC/MS screening of psychoactive substances in urine Danijela Konforte^a, Difei Sun^a, **Jan Palaty**^b a)LifeLabs Medical Laboratories, Toronto ON b) LifeLabs Medical Laboratories, Burnaby BC

Situation

Broad-spectrum LC/MS drug screen for ~600 urine sample per day from addiction patients.

Goals

- Automated data review using MS Excel middleware
- Simple, exception-based, semi-quantitative report format
- Graded identification scheme
- Use known metabolites to strengthen ID confidence
- Built-in controls for carryover, crosstalk, %hydrolysis, adulteration, unusual compounds



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 \uparrow retention & \downarrow concentration than Creatinine Normal constituent of urine (and calibrators!) Verification of pipetting & sample integrity

		Norovucadana
	Oxycodone	Oxymorphone
	Paroxetine	oxymorphone
	PCP	
	Pentazocine	
	Pentedrone NE	
	PMA	
	Pregabalin	
	Promethazine	
	Pseudoephedrine	
	PVP	
		Norquetiapine
	Quetiapine	HO-Quetiapine
	Risperidone	HO-Risperidone
	Ritalinic_acid	
	Sertraline	
	Sufentanil	
zapine	Tapentadol	Desmethyltapentadol
	Temazepam	Oxazepam
	TFMPP	
	THCA	
	Tilidine	Nortilidine
	Tramadol	O-Desmethyltramadol
	Trazodone	mCPP
	Trimipramine	Desmethyltrimipramine
	UR-144_5-OH	
	Venlataxine	O-Desmethylvenlataxine
zapine	XLR-11_4-OH	Zelnidens DCA
	Zoipidem	Zoipidem-PCA

Reporting LC/MS results with exception-based middleware adds **speed** consistency and new process control tools.







Report used by Operator for reviewing results



Only 5 of 122,217 reports required correction due to post-analytical error.

Summary

Fast and accurate analysis of > 300, 000 urine samples since 2016 User-friendly – requires no previous toxicology or LCMS knowledge/experience Robust QA – automation of error detection that cannot be done any other way Flexible – user-defined rules; continual improvement since original implementation Client Education Tool – drug-specific interpretive comments added to patient reports

Performance

900 consecutive samples: 89% of Compounds identified without manual review

~90 min to report 90 samples of which ~94% are positive for



"Found" = common Exception invariably proven as a true Foun

Substitution / pipetting error



Flagging rate extremely low

Only 1 case to date traced to pipetting error.

*) Data from our BC lab using virtually identical method.

Hydrolysis

900 consecutive samples: 37 (4.1%) flagged for decreased hydrolysis of Morphine-Glc-D3, typically due to high levels of analyte.

Cross-talk & Carryover				
# plates			2	
# plates with confirmed Cross-talk			7	
	Jul. 201	L9 A	ug. 2019	
Total samples	12,61	5	13,605	
% Repeated: CO flag		.7	3.1	
% Confirmed CO of repeats	7.3		5.3	
% Confirmed CO of Total	0.2	20	0.17	

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