

DeltaSoft's ChemCart



An integrated suite of applications that leverage
ChemAxon components

DeltaSoft, Inc.

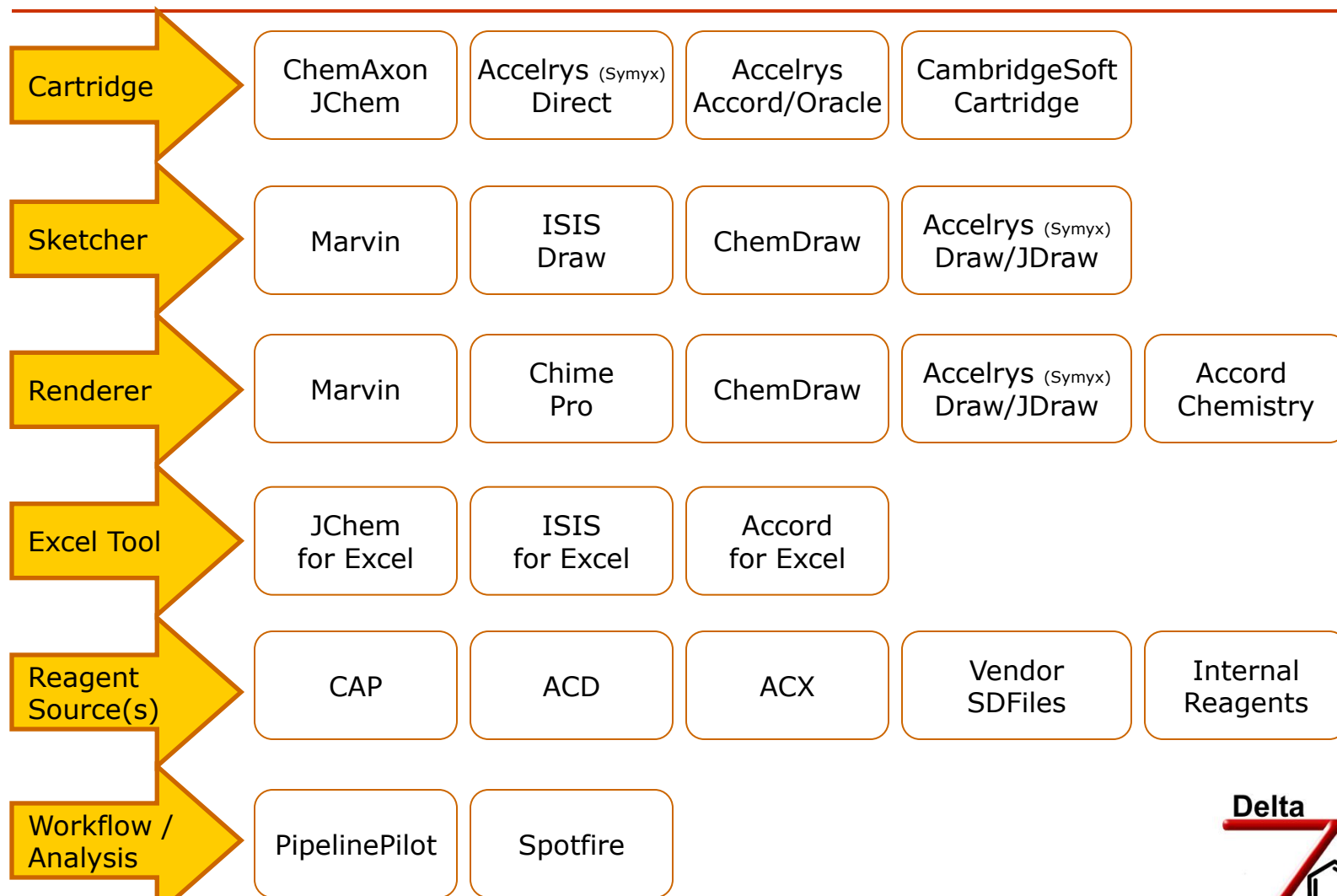
- ❑ Specializing in R&D Informatics since 1996
- ❑ Commercial software applications
 - ChemCart
 - ❑ web interface to research data
 - ChemCart Applications
 - ❑ Compound Registration
 - ❑ Reagent Inventory
 - ❑ Sample Inventory
 - ❑ Electronic Laboratory Notebook
 - ❑ BioAssay
 - ❑ Structure Activity Browser
 - ❑ Custom Synthesis Tracker
- ❑ Services

DeltaSoft's Discovery Informatics Expertise

- ❑ Cheminformatics & Bioinformatics
- ❑ Application Design, Development, Integration
- ❑ Chemistry Cartridge Evaluation and Tuning
- ❑ Oracle Optimization and Support
- ❑ Data Model Design
- ❑ Strategic Planning



Component Approach – Choice!



ChemCart

Project Summary Form

Chemical Structure: CN(C)CC(=O)c1ccccc1

CompID	MW	MF
DS-00001	177.2455	C ₁₁ H ₁₆ N ₂ O

H-Acceptor	H-Donor	LogP
2	0	1.403

LC50 Results

Panel	Cell	sLogIC50
LNS	NCI-H23	4.09
LNS	NCI-H22	4.98
LNS	A549/ATCC	4.00
LNS	ERVX	4.07
LNS	NCI-H226	4.00
LNS	NCI-H223M	4.00
LNS	NCI-H460	4.04
LNS	HDP-62	4.00
LNS	HDP-19	4.08
LNS	HDP-92	4.09
LNS	L5178	4.17
SCL	DMS 114	4.09
SCL	DMS 273	4.00
COL	HT29	4.02
COL	HCC-2998	4.08
COL	NCI-116	4.06
COL	SW620	4.21
COL	COLO 205	4.12
COL	BLD-1	4.08
FOL	HT-10	4.16

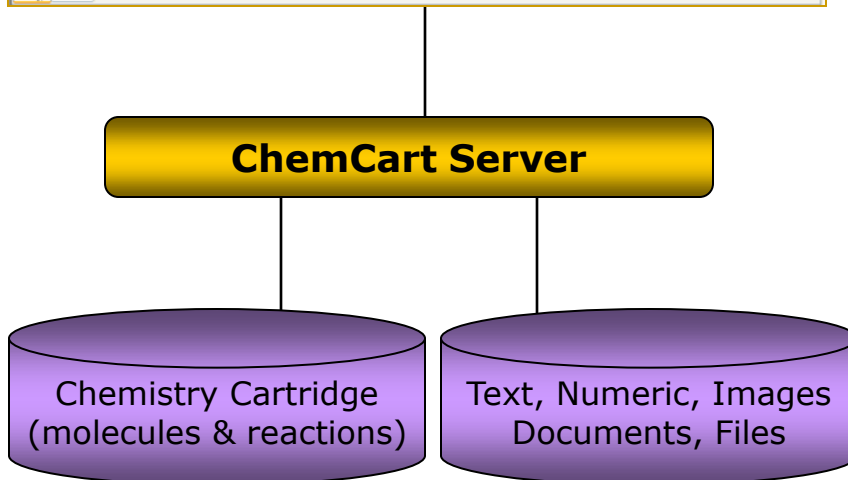
LC50 Details

Point#	LogConc	% Inh
1	-6	0.00
2	-5	0.21
3	-5	4.84
4	-4.5	17.02
5	-4.25	32.56
6	-4	50.16
7	-3.75	66.23
8	-3.5	81.58
9	-3	94.09
10	-2	101.43
11	-1	99.00

Conc. vs % Inh

Mass Spectrum

Dynamic web forms interface to research information, including structures/reactions, data, images, documents & files



Integration with ChemAxon



ChemAxon JChem
Cartridge for Structure
Storage/Searching

ChemAxon JChem
Cartridge for Structure
Calculations (MW, MF)

ChemAxon Marvin for
Structure Sketching/Rendering

ChemAxon Structure
Standardizer / Structure Checker

The screenshot displays the 'Compound Registration' window in ChemAxon JChem. On the left, a chemical structure of N,N-dimethylbenzylamine is shown. The right side contains a registration form with the following data:

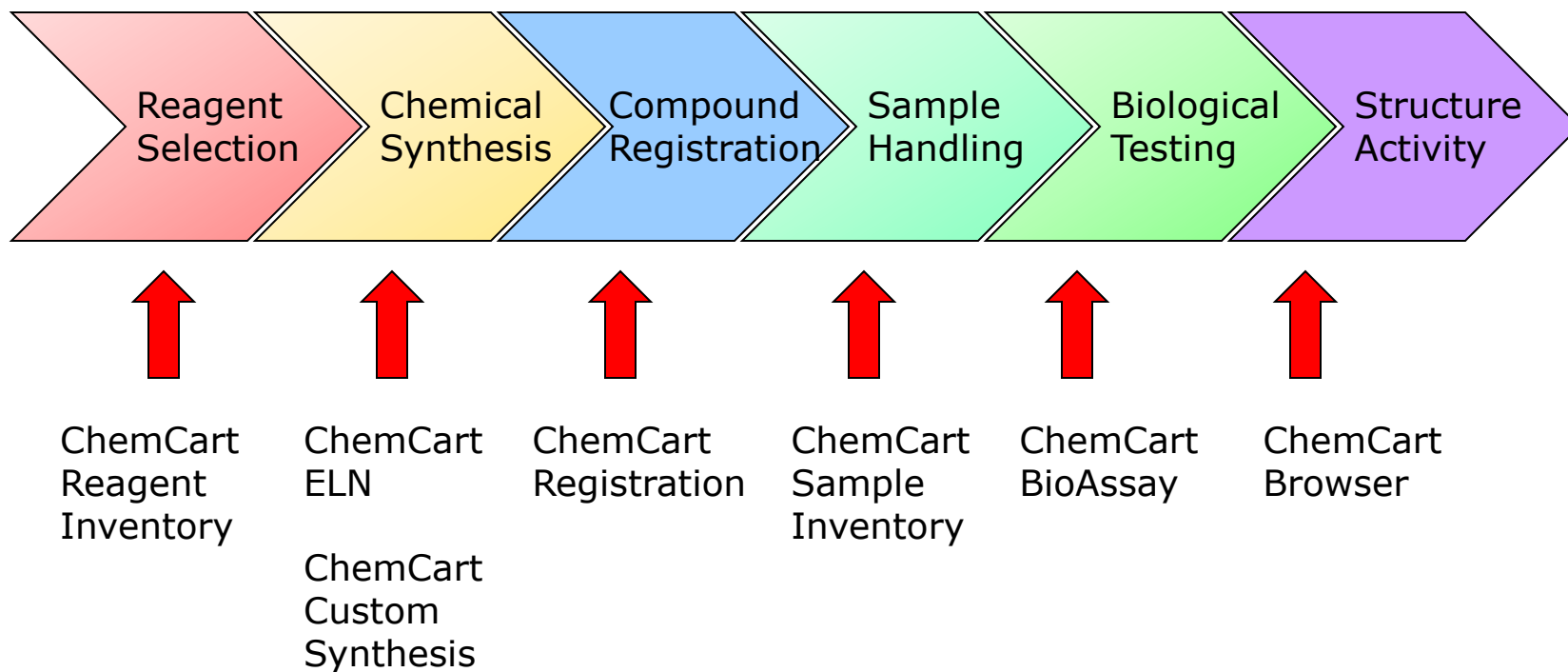
Corp ID	DS1000007	Project	PROJECT1
Reg. No.	1000007	Therapeutic Target	TARGET1
Batch ID	DS1000007-0-1	Solvent	
Mol Formula	C ₁₁ H ₁₅ N O	Solubility	DMSO
Batch Formula	C ₁₁ H ₁₅ N O	Purity	>90%
Mol Weight	177.24	Purification Method	Crystallization
MW with Salt	177.24	Melting Point (°C)	110-111
Exact Mass		Boiling Point (°C)	
Reg Date	21-Apr-2008	Library	Library 105
Reg By	CCADMIN6	External Source	
Alias		External Reg. #	ER 3726

Below the registration form, there are fields for 'Salt Form' (No Salt), 'Notebook Ref' (268-1), 'Amount Submitted' (57 mg), 'Submitter' (CCUSER6), 'Stereochemistry', 'Appearance' (white solid), 'Reference' (JACS, 2006), 'Chemical Name' (amine), and 'Comments' (reserved for Project 1, keep in cold storage).

- Partnered since 2006
- Fully integrated, supporting latest version
- Joint customers using ELN, Registration, BioAssay, Inventory, Search & Browse, Inventory in production



ChemCart Applications



Case #1: Registration

- ❑ Problem: Large chemical company needed to replace aging compound registration system used by several thousand scientists.
- ❑ Solution: ChemCart Registration, JChem Cartridge, Marvin
- ❑ Project Details
 - Standardized and migrated structures from another chemistry engine to JChem
 - Mapped and migrated legacy data to ChemCart Registration
 - Implemented customer specific business rules
 - ❑ Required/optional fields
 - ❑ Controlled vocabulary picklists
 - Integrated with LDAP
 - Configured user interface
- ❑ Application Key Features
 - Registration of parent compounds
 - ❑ and components
 - Duplicate structure checking
 - Validation of field formats
 - Registration reports

The screenshot displays the 'Compound Registration' window in the ChemCart software. It features a menu bar (File, Edit, Form, List, Search, Sort, Update, Tools, Options, Help) and a toolbar with navigation icons. The main area is divided into several sections:

- Structure:** A chemical structure viewer showing a benzamide derivative (N,N-dimethyl-2-phenylacetamide).
- Buttons:** 'New Compound' and 'New Batch' buttons.
- Metadata Table:** A table with fields for Corp ID, Reg. No., Batch ID, Mol Formula, Batch Formula, Mol Weight, MW with Salt, Exact Mass, Reg Date, Reg By, Alias, Project, Therapeutic Target, Solvate, Solubility, Purity, Purification Method, Melting Point (°C), and Boiling Point (°C).
- Form Fields:** Fields for Salt Form, Notebook Ref, Amount Submitted, Submitter, Stereochemistry, and Appearance.
- Reference Section:** Fields for Reference, Chemical Name, and Comments.

At the bottom, there is a status bar with tabs for 'Compound', 'Batch', 'Sample', and 'Spectra'.

Case #2: Reagent Inventory

- ❑ Problem: Multi-site pharmaceutical company needed to streamline reagent inventory tracking processes.
- ❑ Solution: ChemCart Reagent Inventory, JChem Cartridge, Marvin
- ❑ Project Details
 - Loaded supplier catalog information into JChem
 - Mapped and migrated legacy bottle data to ChemCart Reagent Inventory
 - Integrated with existing stockroom request application
 - Configured with barcode readers
 - Integrated with LDAP
- ❑ Application Key Features
 - Access supplier and in-house data
 - Structure searching
 - Configurable categories
 - ❑ Compound
 - ❑ Bottle
 - Safety reports
 - Phase 2: link to purchasing

The screenshot displays the 'Reagent Inventory' application window. At the top, there is a menu bar (File, Edit, Form, List, Search, Sort, Cart, Commercial, In-house, Tools, Options, Help) and a toolbar with navigation icons. The main content area is divided into several sections:

- Header:** Compound ID: MFCD0000653, Formula: C₇H₅ClO, CAS Number: 98-88-4, Mol. Wt.: 140.568.
- Chemical Structure:** A chemical structure of Benzoyl Chloride (C₆H₅COCl) is shown in a box.
- Commercial Sources:** A table listing suppliers, catalog numbers, package sizes, units, prices, currencies, purities, and concentrations.
- In-house Sources:** A table listing internal inventory with columns for Barcode, Supplier, Catalog#, Lot No, Orig Amt, Curr Amt, Units, Date Recd, Date Ordered, Owner, Location, and Exp Date.
- Chemical Name:** BENZOYL CHLORIDE
- Supplier Comment:** CORROSIVE; LACHRYMATORY; MOISTURE-SENSITIVE; TOXIC
- Compound Categories:** corrosive
- Bottle Categories:** reserved

At the bottom of the window, there is a status bar with 'Main History Supplier Info Safety' and a 'Delta' icon.

Case #3: Cloud Implementation

- ❑ Problem: University needed to track experiments, register compounds and associated biological test results, manage compound samples and chemical reagents. No dedicated IT support.
- ❑ Solution: ChemCart Suite (ELN, Reagent Inventory, Registration, Sample Inventory, BioAssay, Browser), JChem Cartridge, Marvin, Amazon Cloud
- ❑ Project Details
 - Installed ChemCart Suite and ChemAxon components in the cloud
 - Migrated structures and biology from local database to enterprise JChem
- ❑ Application Key Features
 - Register from ELN
 - ❑ Record reaction, reagents, products
 - ❑ Track experimental detail
 - ❑ Add documents and images
 - ❑ Submit new compounds / batches

The screenshot displays the ChemCart Suite software interface for recording a chemical reaction. The title is "Synthesis of Aspirin". The reaction is shown as salicylic acid reacting with acetic anhydride to form aspirin and acetic acid. The interface includes a reagent table and a product table.

Structure	Name	Lot#	MF	LR	MW	Act MW	Eq	Theo Mass	Act Mass	mmol	d	Vol
	acid	1-1	C ₇ H ₆ O ₃	Y	138.12	138.12	1	138.12	2.90	18.10		
	anhydride	21-3-4	C ₄ H ₆ O ₃	N	102.09	102.09	1	1.85	1.85	18.10		

Lot#	ID	Structure	MF	MW	Act MW	Eq	Theo Mass	Act Mass	Purity	mmol	% Yield
17-1			C ₉ H ₈ O ₄	180.16	180.16	1	3.261	3.000	100	16.65	92.0
			C ₂ H ₄ O ₂	80.05	80.05	1	1.067	0.000			

Experimental Procedure: A test tube containing salicylic acid was placed in a water bath at 90 C. One drop of 85% phosphoric acid was added from a plastic dropper, followed by 0.3 mL of acetic anhydride. The reactants were mixed and heated at 90 C. When the contents of the test tube were dissolved and colorless, H₂O was added, and the test tube was cooled in an ice bath. The crystalline product was collected in a Hirsch funnel.

Case #4: External Collaborator

- ❑ Problem: Mid-size US pharmaceutical company needed an informatics system that could be accessed in a limited way by external collaborator located in Europe.
- ❑ Solution: ChemCart Suite (ELN, Reagent Inventory, Registration, Sample Inventory, BioAssay, Browser), JChem Cartridge, Marvin
- ❑ Project Details
 - Migrated data from Excel spreadsheets to enterprise JChem
 - Configurable categories Created collaborator-specific applications
 - ❑ ChemCart application level security
 - ❑ Oracle roles and data views
- ❑ Application Key Features
 - BioAssay
 - ❑ Binding, functional, in vivo, DMPK
 - ❑ Documents
 - ❑ Images
 - ❑ Insert from Excel
 - ❑ Bulk loading from CSV

The screenshot displays the ChemCart Suite software interface. At the top, there is a menu bar with options: File, Edit, Form, List, Search, Sort, Update, Tools, Options, Help. Below the menu bar is a toolbar with various icons. The main window is titled "Test Results" and contains a form with the following fields:

- Corp ID: DS-5615
- Lot: 43-1
- Sample (barcode): 100012

Below the form is a table titled "Biological Test Results" with the following columns: Project, Assay Name, Version, Notebook, Page, Cell Line, Result Type, Qualifier, Result Value, Units, Date Created, Entered By.

Project	Assay Name	Version	Notebook	Page	Cell Line	Result Type	Qualifier	Result Value	Units	Date Created	Entered By
CytoTox	CT-1	1	15-1	23	AD38	IC50	=	0.5	uM	21-Apr-2008	CHEMCART
CytoTox	CT-2	1	15-2	34	AD38	IC50	=	0.4	uM	21-Apr-2008	CHEMCART
MitoTox	MT-1	1	16-3	65	MTL	EC90	=	1.4	uM	21-Apr-2008	CHEMCART
Enzyme	E1	1	16-6	14	CEM	IC50	=	10	uM	21-Apr-2008	CHEMCART
Enzyme	E1	1	19-5	45	CEM	IC50	=	11	uM	21-Apr-2008	CHEMCART
Enzyme	E2	1	19-7	37	CEM	IC50	=	8.6	uM	21-Apr-2008	CHEMCART

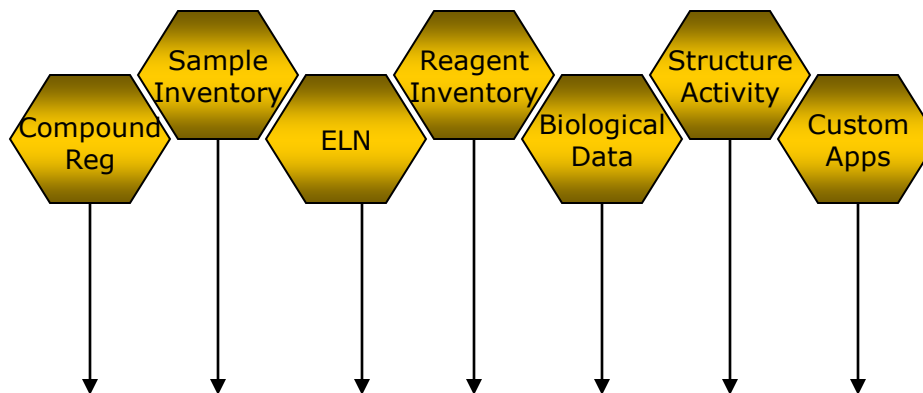
Below the table are three panels:

- Result Image:** A circular image showing a cell-based assay with blue fluorescent spots.
- Document Description:** A table listing documents and their file names:

Document Description	Document
uv spectra	UV.pdf
assay protocol	Protocol.doc
reader file	RawData.txt
excel data	RawData.xls
- Structure:** A chemical structure diagram of a molecule, specifically a substituted benzene ring with a side chain.

ChemCart Informatics Solution

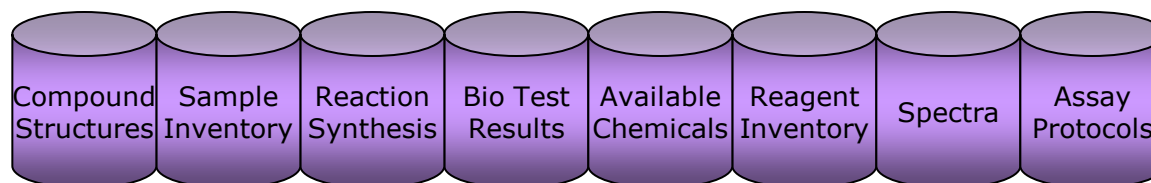
Web Served Applications



Middle Tier



Oracle & Data Cartridge



ChemCart Summary

- ❑ Web-based, configurable forms interface to Oracle
 - Benefit to Scientist
 - ❑ Provides easy access to data necessary for decision making
 - ❑ Enhances communication & collaboration by use of sharable objects (forms, searches, hit lists...)
 - ❑ Facilitates acceptance by integration with scientist-familiar chemical sketchers/renderers, search engines
 - Benefit to IT
 - ❑ Reduces deployment & maintenance overhead
 - ❑ Provides Rapid Application Development capabilities that do not require programming
 - ❑ Integrates with corporate standards (chemistry cartridge, sketcher/renderer, platform)
- ❑ Integrates with pipelining and analysis tools

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Please stop by the partner table to see more!

