



HYDRA

a live demo

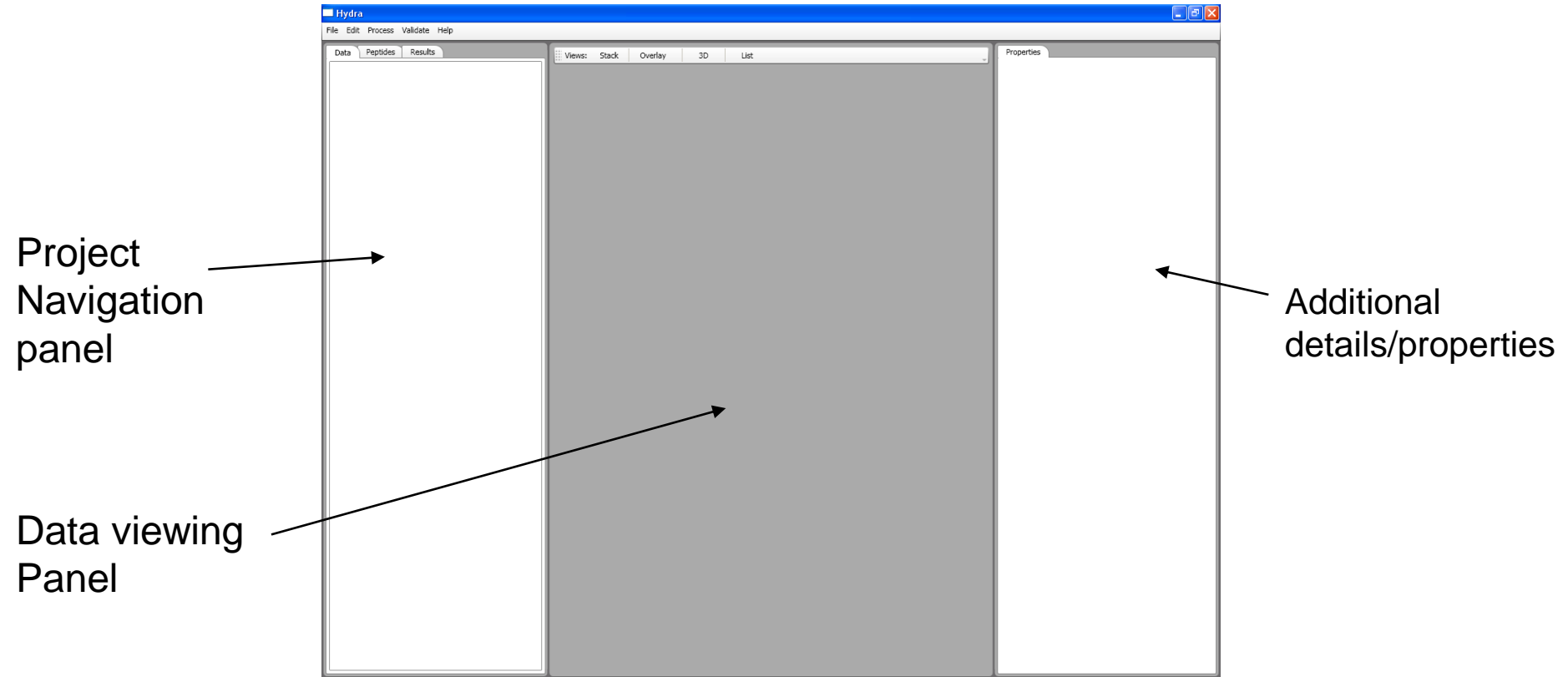


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** note: This was originally presented as a live demo. Here, three Scenerios will represent that which was presented at the HDX-MS Workshop

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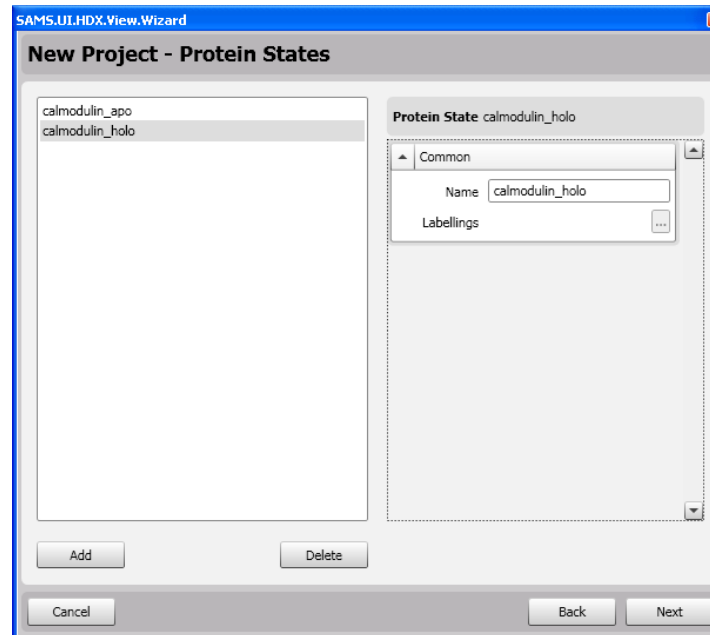
HYDRA's Layout



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Scenerio 1: Defining the Project

Step 1: Define protein states



Scenerio 1: Defining the Project

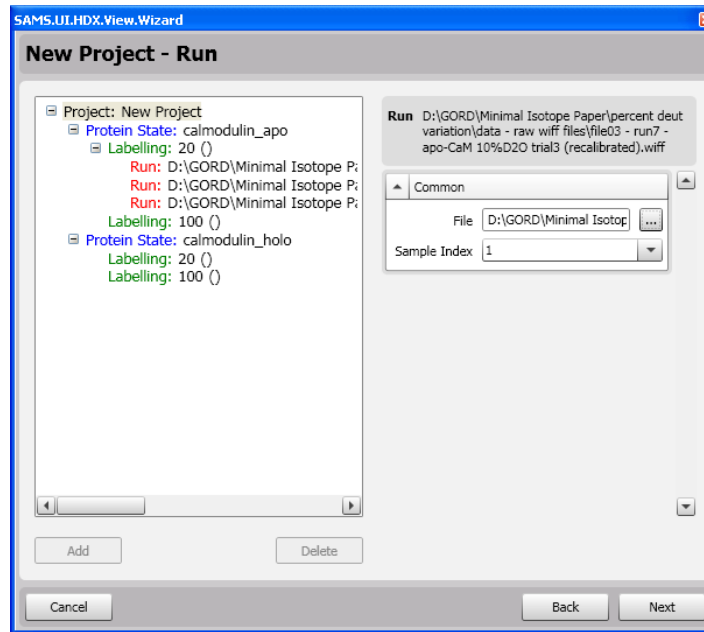
*Step 2: Define
labelling conditions*

The screenshot shows a software window titled "SAMS.U.I.HDX.View.Wizard" with a sub-dialog titled "New Project - Labelling". On the left, a list box contains the numbers "20" and "100". Below this list are "Add" and "Delete" buttons. On the right, a "Labelling" section shows a value of "100". Below it is a "Common" section with a dropdown arrow, containing three fields: "Time" with the value "100", "Percentage" with the value "0", and "Runs" with a three-dot menu icon. At the bottom of the dialog are "Cancel", "Back", and "Next" buttons.

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Scenerio 1: Defining the Project

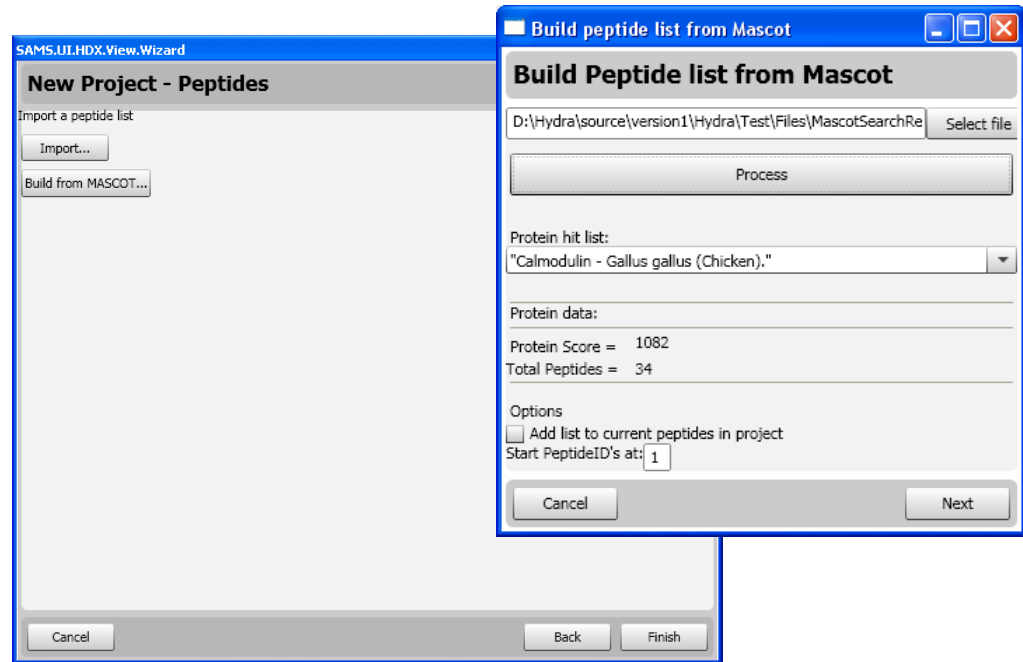
*Step 3: Associate
Experiment Runs with
Protein State and
Labelling Condition*



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Scenerio 1: Defining the Project

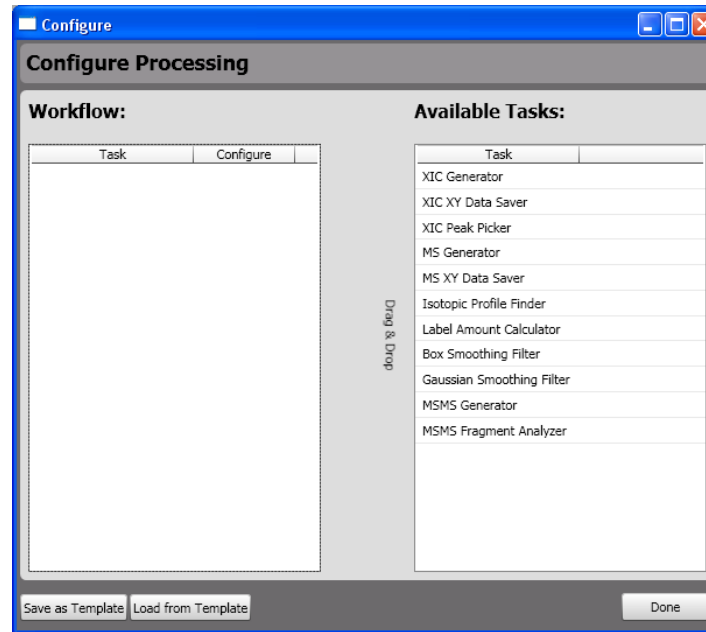
*Step 4 (Final step):
Generate Peptide list
by either importing a
previous list or building
a list from a MASCOT
search result*



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Scenerio 2: Defining the Data Processing Workflow

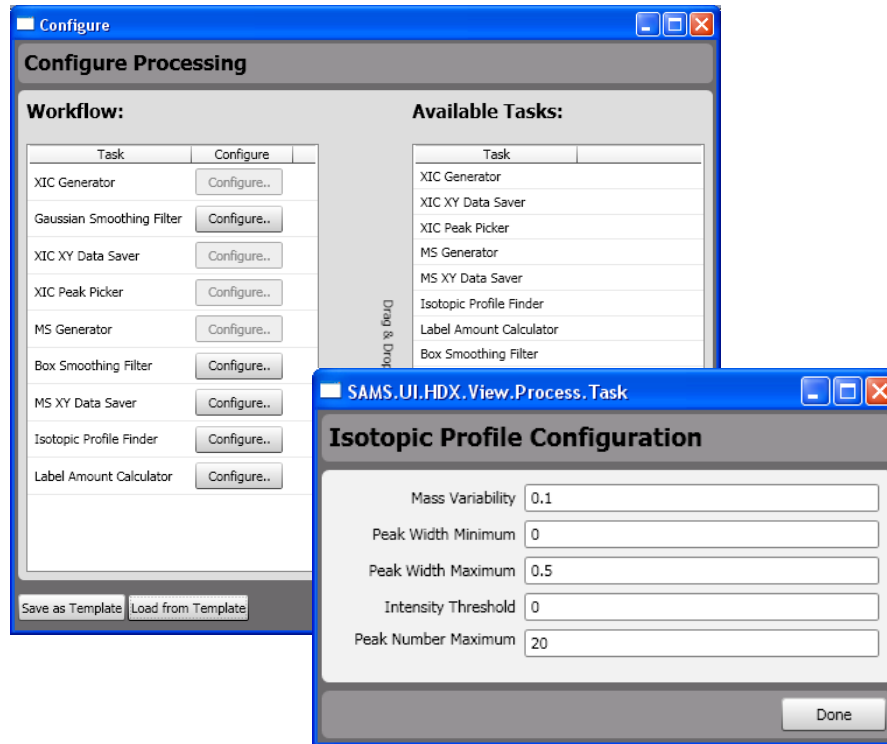
Step 1: Drag and drop Tasks from Available tasks OR load a previously saved Workflow



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Scenerio 2: Defining the Data Processing Workflow

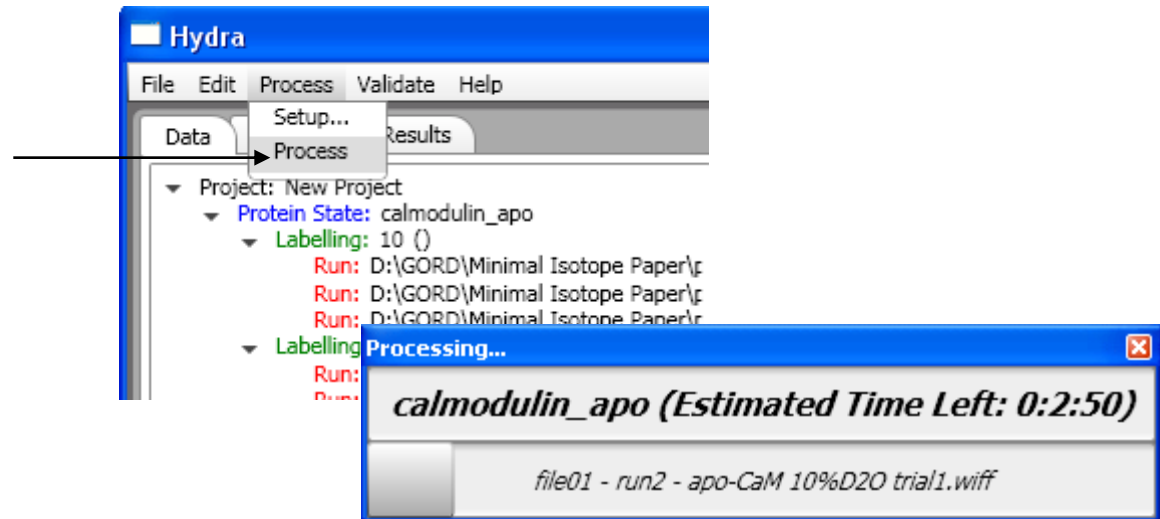
Step 2: Configure tasks



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Scenerio 2: Defining the Data Processing Workflow

*Step 3: Perform
'Single-click' to
process data*



Scenerio 3: Data Viewing

Primary output: Table of Deuterium Incorporation values, showing general Stats of replicates (Exportable)

The screenshot displays the Hydra software interface. The main window has a menu bar (File, Edit, Process, Validate, Help) and a toolbar with 'Views: List' and 'Chart' options. The left sidebar contains a 'Views' section with buttons for 'Peptide Deuteration', 'Deuteration vs Time', 'Spectrum View', and 'Deuteration Distribution', and a 'Filter' section with a table for 'Labelling Time' and 'Percent'.

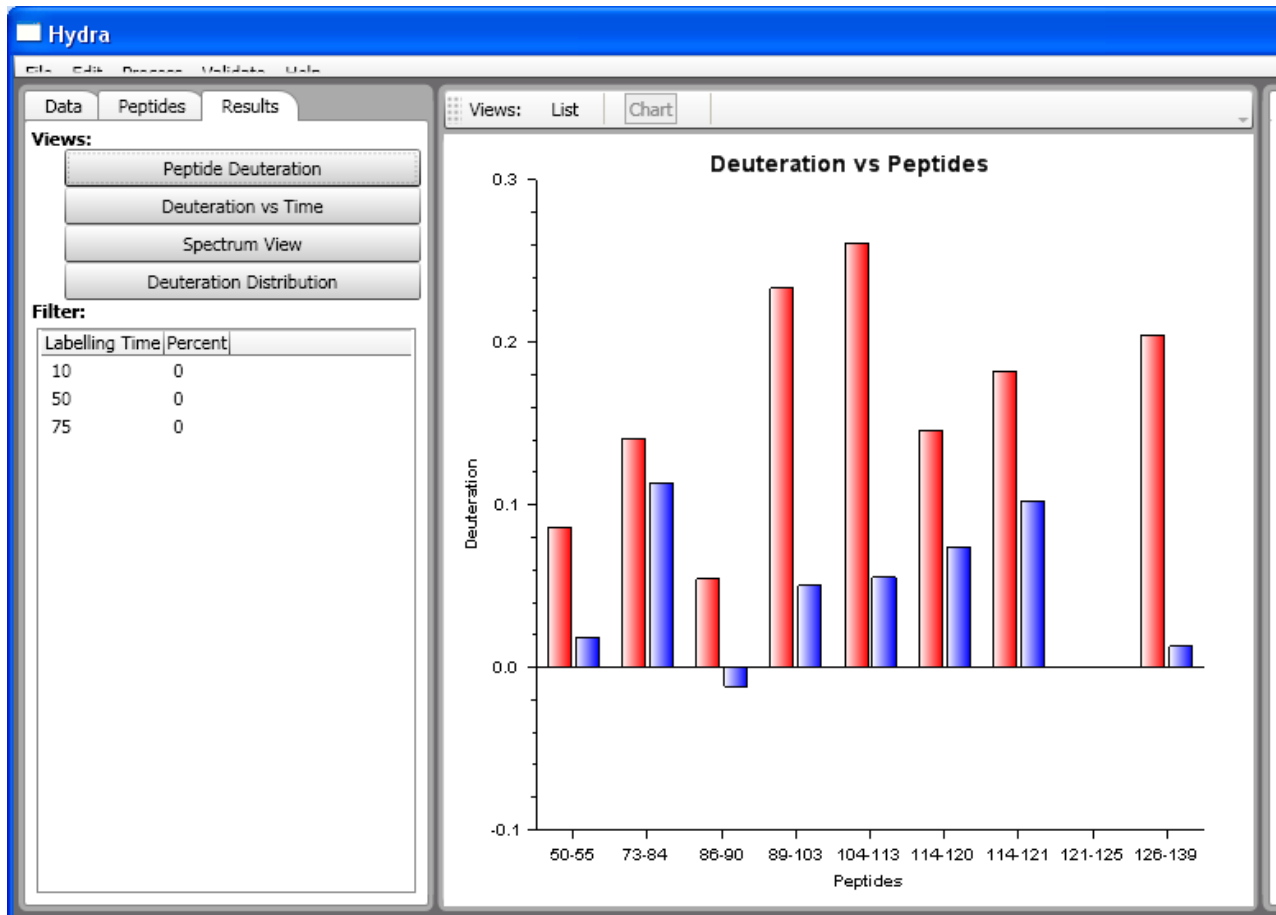
The main data table is titled 'calmodulin_apo' and 'calmodulin_holo' with a 'Comparisons' section. The table contains the following data:

Peptide	calmodulin_apo			calmodulin_holo			Comparisons			
	Deut	StDev	#Peaks	Deut	StDev	#Peaks	Ratio	RatioSD	T Test	P-Valu
50-55	0.086	0.077	3	0.018	0.021	3	0.214	0.313	-4.354	0.049
73-84	0.140	0.123	3	0.114	0.099	3	0.811	0.999	-0.327	0.774
86-90	0.054	0.047	2	-0.012	0.012	2	-0.214	-0.294	7.141	0.019
89-103	0.233	0.203	3	0.050	0.045	3	0.217	0.269	-5.044	0.037
104-113	0.261	0.227	4	0.055	0.048	4				
114-121	0.146	0.127	4	0.074	0.064	4				
114-120	0.182	0.157	4	0.102	0.090	4				
121-125	0.000	0.000	2	0.000	0.000	2				
126-139	0.205	0.178	3	0.013	0.014	3				

An 'Export results' dialog box is open in the foreground, featuring a checked checkbox for 'Export data for each replicate' and 'Cancel' and 'Next' buttons.

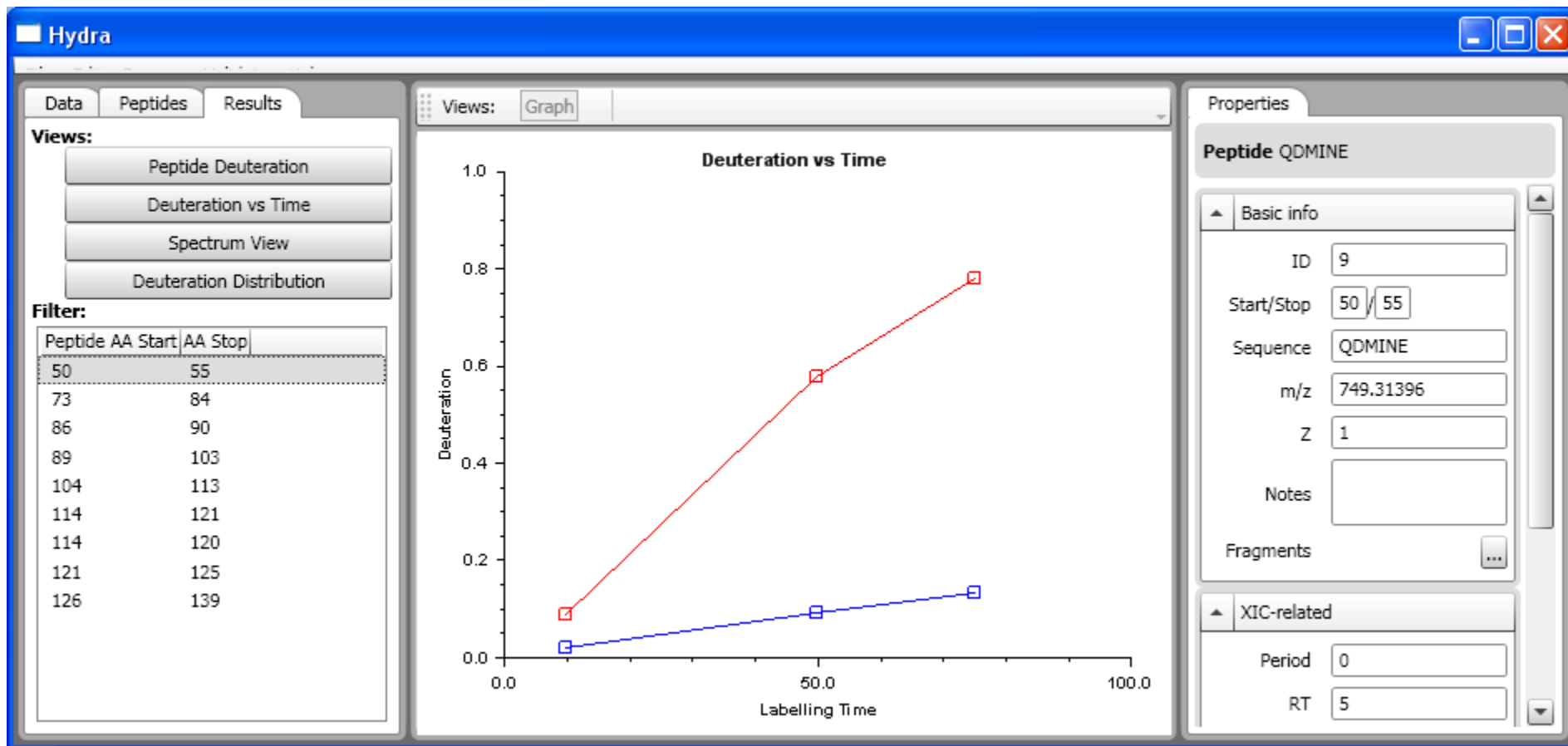
Scenerio 3: Data Viewing

Graphical view of all peptides:



Scenerio 3: Data Viewing

Other views: *Kinetic plot*



Scenerio 3: Data Viewing

Other views: *Spectrum view*

The screenshot displays the Hydra software interface. On the left is a 'Filter' panel with a tree view showing project settings for 'calmodulin_apo' and 'Labelling: 10 ()'. The main area contains three rows of plots, each with a chromatogram (Intensity vs. time) and a mass spectrum (Intensity vs. m/z). The right panel shows a 'Properties' table with three data tables.

Properties Table 1:

Rt	Peak Area	Peak Width	Peak Height
4.317	20	0.667	0.5
5.440	2065	0.967	124.6
6.741	258	0.517	15.0
7.038	473	0.633	24.9
8.056	43	0.500	2.8
8.646	68	0.717	2.9
10.445	346	0.900	17.3

Properties Table 2:

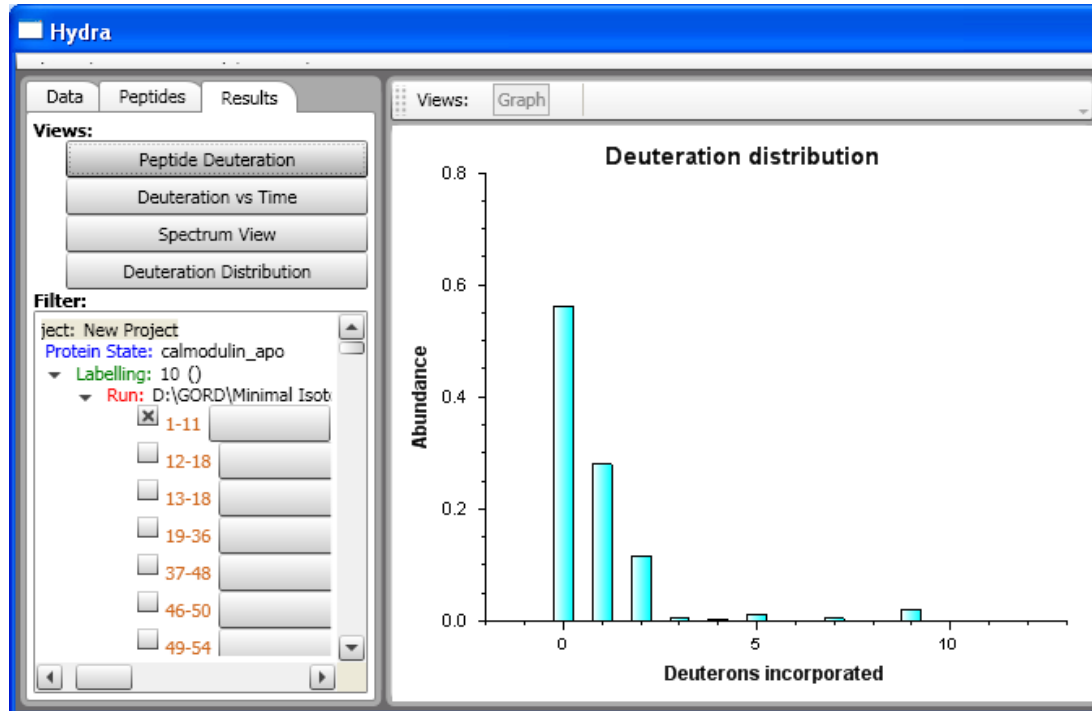
Rt	Peak Area	Peak Width	Peak Height
3.384	27	0.483	2.1
4.494	3189	1.183	186.5
5.727	102	0.600	4.1
6.021	74	0.450	4.7
9.579	145	0.700	8.0

Properties Table 3:

Rt	Peak Area	Peak Width	Peak Height
3.745	14	0.333	1.3
4.695	3936	0.867	233.7
5.781	289	1.217	7.6
6.638	24	0.483	1.7
7.125	15	0.367	1.4
8.097	13	0.350	1.2
9.587	316	0.867	16.6

Scenario 3: Data Viewing

Other views: *Deuterium Distribution Analysis*



HYDRA

Summary and Key Features

- HYDRA uses step-by-step wizards to walk users through project configuration, and thus requires little training.
- HYDRA provides an automated means of extracting deuterium incorporation data including distribution information.
- Visual tools provide a quick way of validating results.
- Flexibility shown by the ability to adapt or add new data processing workflows.

SOFTWARE AVAILABILITY:

- Requests for HYDRA should be directed to Dr. David Schriemer (dschriem@ucalgary.ca)

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Acknowledgements

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*Thanks for your
interest!*