



Laboratory Data Management and Reporting

Mid-Atlantic EQUIS Users Group Meeting

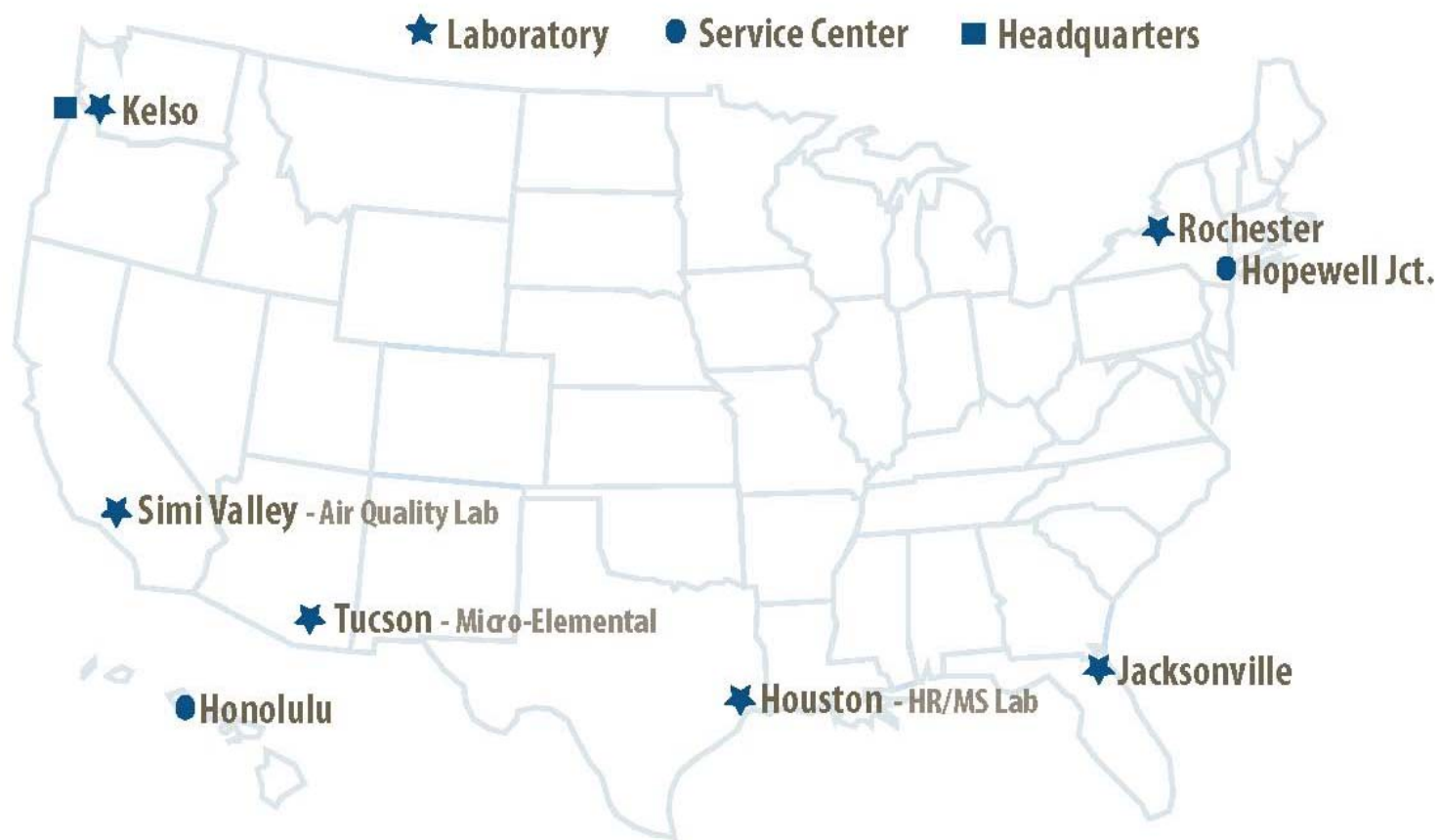
August 2011

Company Information

Founded	1986
Employee-owned since	1997
Laboratories	Six
Service Centers	Two
Total Staff	450
Annual Revenue	\$45M

In the Top 5 Labs Nationwide

Columbia Analytical Network



Columbia Analytical Services

- Routine Full Service Analysis
 - Low-Level Trace Analysis
 - Sediment / Tissue Programs
 - Porewater /Elutriate Testing
 - Drinking Water Testing
 - HR/MS - Dioxins/Furans, PCB congeners
-



Columbia Analytical Services

- Mining / Treatability Testing
- Emergent Contaminants
- Endocrine Disruptors
- Pharmaceutical and Personal Care Product Residues (PPCPs)



Columbia Analytical Services

- Fuels / Product Testing
- Passive Sampling Devices
- Import/Export Permits
- Boiler MACT Testing
- Air Quality Testing Programs



Air Quality Services

- AIHA and NELAP accredited
 - Ambient Air Testing
 - Stationary Source Testing
 - Indoor Air Quality
 - Soil Vapor Testing
 - Vapor Intrusion Testing
 - Industrial Hygiene Consulting
 - Landfill Gas Testing
 - New “Odor Scan”™ Testing
 - Sulfur Speciation Testing
-



Certifications / Accreditations

- NELAP Accredited Network
- Certified in 40 States
- DOD-ELAP Accredited
- U.S. Air Force /AFCEE
- U.S. Navy / NFESC
- U.S. Army / ASCE
- American Industrial Hygiene Association (AIHA)



US Army Corps
of Engineers®



Technical Expertise

- Industrial Process Testing
- Import / Export testing
- Pharmaceutical and Life Sciences Testing (FDA / R&D)
- Creative Problem Solving

Technical Expertise

- Method Research and Development
 - Emergent Chemicals
 - Unregulated Compounds
 - Analytical Consulting
 - Forensics and Litigation Support
 - Electronic Data Management
-

Data Management and Reporting

- How do we manage all these data ?
- Network Data Management
- Project Data Tracking
- Electronic Data Reporting
- Work Flow Process
- Hardware + Software Infrastructure



What is a LIMS?



- Laboratory Information Management System (LIMS) = Network-wide System + Modules for Data Reporting, etc.
 - Sample ID, Matrix, Test, Analyte, DQOs
 - Analyte-specific Data for each Sample
 - Tracks all data review /rework / release / data reporting / report revisions
 - Queries / Management Reports
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System Platform

- Columbia Analytical uses Server / Local Area network (LAN) configuration
- Columbia Analytical standardized on Microsoft (MS) Windows applications (i.e., Word, Outlook, Excel, Access, MS Exchange)
- Columbia Analytical Oracle® database LIMS

Data Management Tools

- Virtually every piece of information in the laboratory network is managed electronically in LIMS
- Data are generated and stored electronically on a single network-wide LIMS
- Data move from department to department electronically via the LIMS
- Data reports generated electronically from LIMS
- Data uploads via LIMS to client / agency database

Data Management Work Flow

Project Set-up / Sample Receipt



Data Analysis / Acquisition / Review

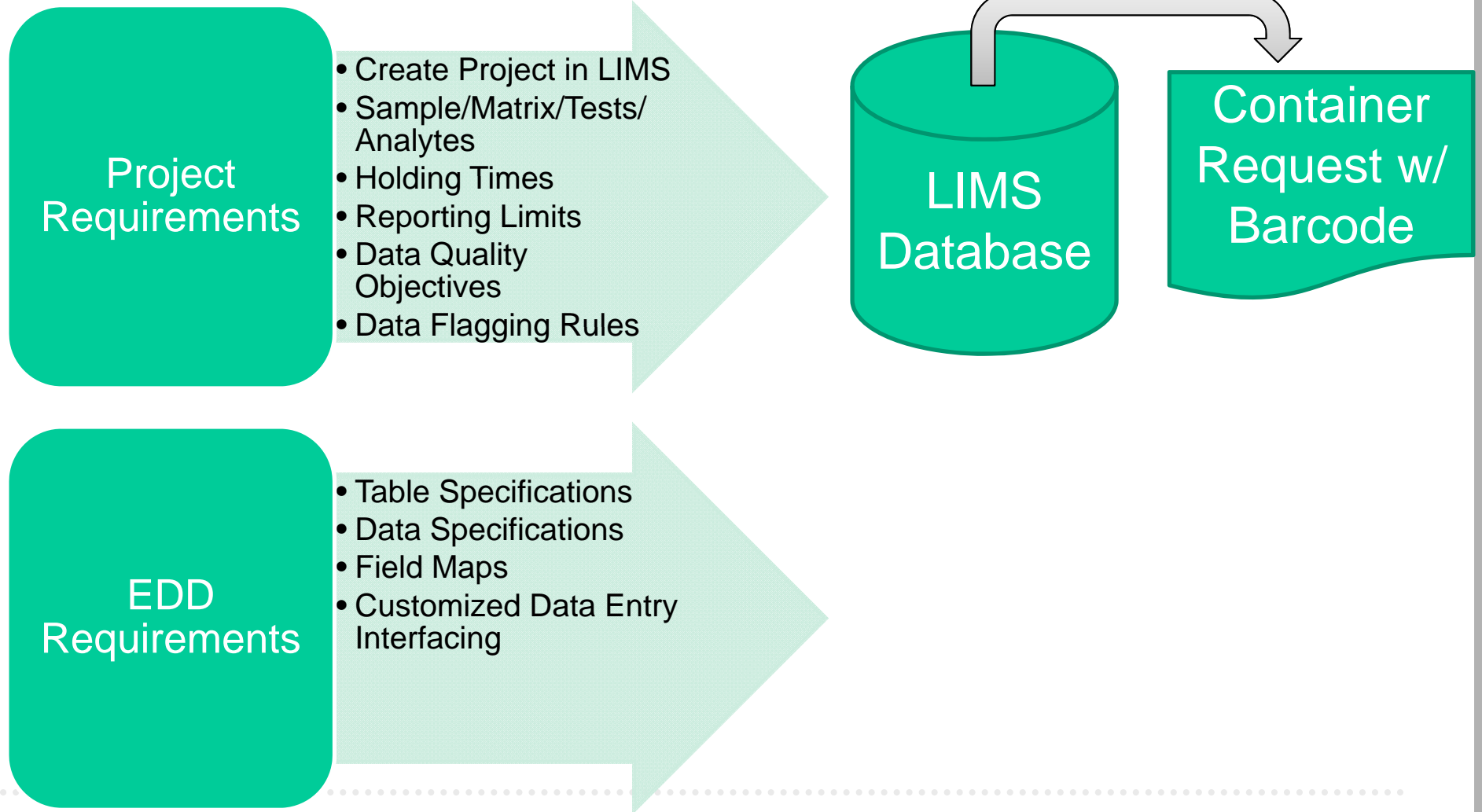


Report Generation / Production



Sample Disposal / Archiving

Project Setup



Data Reporting Levels

	Tier I	Tier II	Tier III	Tier IV
Transmittal Letter	✓	✓	✓	✓
Case Narrative	*	✓	✓	✓
Method Blank Results	✓	✓	✓	✓
Surrogate Recovery Results	✓	✓	✓	✓
Chain-of-Custody Documentation	✓	✓	✓	✓
Matrix Spike Results		*	✓	✓
Duplicate Results		*	✓	✓
Laboratory Control Sample (LCS & Dup) Results		✓	✓	✓
CLP Data Forms			✓	✓
Raw Data				✓

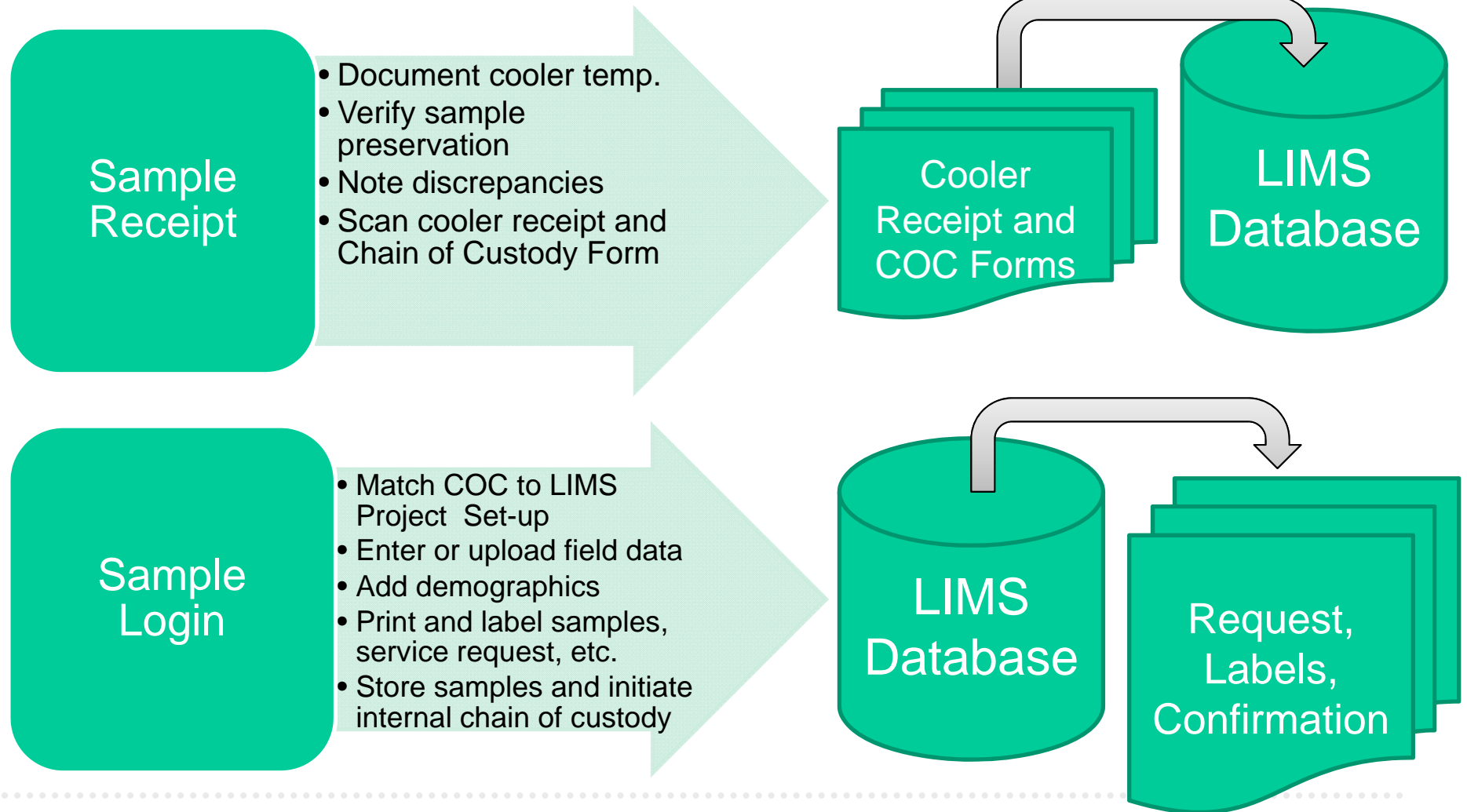
* Client Specific Only

Basic EDD Specifications

Electronic Data Deliverable (EDD) Sample

COL #	COLUMN TITLE	DESCRIPTION
1	Client	Client name as it appears on the chain of custody.
2	Project	Project name and number as it appears on the c.o.c.
3	Service Request	Lab. Service Request number
4	Sample	Client Sample ID
5	Lab Code	Lab. Sample ID
6	Sample Type	i.e. SMPL, MS, DMS, DUP, LCS, DLCS
7	Date Collected	Date sample was collected (mm/dd/yyyy)
8	Date Received	Date sample was received by lab (mm/dd/yyyy)
9	Date Extracted	Date sample was extracted/preped (mm/dd/yyyy)
10	Date Analyzed	Date sample was analyzed (mm/dd/yyyy)
11	Extraction Method	Extraction or prep method code
12	Method	Analysis method code
13	Matrix	Sample matrix
14	Basis	Dry, Wet, NA
15	Units	Unit of measure for result
16	Component	Compound or Analyte name
17	Dilution Factor	Factor of dilution i.e. for a 10:1 dilution, the dilution factor is 10
18	Reporting Limit	Method Reporting Limit i.e. MRL, PQL
19	Detection Limit	Method Detection Limit i.e. MDL, IDL
20	Result	Concentration of component found in sample
21	Result Notes	Qualifiers and footnote flags
22	Spike	Concentration of spike compound (spike conc) Concentration
23	Percent Recovery	Percent amount recovered
24	Acceptance Limits	Upper and Lower acceptance limits
25	Average	
26	RPD	Relative Percent Difference
27	Retention Time	For TICs
28	Regulatory Limit	For TICs

Sample Receipt and Log-In



Log Samples into LIMS

- Project bar code report facilitates matching samples to SDG in LIMS
- Log sample information, field data, and demographics to LIMS



T002385

Client Name:

Project Name:

Project Number:

Sample Group:


Project Manager:

Project Chemist: Jerry Allen

CAS Location: Columbia Analytical Services, Inc.
9143 Philips Highway
Suite 200
Jacksonville, FL
32256

Please return this report along with the Chain of Custody or set of samples.

Sample Receipt Confirmation

- Sample acknowledgement report
- EQUIS EDGE sample receipt EDD as confirmation. 



9143 Philips Highway
Suite 200
Jacksonville, FL 32256

Confirmation of Sample Receipt

To:		From:	Jerry Allen
Email:		Email:	JAllen@caslab.com
Fax:		Fax:	
Phone:		Phone:	904-739-2277 x4410

Samples for analysis have been received by Columbia Analytical Services on 8/18/11 and assigned our Service Request number **J1103645**. Please verify the following information and notify me of any corrections as soon as possible.

The estimated completion date for this work is: 9/1/11

Client:
Project:

PO Number:

EDD Required:

Tier: 1

Report To:

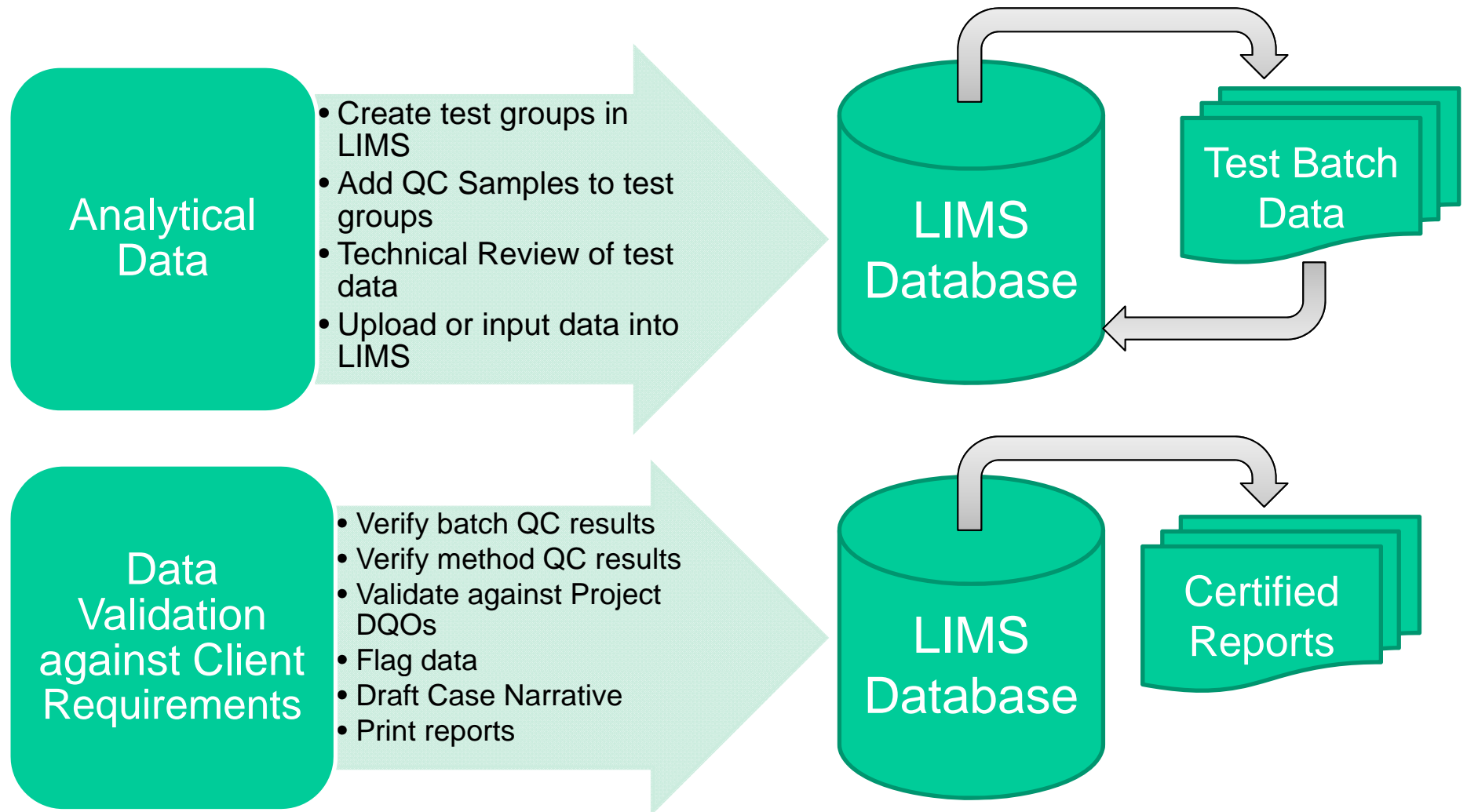
Billing Address:

Comments:

Thank you for your business!



Analytical Testing / Validation



Instrument Data Acquisition

- Metals (MARRS)
- Organics (Stealth)
- Instrument Data Acquisition, Data Reduction, Data Verification, Data Validation, Data Reporting
- Systems Function as LIMS Modules

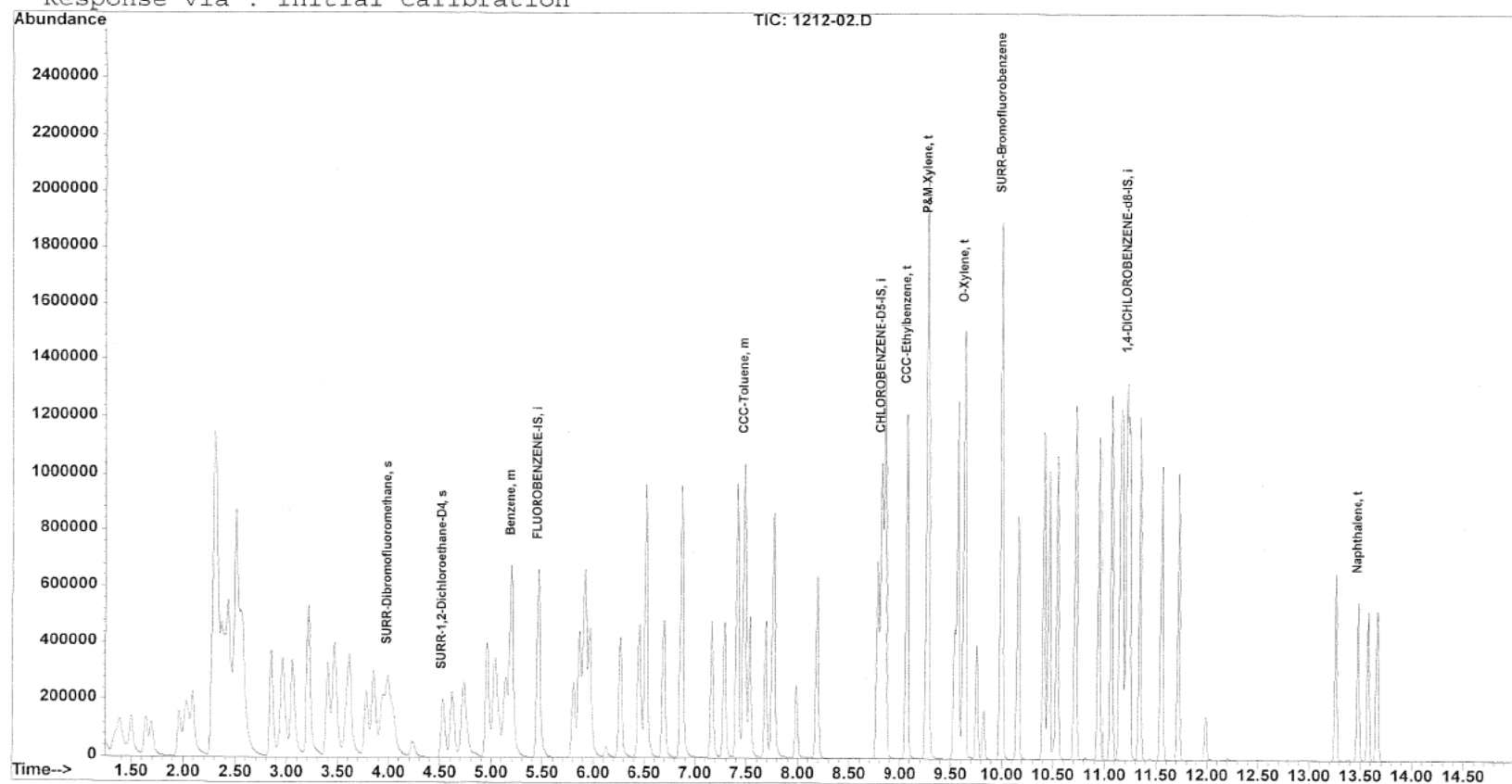
Instrument Data Acquisition Example

Acq On : 12 Dec 2007 4:05 am
Sample : J0701212-CCV
Misc :
MS Integration Params: rteint.p
Quant Time: Dec 12 6:40 19107

Operator: JWA
Inst : MS52
Multiplr: 1.00

Quant Results File: BTEX.RES


Method : D:\HPCHEM\1\METHODS\BTEX.M (RTE Integrator)
Title : VOA by EPA 5030/5035/8260B
Last Update : Mon Dec 08 17:08:54 2003
Response via : Initial Calibration



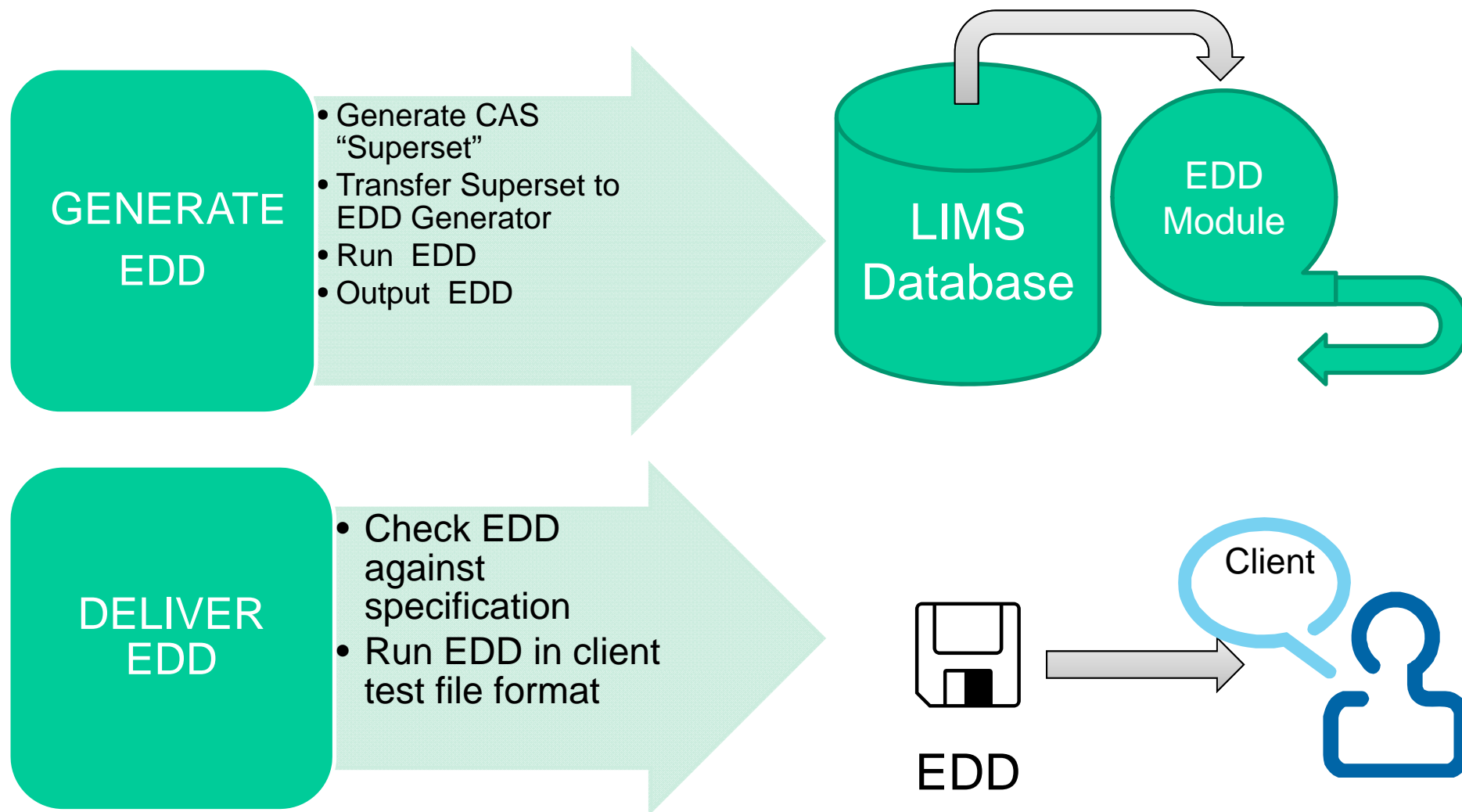
Data Validation to Project DQOS

- Validation routine compares test data, batch QC, Initial and Continuing Calibrations (ICAL / CCV), etc. against project requirements
 - System returns a set of validation reports to the analyst for review
 - Validated data is ready for reporting
 - Data “Superset” generated for EDD
-

Data “Superset” File

- Data “Superset” file has 105 fields including: project information, sample demographics, matrix, test, analyte, chemical abstract number, analytical results, result demographics, QC results, QC criteria, data qualifiers, and raw data records 
 - Large data set allows flexibility to meet most client EDD requirements
-

EDD Generation and Delivery



EDD Module for Data Reporting

- EDD Module can be part of a LIMS or custom software developed by a Lab
- Three primary functions:
 - Translate laboratory data to client-specified format (e.g., naming conventions, field order, field formats, etc.)
 - Organize laboratory data into custom client-specific EDD format
 - Standardize process to produce EDDs

Data Reduction / Reporting

- Data “Super Set” is created
 - Proprietary program Electronic Data Deliverable Generator (EDDGE)
 - EDDGE program normalizes data and translates necessary Columbia Analytical internal valid values into Client-specific valid values
 - EDDs created from EDDGE System
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Project Specifications / DQOs

- QAPPs
- Data Quality Objectives
- Project Limits Tables
- Data Reporting detail
- EDD Specs
- Project specifications stored in LIMS



Project DQOs / QAPPs / Specs

- Project-specific data quality objectives are used to build project-specific table of data validation criteria
- Project-specific criteria are used to verify data is generated / reported compliant with project data quality objectives

Example DQO Table in LIMS

Method ID	Analytical Method	Preparation Method	Matrix	Level	Active	Method Title	Method Comment	Last Date/Time	Last User	Liter. Sour
MJ100	160.3M	NONE	SOIL	LOW	Y	Total Solids		04/04/2001 18:20:03	WNagel	SW-4
MJ101	524.2	METHOD	WATER	LOW	Y	GC/MS Volatiles in Drinking Water		08/16/2011 15:11:34	JJames	40 C
MJ102	608	EPA 3520C	WATER	LOW	Y	Organochlorine Pesticides		04/06/2011 13:46:10	LPortwo	40 C
MJ104	625	EPA 3520C	WATER	LOW	Y	Semivolatile GCMS for Waste Water		08/08/2011 10:53:48	CDegner	40 C
MJ106	8082A	EPA 3520C	WATER	LOW	N	PCB Congeners in Water		07/14/2006 15:47:17	JHeston	SW-4
MJ107	8081B	EPA 3520C	WATER	LOW	N	OC Pest in Water		04/30/2009 15:17:46	AKamawal	SW-4
MJ108	8081B	EPA 3545	SOIL	LOW	N	OC Pest in Soil		03/20/2006 09:30:44	JHeston	SW-4
MJ109	8081B	EPA 3540C	SEDIMENT	LOW	N	OC Pest in LL-Sediment/Soil		11/03/2009 16:52:04	AKamawal	SW-4
MJ110	8081B	EPA 3510C	WATER	LOW	N	OC Pest in TCLP-Water		04/30/2009 15:19:13	AKamawal	SW-4
MJ111	8081B	EPA 3520C	WATER	LOW	N	AFCEE V 3.1 OC Pest Waters		04/30/2009 15:19:17	AKamawal	SW-4
MJ112	8081B	EPA 3545	SOIL	LOW	N	AFCEE V 3.1 OC Pest Soil		03/20/2006 09:30:47	JHeston	SW-4
MJ119	8260C	EPA 5030B	WATER	LOW	Y	Volatile Organics in Water		08/10/2011 10:11:00	KReasone	SW-4
MJ120	8260C	EPA 5030A	SOIL	LOW	Y	Volatile Organics in Soil		08/16/2011 16:26:49	KReasone	SW-4
MJ121	8270C	EPA 3520C	WATER	LOW	Y	Base Neutral/Acid Semivolatile Organic compounds		08/16/2011 12:35:41	CDegner	SW-4
MJ126	AK102	EPA 3510C	WATER	LOW	Y	Alaska Diesel Range for Water		07/28/2010 11:39:25	JMSmith	

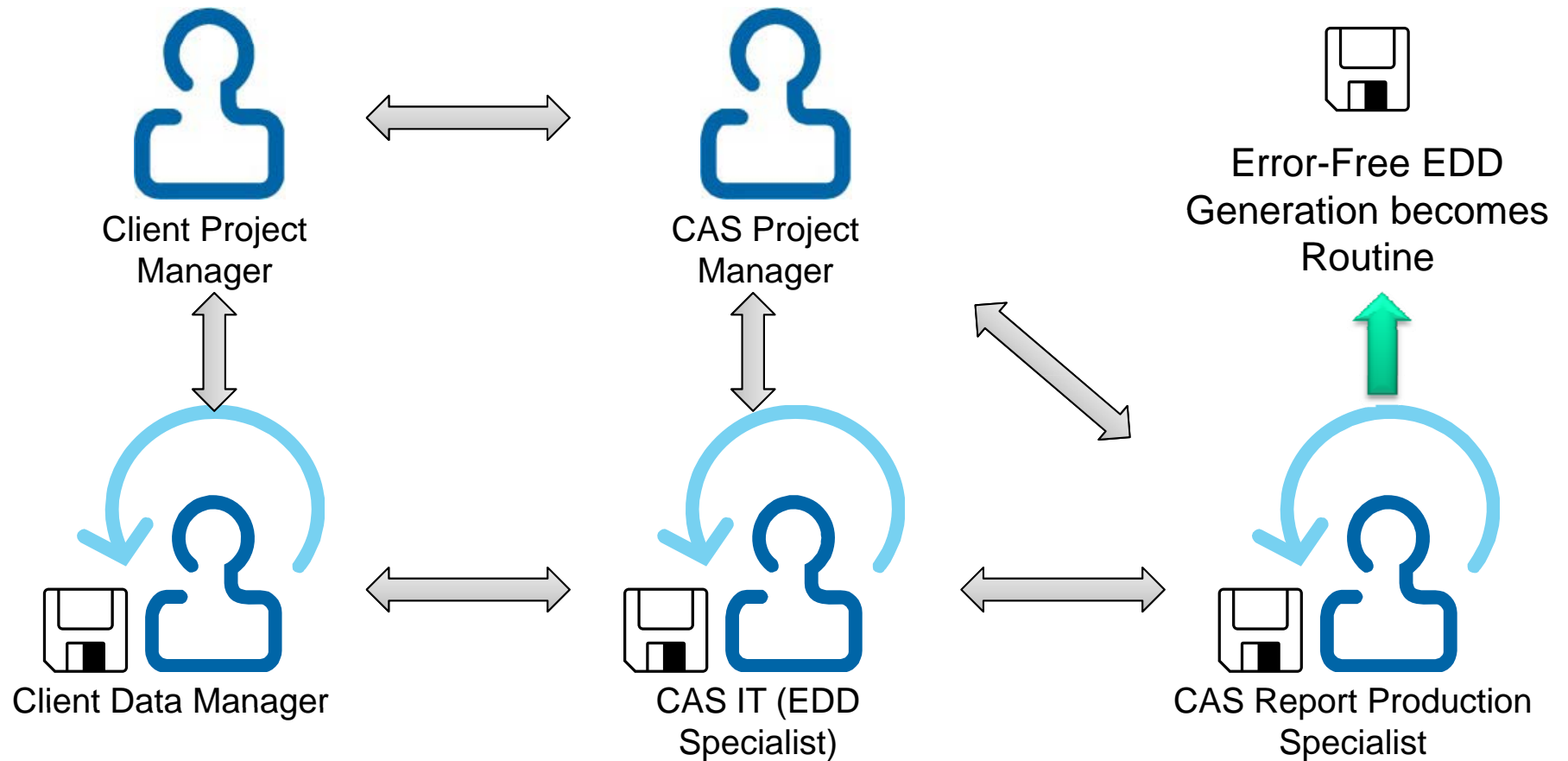
Compound Name	Type	Cal Type	MDL	MRL	LOD	Low MS/Sur	High MS/Sur	DMS %Diff	Low LCS	High LCS	DLCS %Diff	Rpt. Units	Spike Amount	Surr X Dif	Surr Ref Name
1,4-Dichlorobenzene-d4	INT_STD					.5	2					ug/L	40		
Acenaphthene-d10	INT_STD					.5	2					ug/L	40		
Chrysene-d12	INT_STD					.5	2					ug/L	40		
Naphthalene-d8	INT_STD					.5	2					ug/L	40		
Perylene-d12	INT_STD					.5	2					ug/L	40		
Phenanthrene-d10	INT_STD					.5	2					ug/L	40		
1,2,4-Trichlorobenzene	MS	CCC	0.355	10		49	97	30	51	103	30	ug/L	100		
1,4-Dichlorobenzene	MS	CCC	0.317	10		47	93	30	54	96	30	ug/L	100		
2,4-Dinitrotoluene	MS	CCC	0.274	10		62	123	30	61	126	30	ug/L	100		
2-Chlorophenol	MS	CCC	0.311	10		49	100	30	59	101	30	ug/L	100		
4-Chloro-3-methylphenol	MS	CCC	0.490	10		61	111	30	65	111	30	ug/L	100		
4-Nitrophenol	MS	SPCC	1.92	25		57	119	30	55	126	30	ug/L	100		
Acenaphthene	MS	CCC	0.281	10		57	107	30	61	110	30	ug/L	100		
N,N-Dimethylaniline	MS	CCC	2.22	10		70	130	30	70	130	30	ug/L	100		
N-Nitrosodi-n-propylamine	MS	SPCC	0.496	10		53	109	30	56	115	30	ug/L	100		
Pentachlorophenol	MS	CCC	2.44	25		42	127	30	60	116	30	ug/L	100		
Phenol	MS	CCC	0.324	10		47	101	30	48	105	30	ug/L	100		
Pyrene	MS	CCC	0.731	10		52	121	30	53	124	30	ug/L	100		
2,4,6-Tribromophenol	SURR					46	127					PERCENT	150	Yes	
2-Fluorobiphenyl	SURR					48	114					PERCENT	100	Yes	
2-Fluorophenol	SURR					39	103					PERCENT	150	Yes	
Nitrobenzene-d5	SURR					46	115					PERCENT	100	Yes	
Phenol-d6	SURR					38	107					PERCENT	150	Yes	
Terphenyl-d14	SURR					22	146					PERCENT	100	Yes	
1,4-Dinitrobenzene	TIC_TRG		10	10		70	130	30	70	130	30	ug/L	100		
1-Methylnaphthalene	TIC_TRG		10	10								ug/L	100		
2,3,7,8-Tetrachlorodibenzo-p	TIC_TRG		50	50								ug/L	100		
4,4'-Methylenebis[2-chloroa	TIC_TRG		25	25		70	130	30	70	130	30	ug/L	100		
alpha-Terpineol	TIC_TRG		10	10								ug/L			
Chloroacetaldehyde	TIC_TRG		10	10								ug/L			
HPMD	TIC_TRG		6.15	25								ug/L			
DPMD	TIC_TRG		3.86	25								ug/L			
Paraldehyde	TIC_TRG		10	10								ug/L			
Iotbene diisocyanate	TIC_TRG		10	10								ug/L			
1,2,4,5-Tetrachlorobenzene	TRG		0.26	10		70	130	30	70	130	30	ug/L	100		
1,2-Dichlorobenzene	TRG		0.431	10		47	94	30	55	97	30	ug/L	100		
1,2-Diphenylhydrazine	TRG		0.509	10		54	118	30	58	117	30	ug/L	100		
1,3,5-Trinitrobenzene	TRG		0.38	25		70	130	30	70	130	30	ug/L	100		
1,3-Dichlorobenzene	TRG		0.352	10		45	92	30	55	95	30	ug/L	100		

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MJ120	8260C	EPA 5030A	SOIL	LOW	Y	Volatile Organics in Soil		08/16/2011 16:26:49	KReasone	SW-1
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MJ126	AK102	EPA 3510C	WATER	LOW	Y	Alaska Diesel Range for Water		07/28/2010 11:39:25	JMSmith	

Reg. Limit	Min RF	Max RT Shift	Max RRT Shift	Max %RSD	Min Linear R2	Min Quadratic R2	CCV %Diff	ICV Amount	ICV Units	ICV %Diff	Chem. Abs. #	Comment	Last Dat
		0.5						40	ug/ml		3856-83-1		03/30/2
		0.5						40	ug/ml		15067-26-2		07/07/2
		0.5						40	ug/ml		1719-03-5		03/30/2
		0.5						40	ug/ml		1146-65-2		03/30/2
		0.5						40	ug/ml		1520-96-3		03/30/2
		0.5						40	ug/ml		1517-22-2		03/30/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	120-82-1		07/26/2
0.01	0.5	0.06	15	0.990	0.990		20	100	ug/ml	20	106-46-7		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	121-14-2		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	95-57-8		07/26/2
0.01	0.5	0.06	15	0.990	0.990		20	100	ug/ml	20	59-50-7		07/26/2
0.05	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	100-02-7		07/26/2
0.01	0.5	0.06	15	0.990	0.990		20	100	ug/ml	20	83-32-9		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	121-69-7		07/26/2
0.05	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	621-64-7		07/26/2
0.01	0.5	0.06	15	0.990	0.990		20	100	ug/ml	20	87-86-5		07/26/2
0.01	0.5	0.06	15	0.990	0.990		20	100	ug/ml	20	108-95-2		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	129-00-0		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	118-79-6		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	321-60-8		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	367-12-4		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	4165-60-0		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	13127-88-3		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	1718-51-0		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	100-25-4		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	90-12-0	This compound is searched	02/01/2
											1746-01-6	This compound is searched	07/07/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	101-14-4	This compound is searched	02/01/2
											10482-56-1	This compound is searched	07/07/2
											107-20-0	This compound is searched	07/07/2
											3375-84-6	This compound is searched	07/07/2
											CASID30031	This compound is searched	07/07/2
											123-63-7	This compound is searched	03/30/2
											CASID30165	This compound is searched	03/30/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	95-94-3		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	95-50-1		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	122-66-7	This compound is	07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	99-35-4		07/26/2
0.01	0.5	0.06	15	0.990	0.990		30	100	ug/ml	30	541-73-1		07/26/2

EDD Development Process



Client EDD Spec is Important

- ✓ EQulS EDD spec is extremely detailed
- ✓ Laboratories address a wide variety EDD requests and formats
- ✓ All client project specifications may not captured in basic EQulS EDD spec

EDD Checker Routines

- EQUIS EDD checker routines
 - State-Specific (NJDEP, NYSDEC, etc.)
 - USEPA Region-specific EDD checkers
 - USEPA SEDD online checker
 - Laboratory Data Consultants (Adapt)
 - Alaska Corps of Engineers (COELT and SEDD Savvy)
 - CA Dept of Water Resources GEOTRACKER
 - U.S. Air Force ERPTOOLS X
-

Electronic Data Deliverable Formats

- EQuIS EZ and 4-file formats (with checker)
- ADR/ADAPT, GIS\Key, Locus EIM, EnviroData
- EDF for GeoTracker (COELT 1.2i w/EDCC)
- State-specific formats (NJ, NY, AZ, CA, TX, etc.)
- Federal Programs formats (ERRIS, etc)
- USEPA formats (SEDD, etc)
- Client-Custom EDD formats

EDD Formats Supported

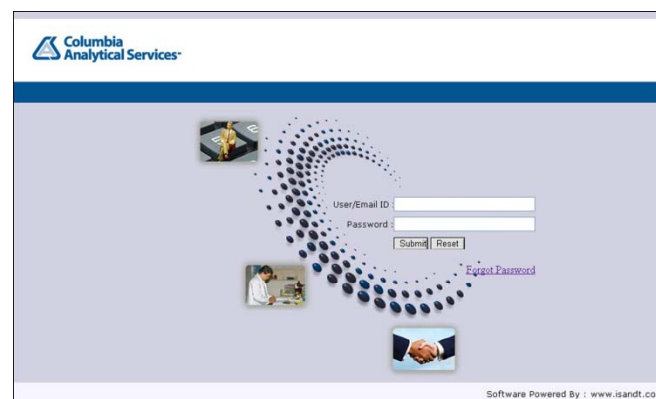
- CAS supports more than 500 EDD formats

- **ADR/Adapt - Laboratory Data Consultants**
- **GISKey - GIS/Solutions**
- **ArcInfo - ESRI GIS + Mapping Software Product**
- **EQiS/EDP Earthsoft Environmental Quality Information System**
- **SEDD - USEPA Staged Electronic Data Deliverable, Level 2a**
- **COELT - Corps of Engineers Loading Tool**
- **EPA Region 3 Format**
- **EPA Region 4 Format**
- **EPA Region 5 Format**
- **Geotracker /EDF - Cal EPA State Water Resources Control Board**

- **ERPIMS/ERPTOOLS - Environmental Resources Program Information Management System**
- **Navy CLEAN - US Navy Comprehensive Long Term Environmental Action Navy**
- **AZDEQ - Arizona Department of Environmental Qualifier**
- **NJPEP / Hazsite EDS - New Jersey Department of Environmental Protection**
- **RIBS - New York Department of Environmental Conservation**
- **TRRP - Texas Commission on Environmental Quality Risk Reduction Program**

Electronic Data Transfer / Delivery

- Data electronic transfer options from LIMS:
 - FTP Web Site <https://clients.caslab.com>
 - Email file attachment
 - Diskette or CD-ROM
 - Hard Copy
 - File Uploads





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