Our Project Data: A Year in the Lab

Batch Data
batch name, instrument name, compound name,
calibration slope, calibration intercept, calibration R^2,
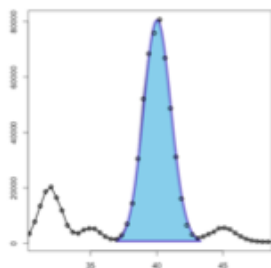reviewer name, collection time, review start time, review complete time

Each batch has 52 samples.

Sample Data
batch name, sample name, compound name, sample type,
ion ratio, response, concentration,
expected concentration, used for calibration, sample flags

Each sample has 24 peaks.

Peak Data
batch name, sample name, compound name, chromatogram name,
peak area, peak quality, manually modified

Batch Level Data

Batch Data
batch name, instrument name, compound name,
calibration slope, calibration intercept, calibration R^2,
reviewer name, collection time, review start time, review complete time

batchName	instrumentName	compoundName	calibrationSlope	calibrationIntercept	calibrationR2	batchPassed	...
b802253	doc	morphine	0.00775	-5.757e-06	0.9965	TRUE	
b802253	doc	hydromorphone	0.00768	-4.379e-05	0.9805	TRUE	
b802253	doc	oxymorphone	0.00798	5.154e-06	0. 9839	TRUE	
...							

20 batches a day. Each batch has six analytes, each analyte has an IS.

Sample Level Data

batchName	sampleName	compoundName	ionRatio	response	concentraiotn	sampleType	...
b802253	s253001	morphine	0	0	0	blank	
b802253	s253001	hydromorphone	0	0	0	blank	
b802253	s253001	oxymorphone	0	0	0	blank	
...							

Sample Data
batch name, sample name, compound name, sample type,
ion ratio, response, concentration,
expected concentration, used for calibration, sample flags

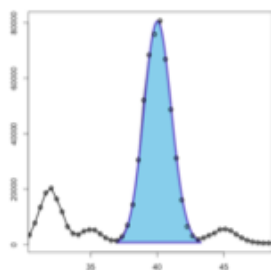*52 samples in a batch = 1040 samples a day.*
7 standards, 3 QCs, 2 blanks, 40 unknowns per batch.

Peak Level Data

batchName	sampleName	compoundName	chromatogramName	peakArea	peakQuality	manuallyModified
b802253	s253001	morphine	quant	0	0	FALSE
b802253	s253001	morphine	qual	0	0	FALSE
b802253	s253001	hydromorphone	quant	0	0	FALSE
…						

24 chromatograms in a sample = 24960 chromatograms a day.
Quant and Qual, for both the Analyte and the IS.

Peak Data
batch name, sample name, compound name, chromatogram name, peak area, peak quality, manually modified