

New

Toxicology Reporting Module

A newly-developed gas chromatography/mass spectrometry reporting module coupled with GCMSsolution enables high-throughput drug testing laboratories to address specific productivity and QA/QC requirements. Corrective action plans established by most regulatory methods can be automated and samples may be evaluated during batch sequence injections for a variety of QA/QC parameters. Intelligent sequencing allows review and real-time corrective action during sample analysis without analyst intervention, increasing the likelihood of successful batch analysis while saving valuable time and minimizing sample loss.

This module allows the user to define the control standards concentration along with the appropriate QA/QC criteria. The QC standards and percent difference from the theoretical concentrations are then analyzed. The end result is a simple, easy-to-read summary that clearly states if the sample has passed or failed. Information such as standards concentration, internal standards, and QC limits are contained in a central point look-up table that can be shared between multiple instruments.



	A	B	C	D	E	F	G	H	I
1	Compounds	Full Compound Name (optional)	ISTD Compound	40% Mean Conc.	125% Mean Conc.	± %Control	Lowest Level of Quantitation		
2	NOR		NOR-d5	120	375	20	120	Import GCMS Data File	
3	OXA		OXA-d5	120	375	20	120		
4	AHA		AHA-d5	60	187.5	20	60		
5									

Customized but flexible reporting formats allow quick and effortless review of each sample result within a batch run to determine QC and target compound identification.

Target analyte results are presented in a well-organized format that allows easy review of target compound results. Identification criteria that do not pass are specifically flagged. The batch summary report contains a concise, one-line summary of results for each sample in a batch.

Batch Summary Report

Quantitation Summary, Amount Units = ng/ml
 Q-Qualifier Ratio Failure
 I - Internal Standard Ratio Failure

Vial	Filename	Sample Name	NOR	OXA	AHA
1	STD-0001_7102006_2	STD-0001	300	300	150
2	40 control UNK-0001_7102006_3	40% UNK-0001	122.205	118.436	114.993
3	125 control UNK-0001_7102006_4	125% UNK-0001	395.257	428.469	213.409
45	Solvent__7102006_1		NF	NF	NF
4	1 Unknown-0001_7102006_5	UNK-0001	NF	NF	252.351
5	2 Unknown-0001_7102006_6	UNK-0001	NF	NF	206.055
6	3 Unknown-0001_7102006_7	UNK-0001	615.189	.000 Q	.000 Q
7	4 Unknown-0001_7102006_8	UNK-0001	.000 Q	.000 Q	.000 Q
8	5 Unknown-0001_7102006_9	UNK-0001	.000 Q	NF	.000 QI
9	6 Unknown-0001_7102006_10	UNK-0001	NF	NF	.000 Q
10	7 Unknown-0001_7102006_11	UNK-0001	NF	272.499	.000 Q



Shimadzu QA/QC Report

Data File C:\Documents and Settings\mjwaller\My Documents\NIDA data\STD-0001_7102006_2.qgd
Method File C:\Documents and Settings\mjwaller\My Documents\NIDA data\BZP_SIM.qgm

ID#	Name	m/z	P.T. Ret Time (min)	Detection Window (min)
1	NOR-d5	347.15	4.94	4.904 - 4.977
2	NOR	341.1	4.947	4.911 - 4.984
3	OXA-d5	435.15	5.18	5.142 - 5.217
4	OXA	429.15	5.186	5.149 - 5.223
5	AHA-d5	386.2	6.677	6.635 - 6.719
6	AHA	381.1	6.685	6.642 - 6.727

ID#: 1 **Name:** NOR-d5 **RT(min):** 4.94

m/z	Area	Conc	Ref Ion Ratio	Ratio Range	Criteria
Type: ISTD 347.15	1650416	300ng/mL			
Ref Ion# 1 348.15	418745		25.37	20.3 - 30.45	Pass

ID#: 2 **Name:** NOR **RT(min):** 4.947

m/z	Area	Conc	Ref Ion Ratio	Ratio Range	Criteria
Type: Target 341.10	1678007	300ng/mL			
Ref Ion# 1 327.10	339825		20.25	16.2 - 24.3	Pass
2 343.10	811942		48.39	38.71 - 58.06	Pass

ID#: 3 **Name:** OXA-d5 **RT(min):** 5.18

m/z	Area	Conc	Ref Ion Ratio	Ratio Range	Criteria
Type: ISTD 435.15	759433	300ng/mL			
Ref Ion# 1 420.15	192657		25.37	20.3 - 30.44	Pass

ID#: 4 **Name:** OXA **RT(min):** 5.186

m/z	Area	Conc	Ref Ion Ratio	Ratio Range	Criteria
Type: Target 429.15	1042338	300ng/mL			
Ref Ion# 1 431.20	608383		58.37	46.69 - 70.04	Pass
2 313.10	313343		30.06	24.05 - 36.07	Pass

ID#: 5 **Name:** AHA-d5 **RT(min):** 6.677

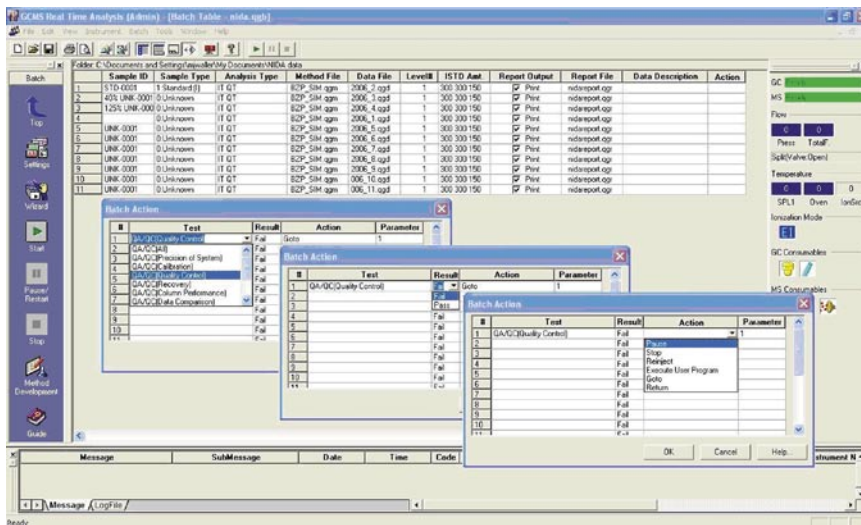
m/z	Area	Conc	Ref Ion Ratio	Ratio Range	Criteria
Type: ISTD 386.20	877187	150ng/mL			
Ref Ion# 1 401.20	315192		35.93	28.75 - 43.12	Pass

ID#: 6 **Name:** AHA **RT(min):** 6.684

m/z	Area	Conc	Ref Ion Ratio	Ratio Range	Criteria
Type: Target 381.10	551912	150ng/mL			
Ref Ion# 1 383.15	270873		49.08	39.26 - 58.9	Pass
2 396.15	246427		44.65	35.72 - 53.58	Pass

This user-friendly tool enhances laboratory productivity by automating the data processing and reporting tasks associated with the daily workflow of drug screening analysis. Coupled with the QA/QC functionality that is available within GCMSsolution software, this powerful tool gives the user the ability to easily analyze their data, and saves time by allowing the sample to be re-injected or analyses to be stopped if QA/QC criteria are not met. Data review can be done immediately after acquisition, and corrective action can take place without user intervention.

Batch sequence injections may be evaluated for a variety of QA/QC parameters, including sample upper/lower limits, precision, recovery, spiked samples, and blank samples. GCMSsolution uses pass/fail criteria to evaluate each injection and automatically executes the appropriate user-defined corrective actions, which include rerun, stop, pause, goto, and return commands. Intelligent batch sequencing allows the end user to save valuable time and minimize the loss of valuable samples.



Fully Automated