



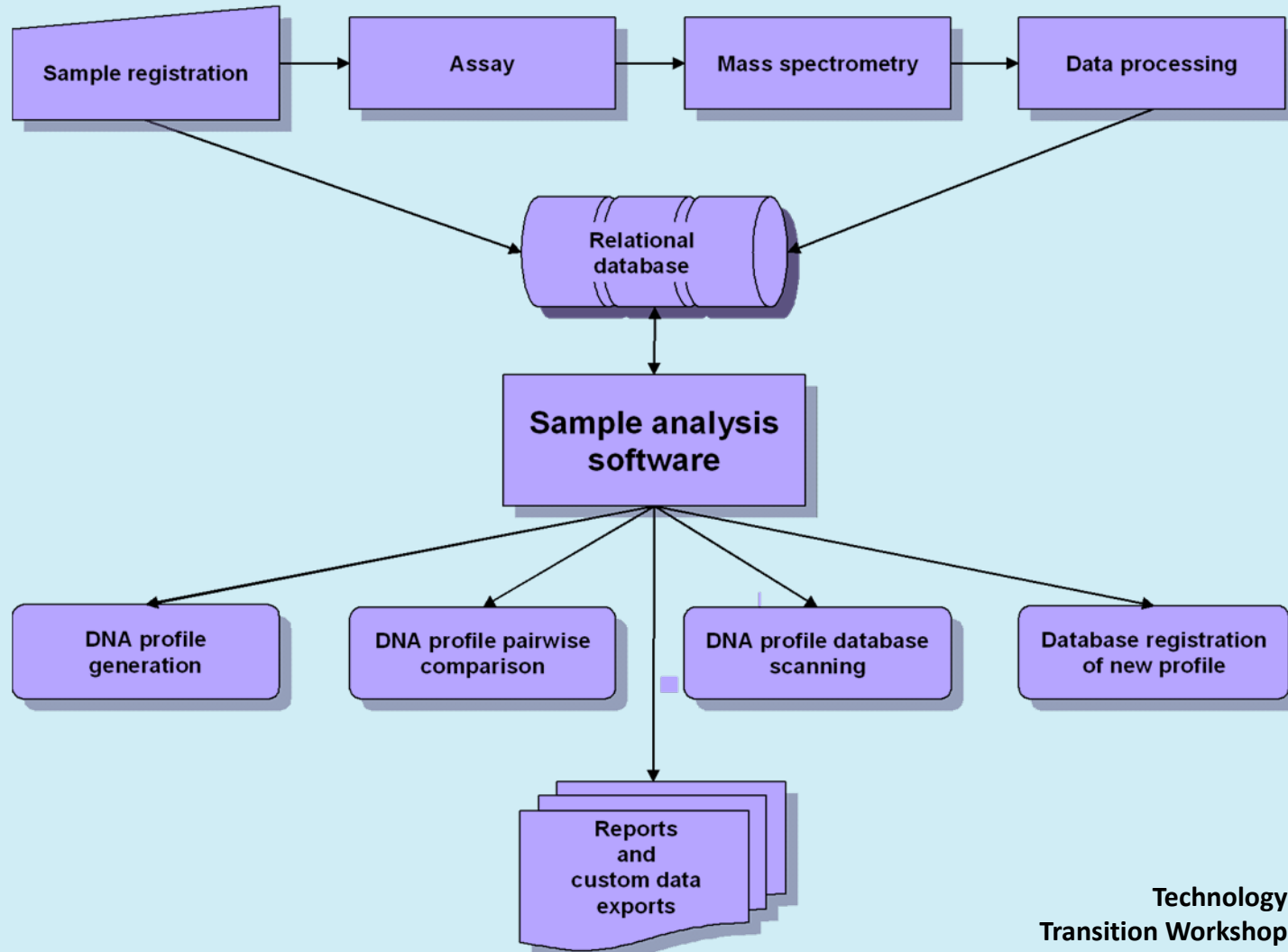
Technology Transition Workshop | *Thomas Hall, Ph.D.*

Overview of Ibis™ Forensic Analysis Software

Outline

- **General software interface**
- **Features**
- **Data processing**
- **Data analysis**
 - **mtDNA**
 - **SNPs**

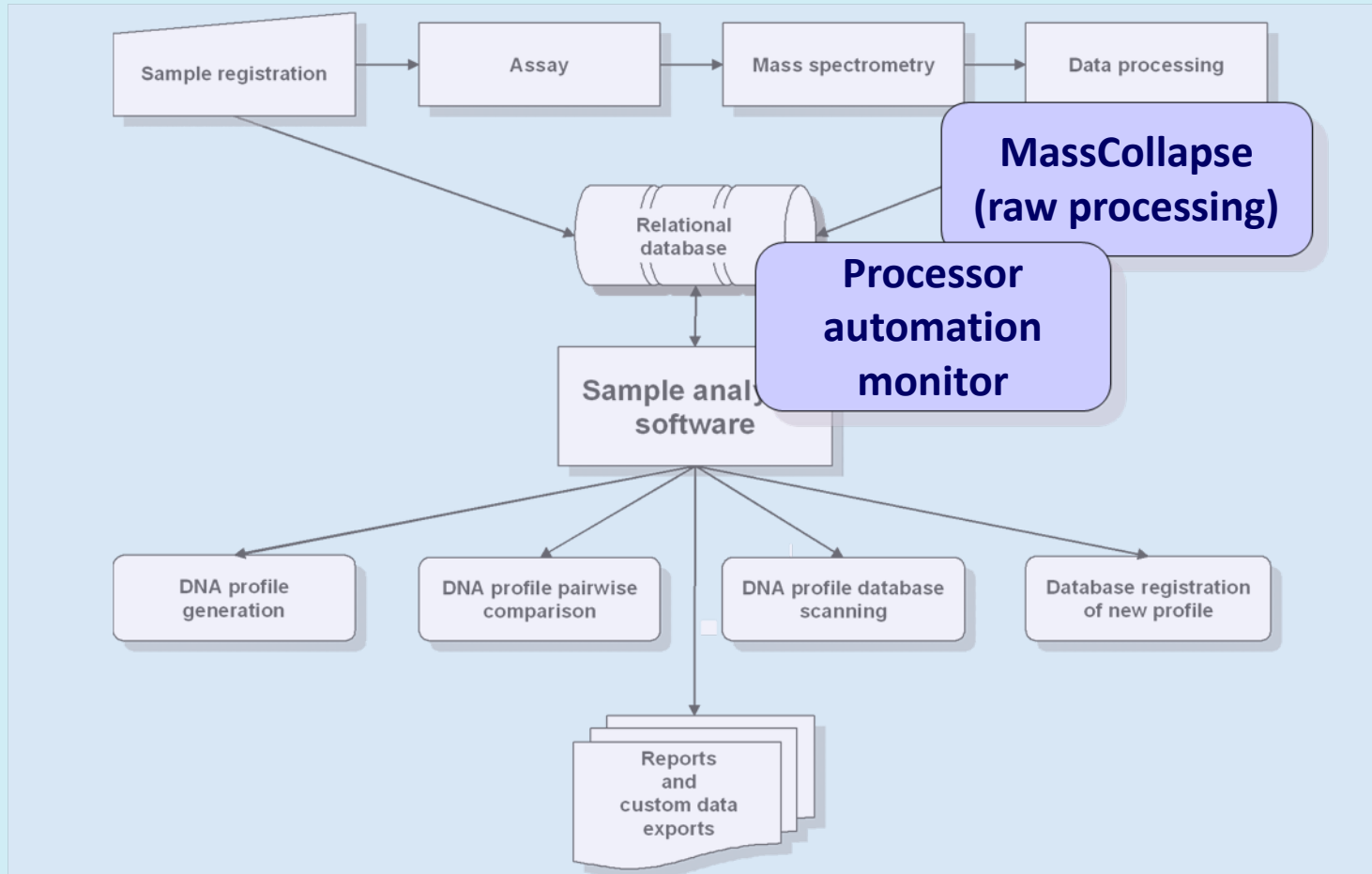
Forensic Analysis Software



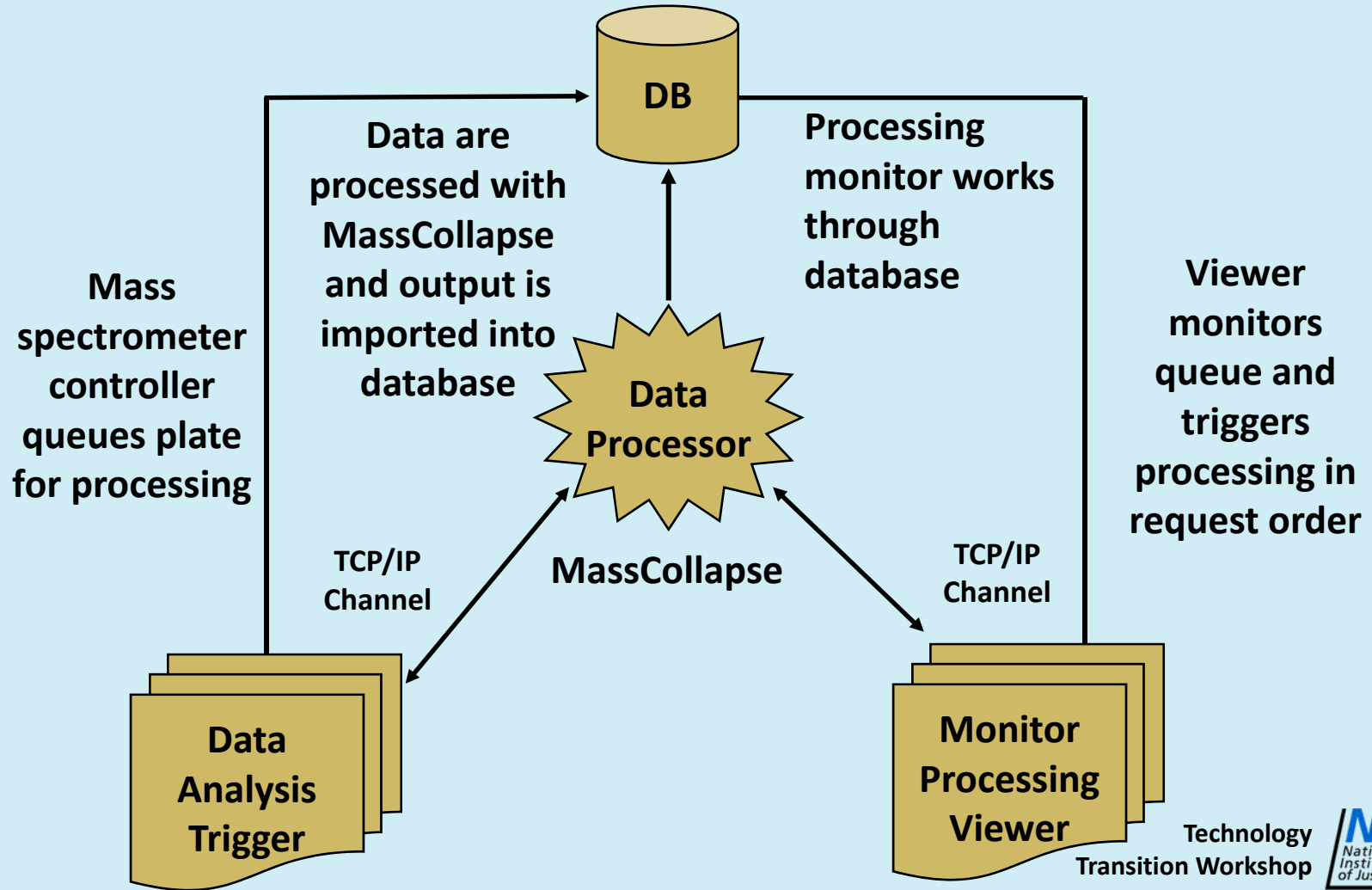
Software Features

- **Utilizes IbisTrack database software for sample tracking**
 - **Integrated system**
 - **MitoDNA analysis module is an independent module**
 - **Updates to MitoDNA → Simply place updated module with most recent IbisTrack; integration is dynamic**
- **Provides functions for:**
 - **Analysis / QC of assay data and registration of profiles**
 - **Adding / removing databases, populations, sequence profiles, and base composition profiles**
 - **Automated conversion of sequence to mtDNA base count profiles**
 - **Population-based searching and reporting for mtDNA**
 - **Plate-based analysis reporting for mtDNA**

Data Processing

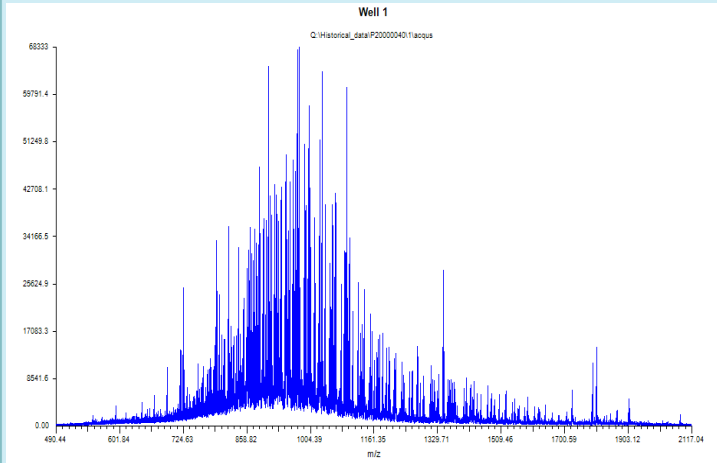


Forensic Data Processing Monitor



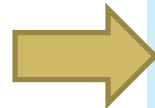
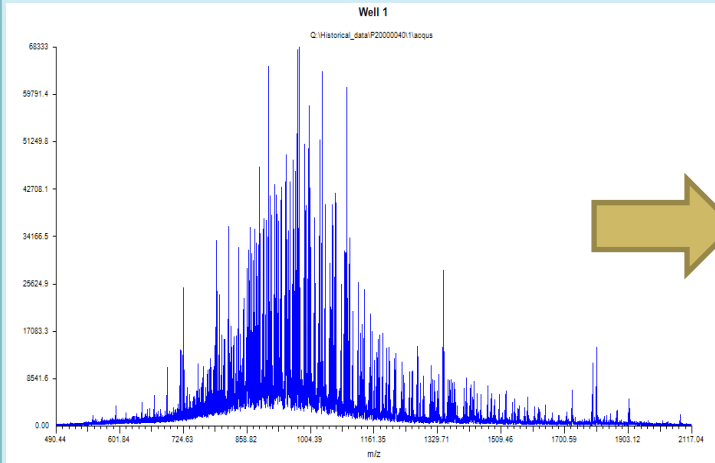
MassCollapse Deconvolution

Raw spectrum

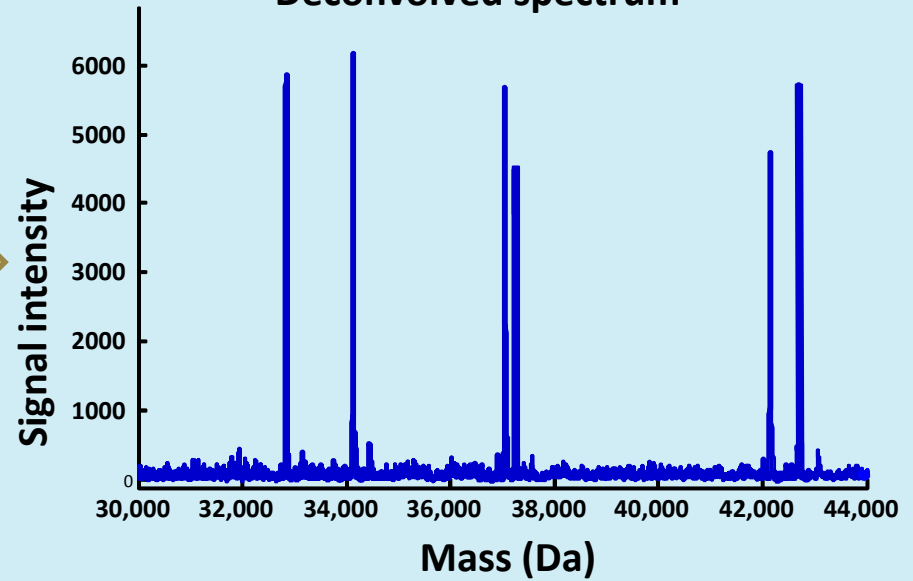


MassCollapse Deconvolution

Raw spectrum

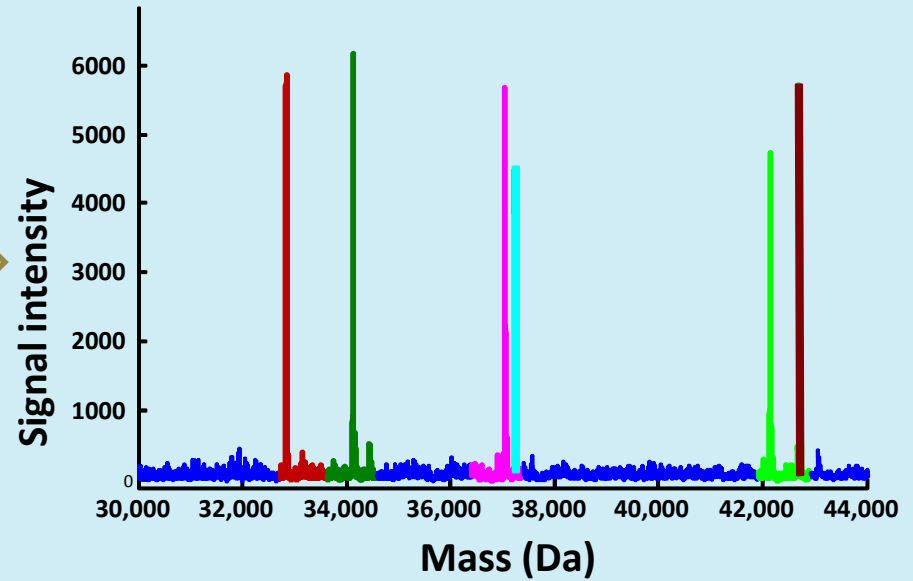
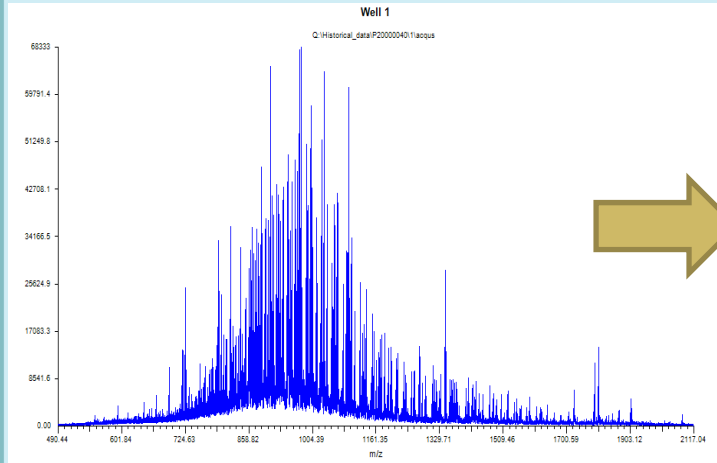


Deconvolved spectrum



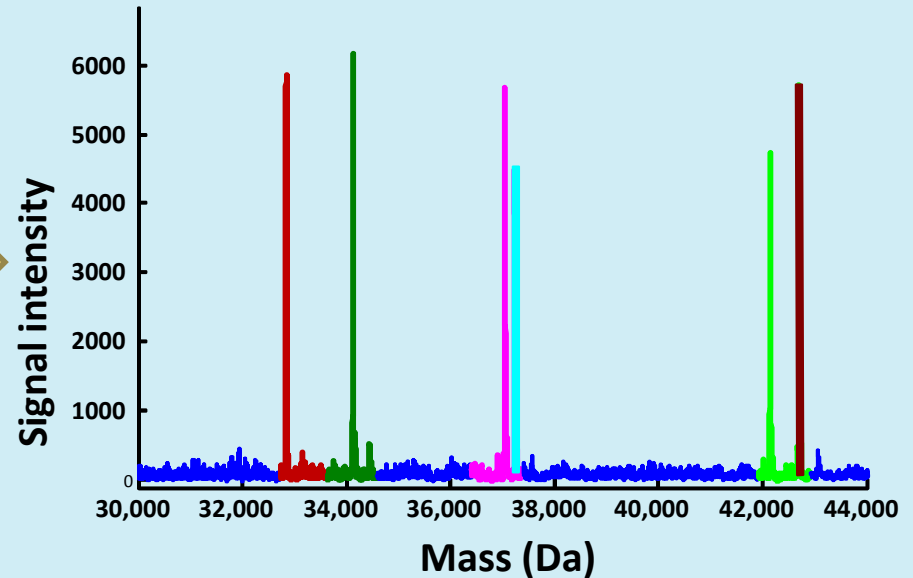
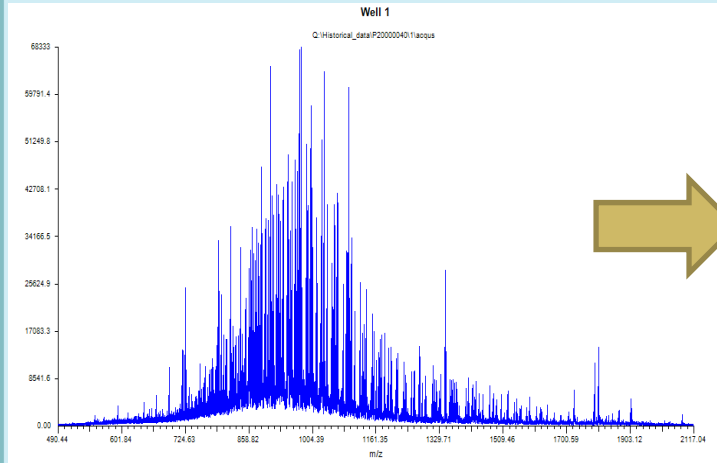
MassCollapse Deconvolution

Raw spectrum



MassCollapse Deconvolution

Raw spectrum



List of masses and intensities

Collapsed data can also be interrogated for fit of base compositions given a model of the Ibis™ mass tag

32855.1 Da

34143.8 Da

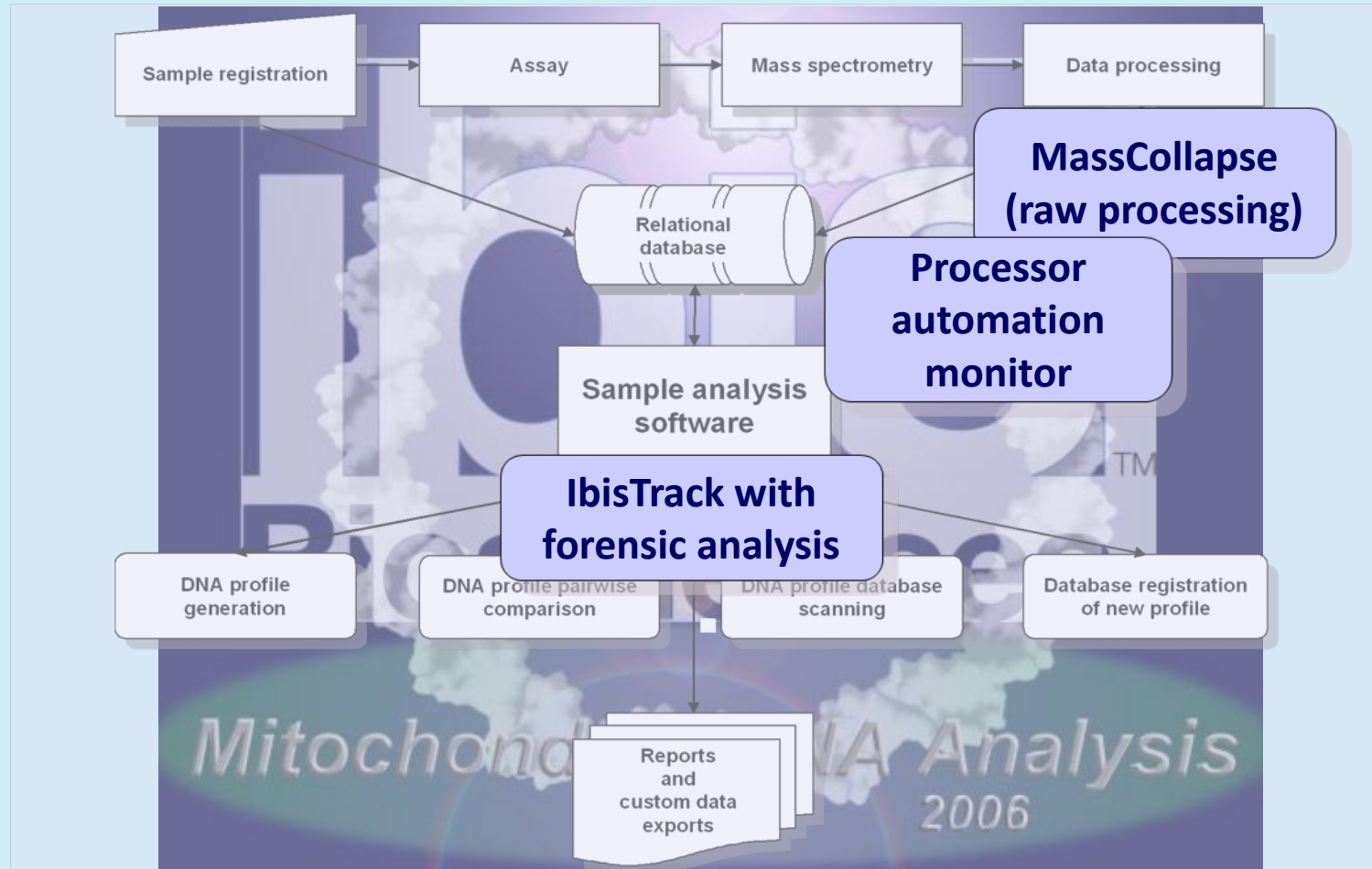
37058.2 Da

37254.2 Da

42162.1 Da

42710.3 Da

Forensic Analysis Software



Basic Application Interface

The screenshot displays the IbisTrack application window. The title bar reads "IbisTrack". The menu bar includes "File", "View", and "Help". The main navigation bar contains icons for "Home", "Casework", "Databasing", "Import", and "Analysis". On the left, a "Tasks" pane is expanded to show "mtDNA Analysis" with sub-items: "Analyze mtDNA", "Import Mass Data", "Add Database Items", "Remove Database Items", "Move Samples to Populations", "Rebuild Unique Products", "Build Amplified BC Database", "Upload data to main server", and "Archive case/plate data". Below this are "STR Analysis" (with sub-items "Analyze STRs" and "Analyze Y-STRs") and "SNP Analysis" (with sub-item "Analyze Autosomal SNPs"). At the bottom of the task pane are "Tasks", "Advanced Tasks", and "In-House Tasks". The main content area features a "Welcome to IbisTrack" message, followed by a description of the software's purpose and a list of four common operations: "Casework", "Database Population", "Import", and "Analysis", each with an icon and a brief description.

Welcome to *IbisTrack*

IbisTrack tracks samples and plates for the Ibis T5000 Biosensor System, from initiating an assay through viewing results.

Please select from one of the following common operations, or select from the tasks in the navigation pane to the left.

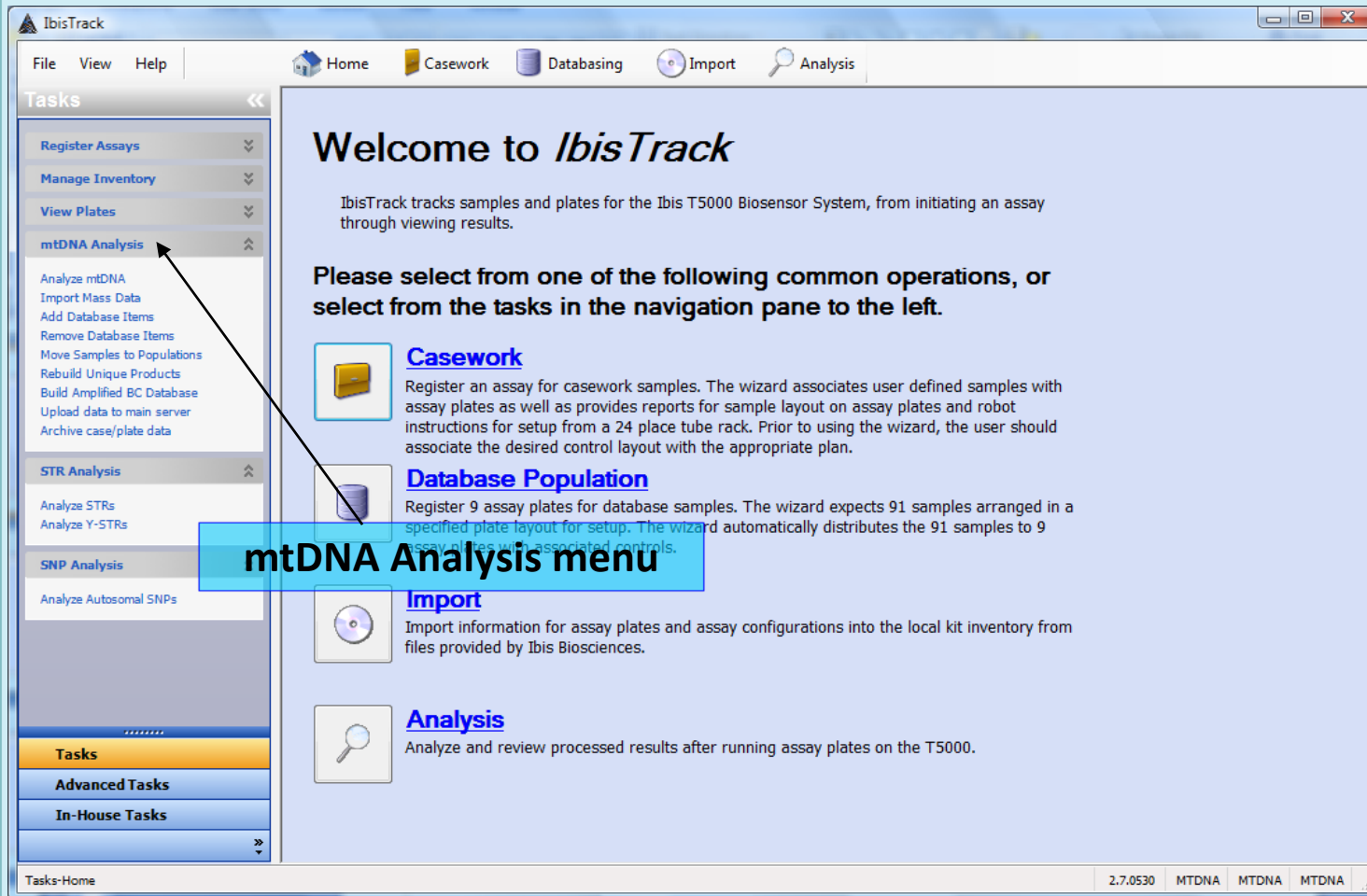
- Casework**
Register an assay for casework samples. The wizard associates user defined samples with assay plates as well as provides reports for sample layout on assay plates and robot instructions for setup from a 24 place tube rack. Prior to using the wizard, the user should associate the desired control layout with the appropriate plan.
- Database Population**
Register 9 assay plates for database samples. The wizard expects 91 samples arranged in a specified plate layout for setup. The wizard automatically distributes the 91 samples to 9 assay plates with associated controls.
- Import**
Import information for assay plates and assay configurations into the local kit inventory from files provided by Ibis Biosciences.
- Analysis**
Analyze and review processed results after running assay plates on the T5000.

Tasks-Home 2.7.0530 MTDNA MTDNA MTDNA

Basic Application Interface



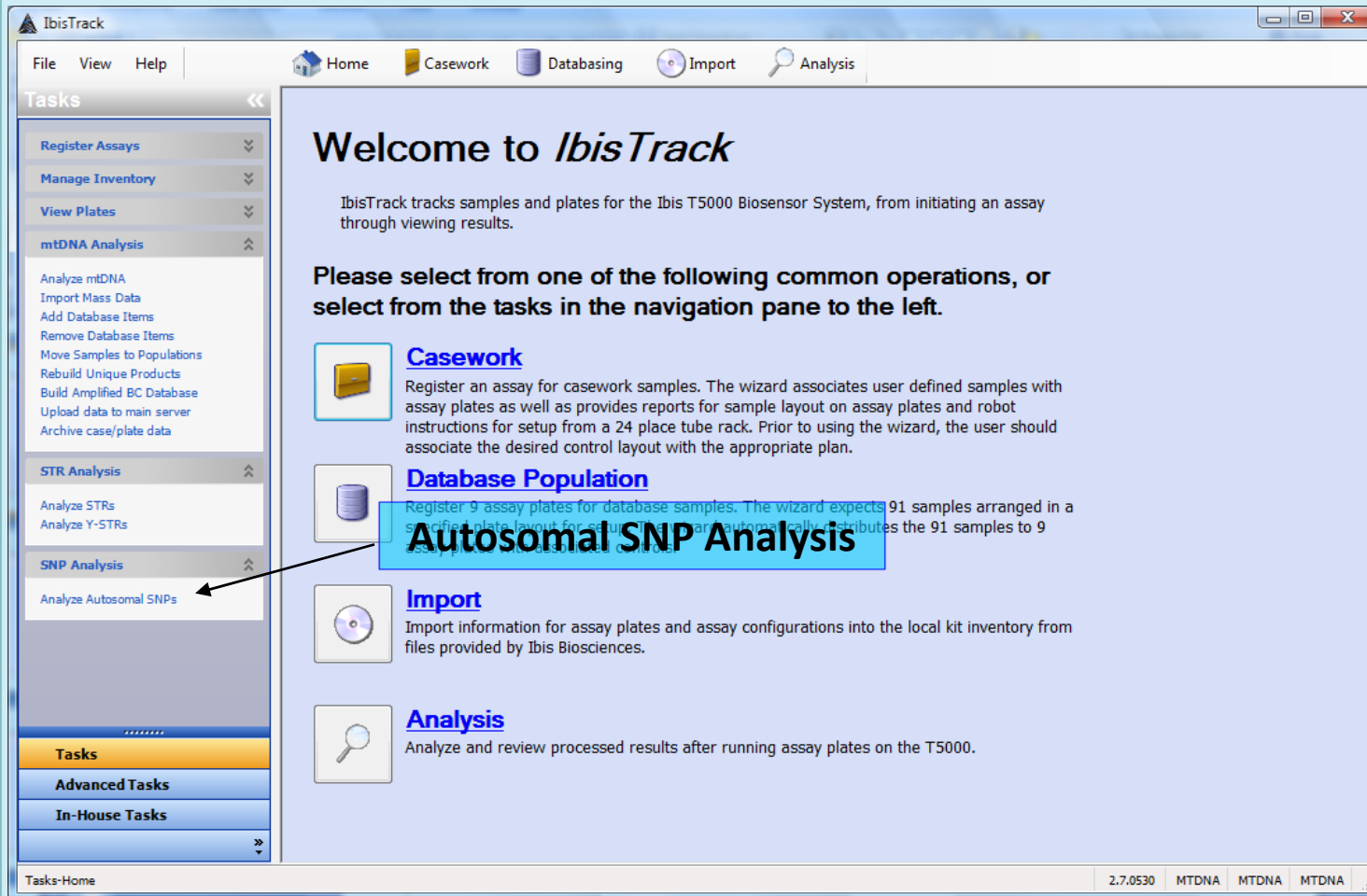
Basic Application Interface



Basic Application Interface

The screenshot displays the IbisTrack application window. The title bar reads 'IbisTrack'. The menu bar includes 'File', 'View', and 'Help'. The main navigation bar contains icons for 'Home', 'Casework', 'Databasing', 'Import', and 'Analysis'. On the left, a 'Tasks' pane lists various operations: 'Register Assays', 'Manage Inventory', 'View Plates', 'mtDNA Analysis' (with sub-items: Analyze mtDNA, Import Mass Data, Add Database Items, Remove Database Items, Move Samples to Populations, Rebuild Unique Products, Build Amplified BC Database, Upload data to main server, Archive case/plate data), 'STR Analysis' (with sub-items: Analyze STRs, Analyze Y-STRs), and 'SNP Analysis' (with sub-item: Analyze Autosomal SNPs). The main content area features a 'Welcome to IbisTrack' message and a list of four common operations: 'Casework', 'Database Population', 'Import', and 'Analysis'. A blue box highlights the 'STR / Y-STR Analysis' sub-section under 'Database Population', and an arrow points from this box to the 'STR Analysis' task in the left pane. The status bar at the bottom shows 'Tasks-Home' and '2.7.0530 MTDNA MTDNA MTDNA'.

Basic Application Interface



Basic Application Interface – mtDNA

Tasks

- Register Assays
- Manage Inventory
- View Plates
- mtDNA Analysis**
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
 - Upload data to main server
 - Archive case/plate data
- STR Analysis
 - Analyze STRs
 - Analyze Y-STRs
- SNP Analysis
 - Analyze Autosomal SNPs

Tasks

- Advanced Tasks
- In-House Tasks

Tasks-Home

2.7.0530 MTDNA MTDNA MTDNA

Welcome to *IbisTrack*

IbisTrack tracks samples and plates for the Ibis T5000 Biosensor System, from initiating an assay through viewing results.

Click please select from one of the following common operations, or select from the tasks in the navigation pane to the left.

Casework

Register an assay for casework samples. The wizard associates user defined samples with assay plates as well as provides reports for sample layout on assay plates and robot instructions for setup from a 24 place tube rack. Prior to using the wizard, the user should associate the desired control layout with the appropriate plan.

Database Population

Register 9 assay plates for database samples. The wizard expects 91 samples arranged in a specified plate layout for setup. The wizard automatically distributes the 91 samples to 9 assay plates with associated controls.

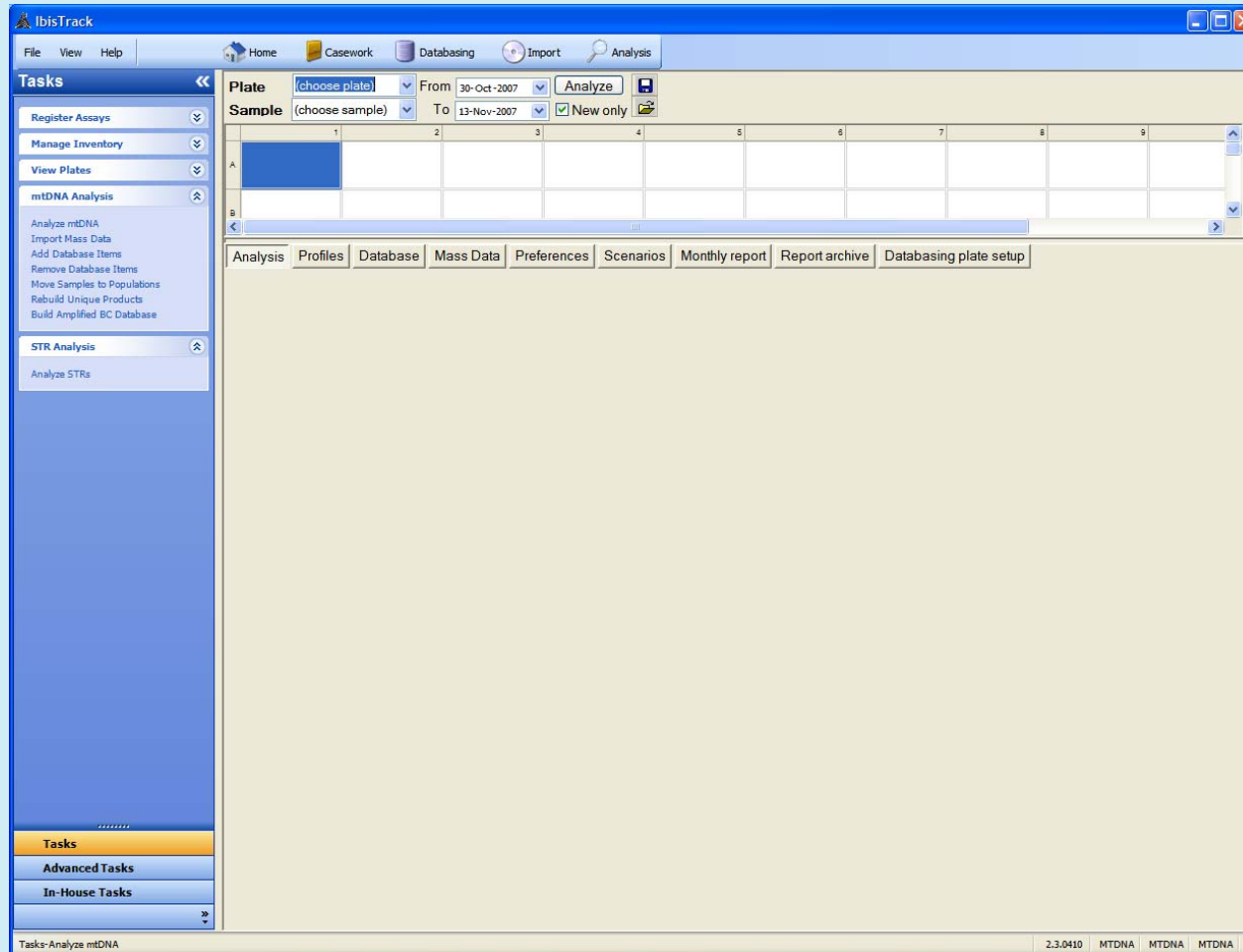
Import

Import information for assay plates and assay configurations into the local kit inventory from files provided by Ibis Biosciences.

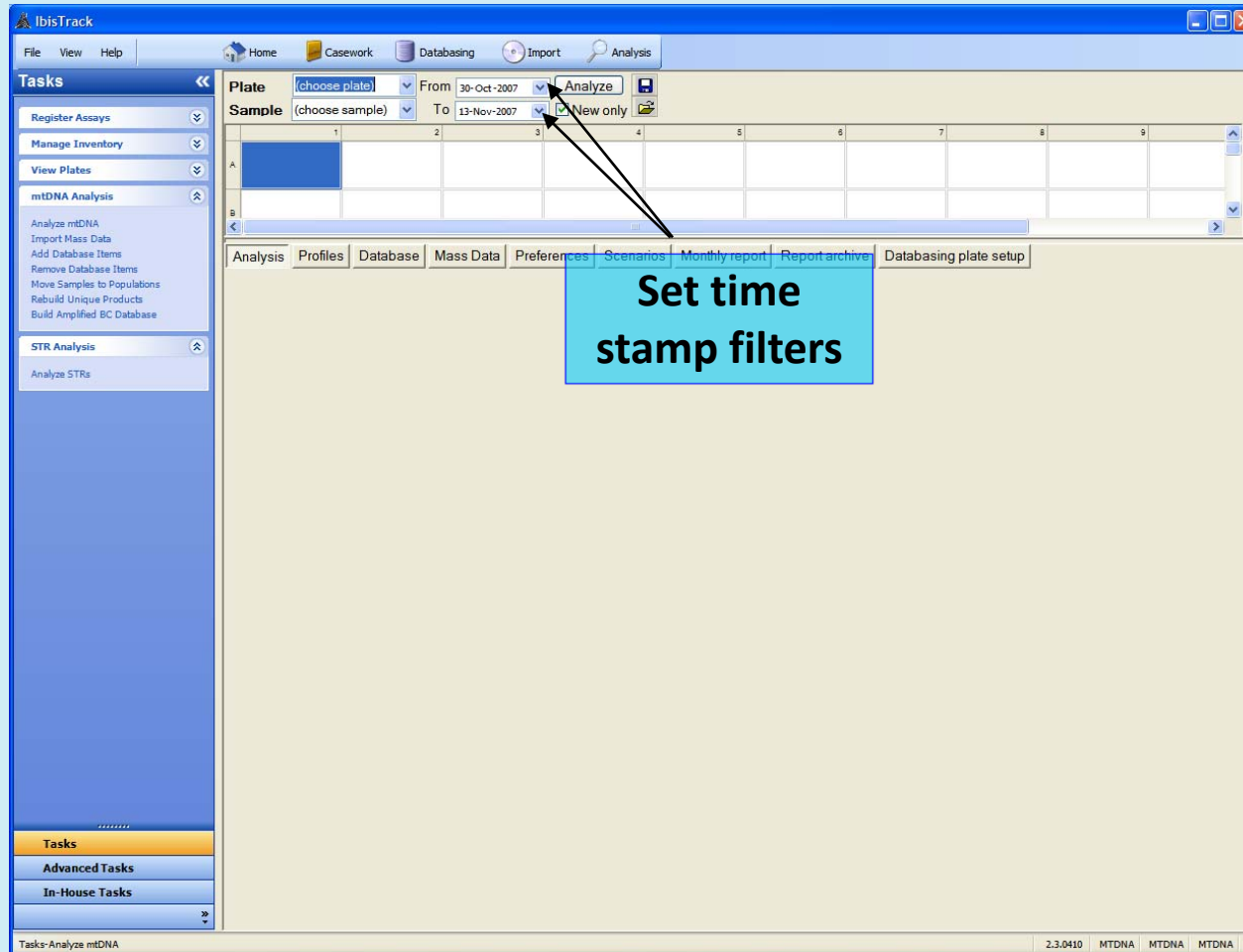
Analysis

Analyze and review processed results after running assay plates on the T5000.

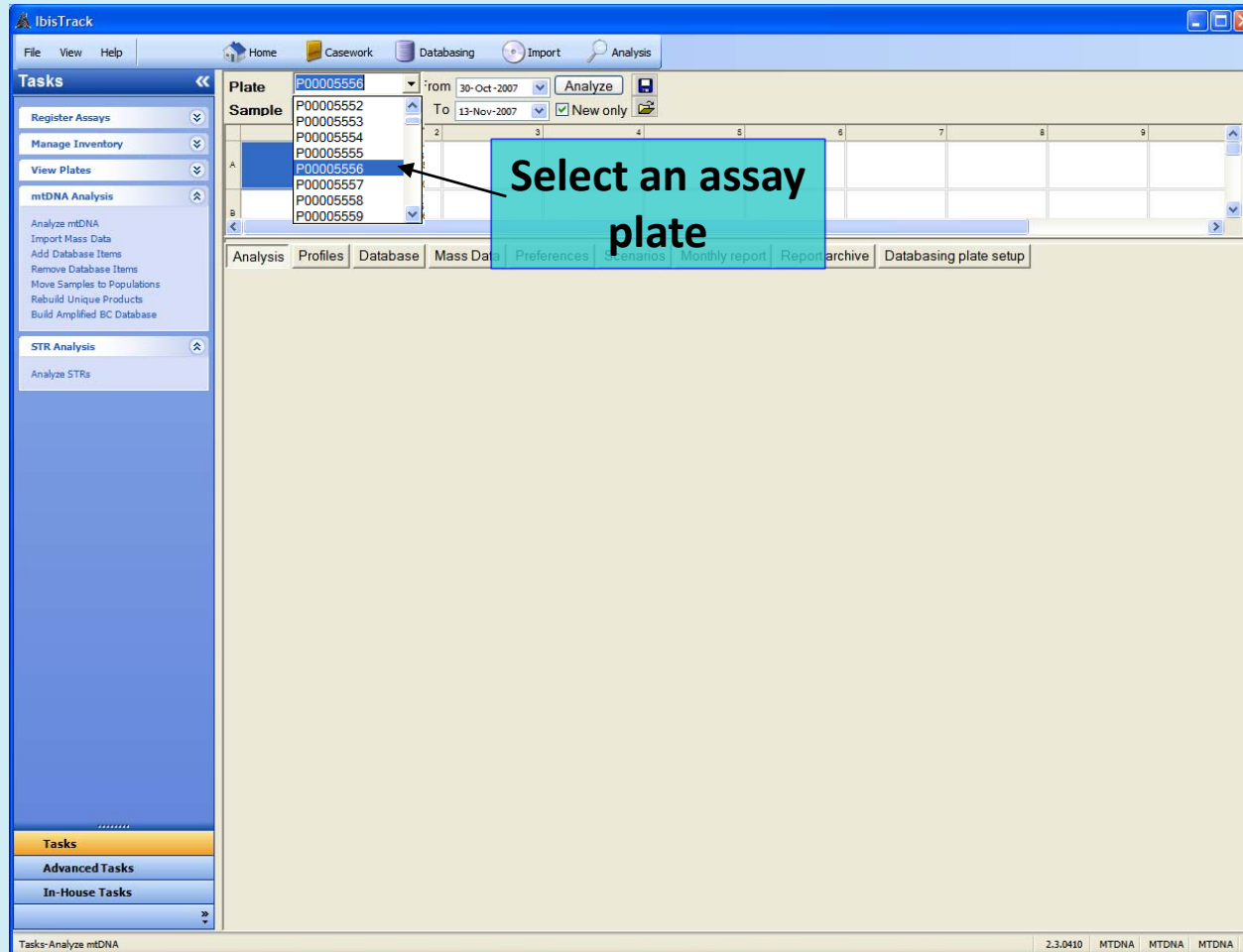
Basic Application Interface – mtDNA



Basic Application Interface – mtDNA



Basic Application Interface – mtDNA



Basic Application Interface – mtDNA

IbisTrack

File View Help Home Casework Databasing Import Analysis

Tasks

- Register Assays
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

Tasks-Analyze mtDNA

Plate: P00005555 From: 30-Oct-2005 To: 13-Nov-2007 Analyze

Sample: All To: New only

	1	2	3	4	5	6	7	8	9	10
A	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70
B	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85	HUM2905 Scenario: 85

Analysis Profiles Database Mass Data Preferences Scenarios Monthly report Report archive Databasing plate setup

2.3.0410 | MTDNA | MTDNA | MTDNA

Basic Application Interface – mtDNA

The screenshot displays the IbisTrack software interface. The main workspace shows a 'Plate' dropdown set to 'P00005555', a 'Sample' dropdown set to 'All', and a date range filter from '30-Oct-2005' to '13-Nov-2007'. Below this is a grid of sample scenarios. The first cell in the grid is highlighted in blue, and a blue callout box with the text 'Select sample' has an arrow pointing to it.

	1	2	3	4	5	6	7	8	9	
A	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70
B	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80	HUM2925 Scenario: 85 HUM2921 Scenario: 80

Basic Application Interface – mtDNA

Tasks

- Register Assays
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

Plate P00005555 **From** 30-Oct-2005 **Analyze** **Sample** 1 **To** 13-Nov-2007 New only

	1	2	3	4	5	6	7	8	9	10
A	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70
B	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70	HUM2925 Scenario: 86 HUM2901 Scenario: 70

Analysis Profiles Database Mass Data Preferences Scenarios Monthly report Report archive Databasing plate setup

Tasks-Analyze mtDNA 2.3.0410 MTDNA MTDNA MTDNA

Basic Application Interface – mtDNA

Click Analyze

Plate: P00005555 From: 30-Oct-2005 To: 13-Nov-2007 Analyze New only

	1	2	3	4	5	6	7	8	9	10
A	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70
B	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70	HUM2905 Scenario: 86 HUM2901 Scenario: 70

Analysis Profiles Database Mass Data Preferences Scenarios Monthly report Report archive Databasing plate setup

Tasks-Analyze mtDNA 2.3.0410 MTDNA MTDNA MTDNA

Basic Application Interface – mtDNA

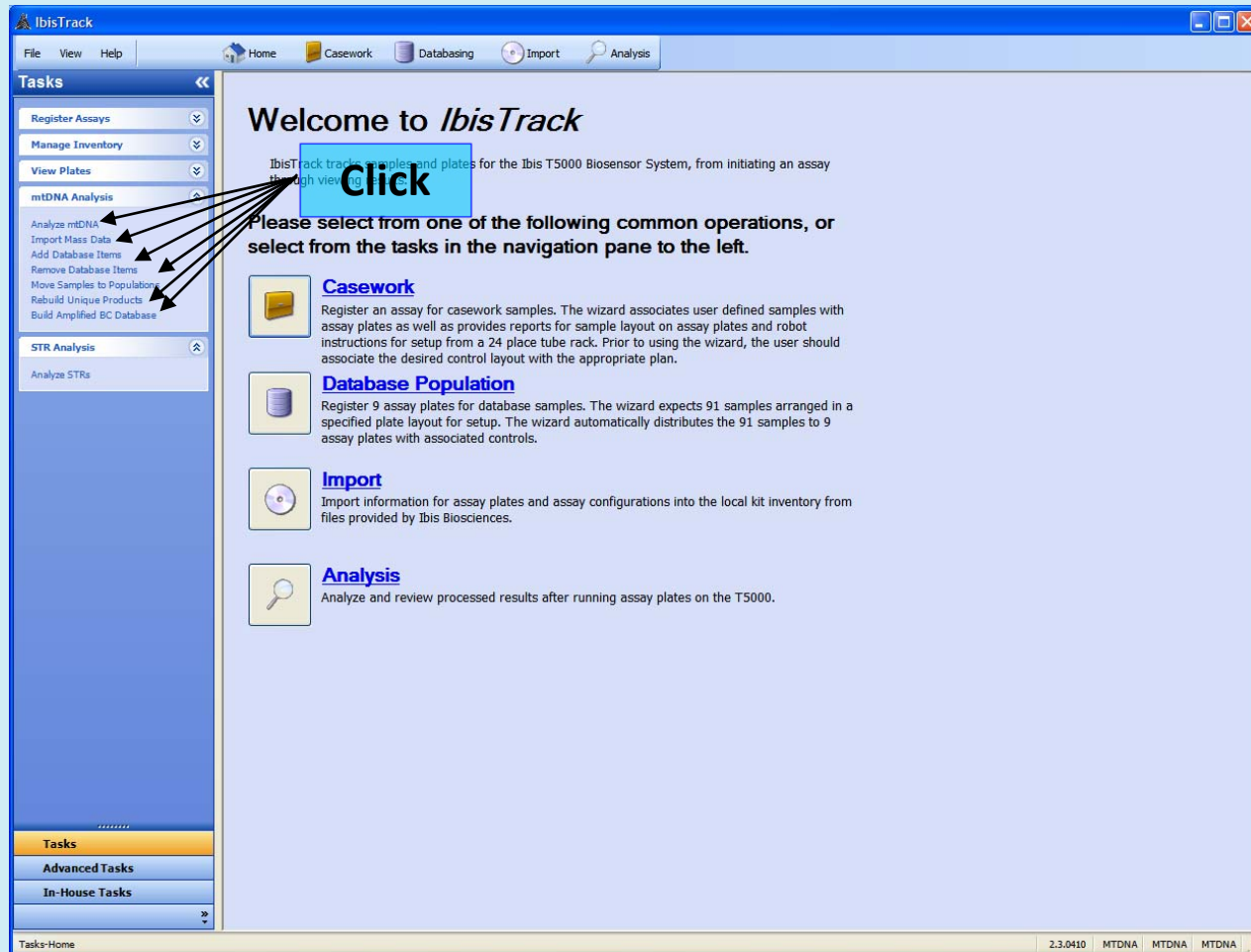
The screenshot displays the IbisTrack software interface for mtDNA analysis. The interface includes a menu bar (File, View, Help), a toolbar (Home, Casework, Databasing, Import, Analysis), and a main workspace. The workspace is divided into several sections:

- Tasks Panel (Left):** A vertical sidebar with options like "Plate selection", "Sample selection", "Advanced Tasks", and "In-House Tasks".
- Header/Filter Area:** Contains fields for "Plate" (P00005556), "Sample" (1), and date ranges ("From 30-Oct-2005", "To 13-Nov-2007").
- Analysis/Database Section:** Lists various analysis parameters and database entries, including "Well 1 (A01)", "Well 13 (B01)", "Well 25 (D01)", "Well 49 (E01)", and "Well 61 (F01)".
- Product assignment info:** A central area showing mass spectra and peak assignments for different wells.
- Base count profile:** A section on the right displaying a list of base counts and their corresponding mass values.
- Mass assignment detail:** A table at the bottom right showing numerical data for mass assignments, including columns for "num", "error", "exp. mass", "obs. mass", and "mod".
- Spectral schematic views:** A large area on the left showing a grid of mass spectra for different wells, with a "Coverage map" overlay.

Annotations with arrows point to the following features:

- Plate selection:** Points to the "Plate" dropdown menu.
- Sample selection:** Points to the "Sample" dropdown menu.
- Plate time-stamp selection:** Points to the date range filters.
- Interface navigation:** Points to the menu bar and toolbar.
- Sample / well navigation:** Points to the "Well" dropdown menu.
- Product assignment info:** Points to the mass spectra and peak lists.
- Base count profile:** Points to the list of base counts and masses.
- Mass assignment detail:** Points to the table at the bottom right.
- Coverage map:** Points to the grid of mass spectra.
- Spectral schematic views:** Points to the overall layout of the mass spectra.

Basic Application Interface – mtDNA



Basic Utilities Interface – mtDNA

Tasks

- Register Assays
 - Register Casework Plates
 - Register New Plate for Database Population
 - Process Repeats for Database
 - Register Quality Control Plates
 - Generate Plate Setup Reports
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

Tasks

- Find Results
- Advanced Tasks
- In-House Tasks

Add items to database | Remove items | Arrange samples | Rebuild Unique Products Table | Build Amplified BC database | Import mass file

Sequence profile | Individual IDs | Base count profile | **Add database** | Add population | ImportXML

Single entry | Batch

Database: IBIS | CRS start: 16024 | Region: --

ID for new entry: IBIS00001 | CRS end: 576 | Source: --

Population: UNKNOWN

Reference: This is really just a test example

Comment: In-house saliva sample

Description (for new sequence): Sequence entry for sample IBIS00001

Import sequence ->

To import a sequence correctly, CRS start and end coords must be entered

Profile:

CRS	Position	Profile Base
A	73	G
T	146	C
T	195	C
A	263	G
-	315.1	C
-	524.1	A
-	524.2	C
-	524.3	A
-	524.4	C
T	16224	C
T	16311	C
T	16519	C
A	16524	G

Register into database | Cancel

Enter a profile in the left box in standard format.
Example:
73 G
263 G
315.1 C

Designate a deletion as lowercase d:
302 d

Use uppercase for UIPAC codes:
263 N
263 R
etc.

Press 'Format ->' and double-check row entries.
Press 'Register into database'

Tasks-Add Database Items | 2.5.0520 | MTDNA | MTDNA | MTDNA

Basic Application Interface – mtDNA

Tasks: Add Database Items

Example: Single addition of a sequence profile

Basic Application Interface – mtDNA

Item addition

Item deletion

Sample arrangement

Database maintenance

Mass data import

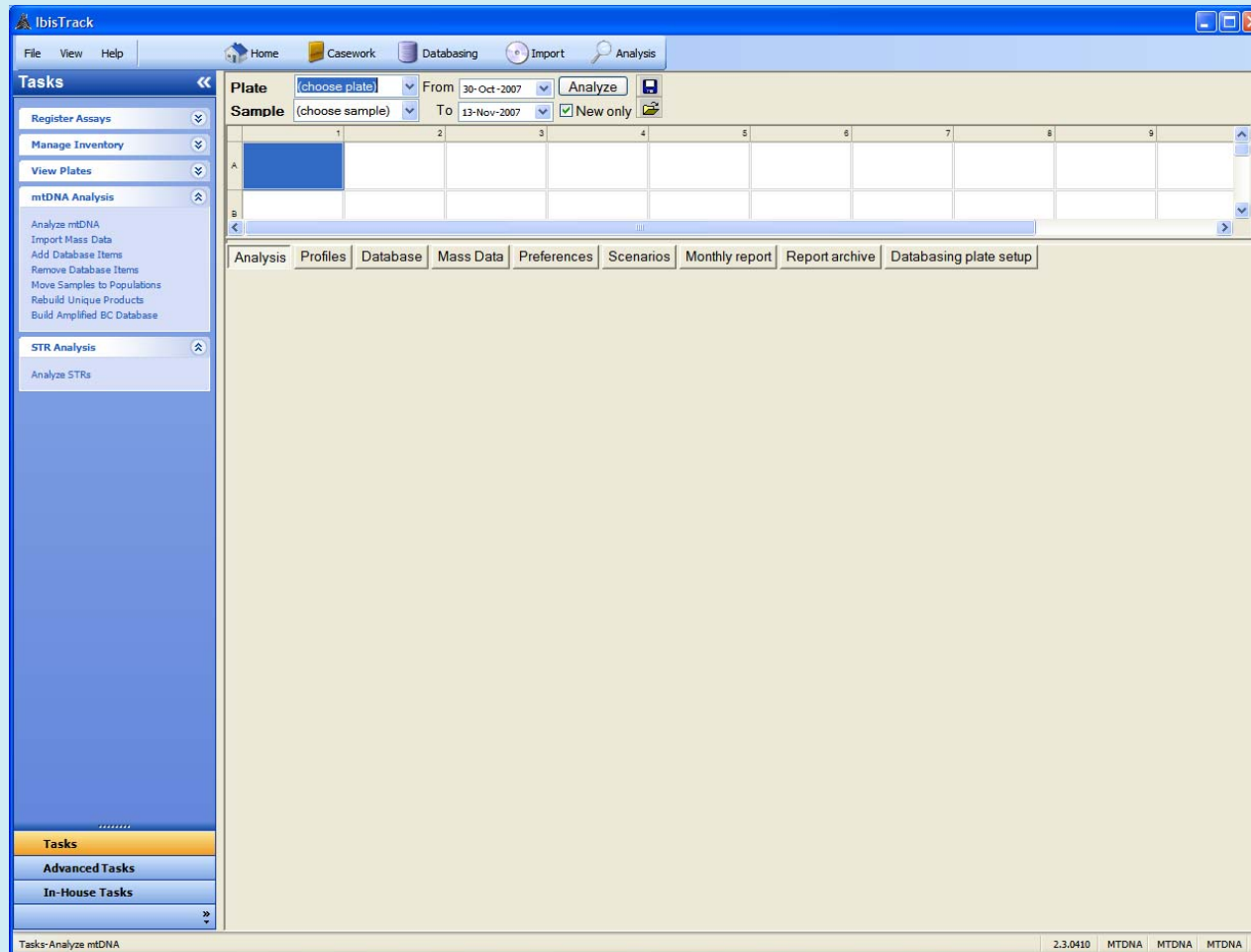
Sequence imports can be done by:

1. Manual profile entry (or copy/paste)
2. Import of raw sequence (software aligns and creates profile automatically)
3. Import LISA-exported profiles (e.g. AFDIL system)
4. Import CMF-formatted profiles (can be done in batch)

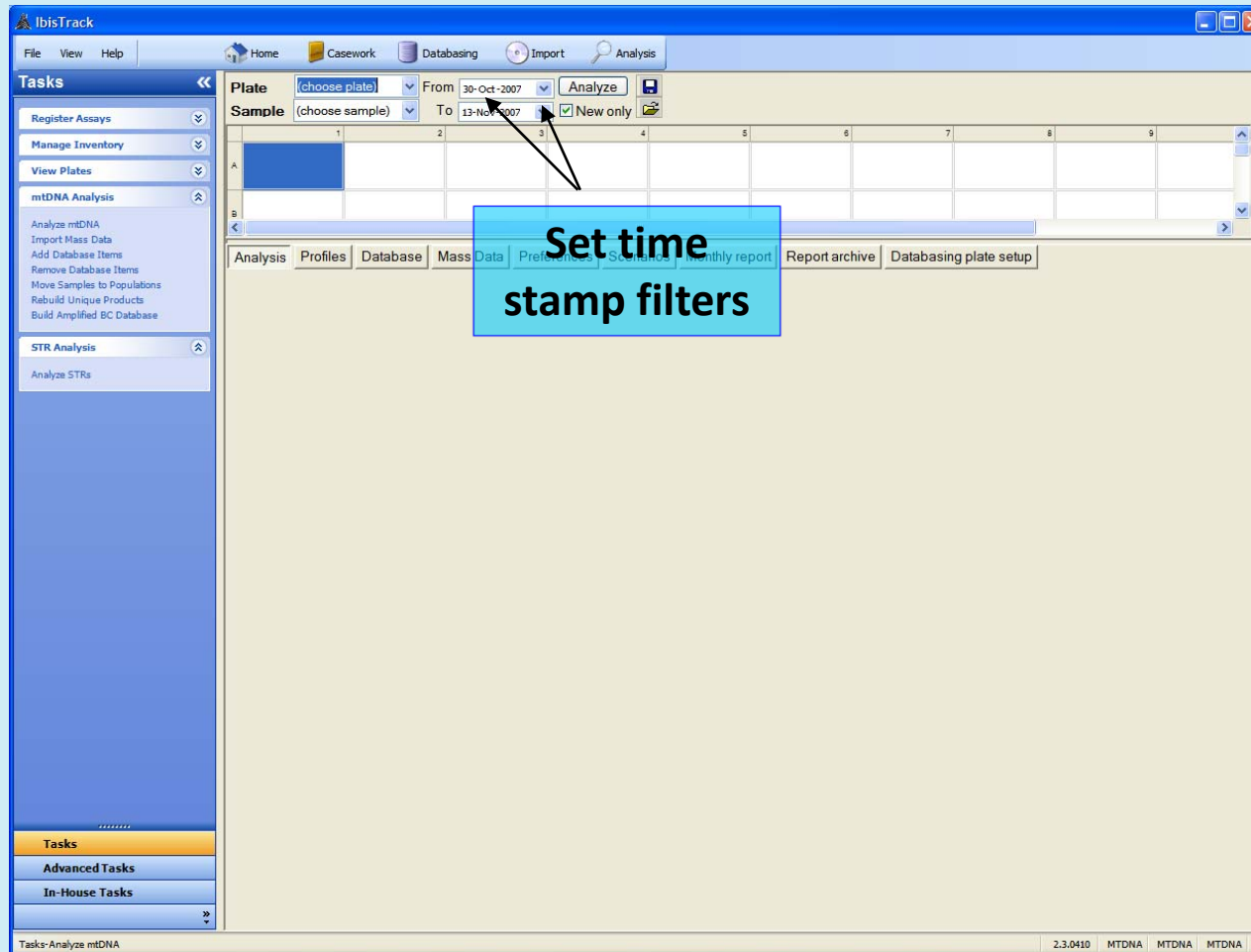
Conversion to base composition profiles is automatic for all

Example: Single addition of a sequence profile

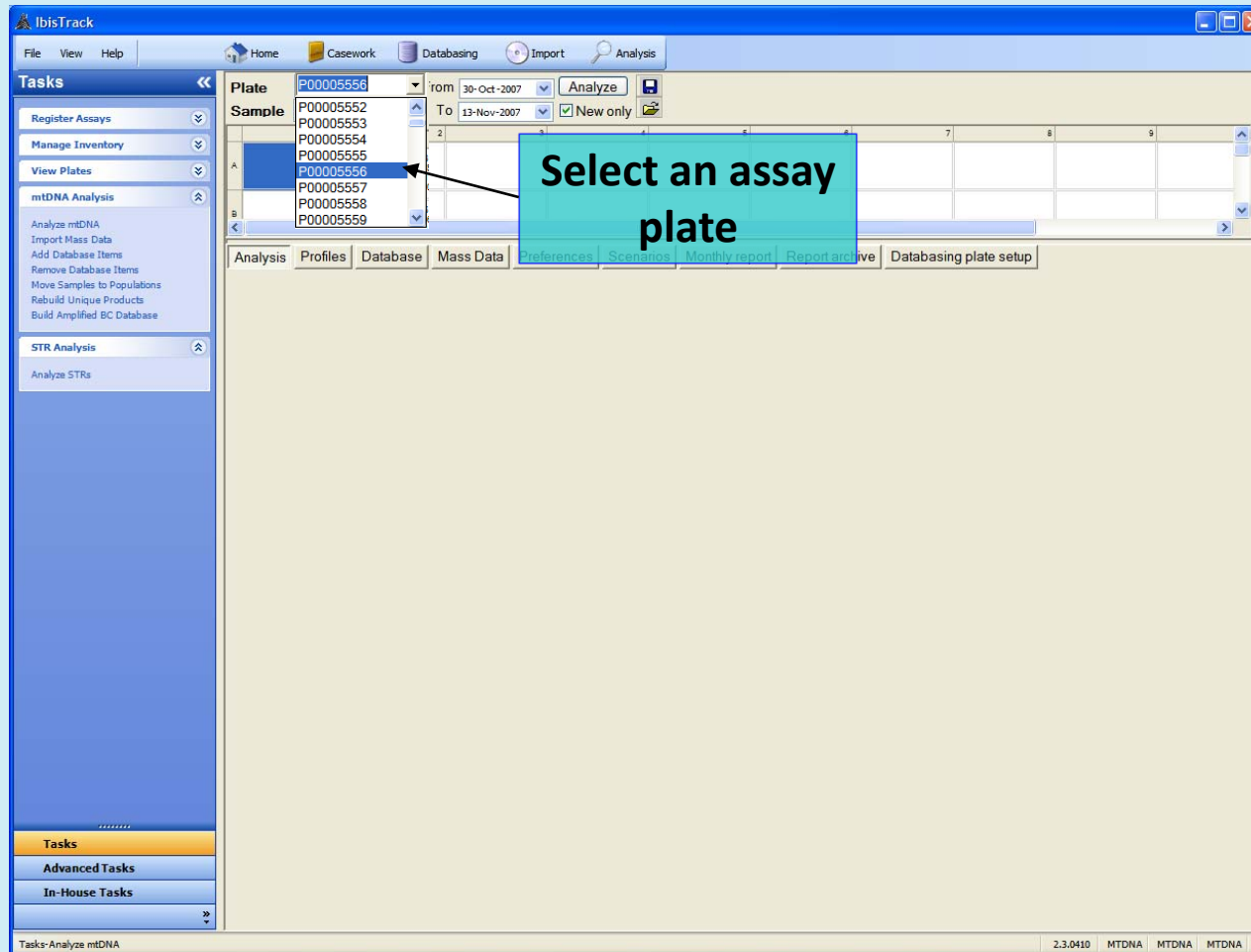
Sample Analysis – mtDNA



Sample Analysis – mtDNA



Sample Analysis – mtDNA



Sample Analysis – mtDNA

The screenshot displays the IbisTrack software interface. The main window is titled "IbisTrack" and features a menu bar with "File", "View", and "Help". Below the menu bar are icons for "Home", "Casework", "Databasing", "Import", and "Analysis".

On the left side, there is a "Tasks" sidebar with the following sections:

- Register Assays
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

The main workspace shows a data grid for mtDNA analysis. At the top, there are filters for "Plate" (P00005555), "From" (30-Oct-2005), and "To" (13-Nov-2007). Below these are "Sample" (All) and "New only" checkboxes. The grid contains two rows of data:

	1	2	3	4	5	6	7	8	9	
A	HUM2996 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2905 Scenario: 75 HUM2901 Scenario: 70
B	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85	HUM2925 Scenario: 85

Below the grid, there are tabs for "Analysis", "Profiles", "Database", "Mass Data", "Preferences", "Scenarios", "Monthly report", "Report archive", and "Databasing plate setup".

At the bottom of the window, the status bar shows "Tasks-Analyze mtDNA" and "2.3.0410 MTDNA MTDNA MTDNA".

Sample Analysis – mtDNA

The screenshot displays the IbisTrack software interface. The top menu bar includes 'File', 'View', 'Help', 'Home', 'Casework', 'Databasing', 'Import', and 'Analysis'. The 'Tasks' sidebar on the left lists various functions such as 'Register Assays', 'Manage Inventory', 'View Plates', 'mtDNA Analysis', and 'STR Analysis'. The main workspace features a grid of sample analysis results. The grid has columns numbered 1 through 9 and rows labeled 'A' and 'B'. Each cell in the grid contains text indicating the sample ID and scenario, such as 'HUM2906 Scenario: 75' or 'HUM2901 Scenario: 70'. A blue box with the text 'Select sample' and an arrow points to the first cell in the grid. Below the grid, there are tabs for 'Analysis', 'Profiles', 'Database', 'Mass Data', 'Preferences', 'Scenarios', 'Monthly report', 'Report archive', and 'Databasing plate setup'. The status bar at the bottom shows 'Tasks-Analyze mtDNA' and '2.3.0410 MTDNA MTDNA MTDNA'.

Sample Analysis – mtDNA

The screenshot shows the IbisTrack software interface. The main window is titled "IbisTrack" and has a menu bar with "File", "View", and "Help". Below the menu bar are icons for "Home", "Casework", "Databasing", "Import", and "Analysis".

The left sidebar contains a "Tasks" panel with the following sections:

- Register Assays
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

The main workspace shows a "Plate" dropdown set to "P00005555" and a "From" date of "30-Oct-2005". Below this is a "Sample" dropdown set to "1" and a "To" date of "13-Nov-2007". There is an "Analyze" button and a "New only" checkbox.

The main area displays a grid of samples. The grid has 10 columns and 2 rows. The first row is labeled "A" and the second row is labeled "B". Each cell in the grid contains text such as "HUM2905 Scenario: 75" or "HUM2905 Scenario: 86".

Below the grid is a navigation bar with tabs: "Analysis", "Profiles", "Database", "Mass Data", "Preferences", "Scenarios", "Monthly report", "Report archive", and "Databasing plate setup".

The status bar at the bottom of the window shows "Tasks-Analyze mtDNA" and "2.3.0410 MTDNA MTDNA MTDNA".

Sample Analysis – mtDNA

Click Analyze

Plate	Sample	1	2	3	4	5	6	7	8	9
A	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75	HUM2906 Scenario: 75
	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70
B	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86	HUM2905 Scenario: 86
	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70	HUM2901 Scenario: 70

Analysis Profiles Database Mass Data Preferences Scenarios Monthly report Report archive Databasing plate setup

Tasks-Analyze mtDNA 2.3.0410 MTDNA MTDNA MTDNA

Single Sample Analysis – mtDNA

Single assignment – bottom strand

Single assignment – top strand

Mass measurement error (ppm)

ppm = Parts per million

ppm error = ((expected – observed)/expected) * 1,000,000

Single Sample Analysis – mtDNA

Tasks

- Register Assays
 - Register Casework Plates
 - Register New Plate for Database Population
 - Process Repeats for Database
 - Register Quality Control Plates
 - Generate Plate Setup Reports
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

Analysis

Plate: P00005556 From: 18-Nov-2005 To: 02-Dec-2007

Sample: 1 To: 7

Analysis Profiles Database Mass Data Preferences Scenarios Monthly report Report archive

P00005556-2003X02368-0001A1D (1)

Filter ambiguous assignments **Single assignment – top strand**

Spectrum viewing mode: Raw Decomposed

Well: 73 (G01)

Scenario: 65, PP 2896 (HUMMTDNA_ASN_161)

Positions: 16102..16224

Amplified coordinates: 16124..16201

Base count: A45 G13 C41 T24

num	error	exp. mass	obs. mass
1	0.7492	37567.2673	37567.2391

Single assignment – bottom strand

Product strand corresponds to a mass peak

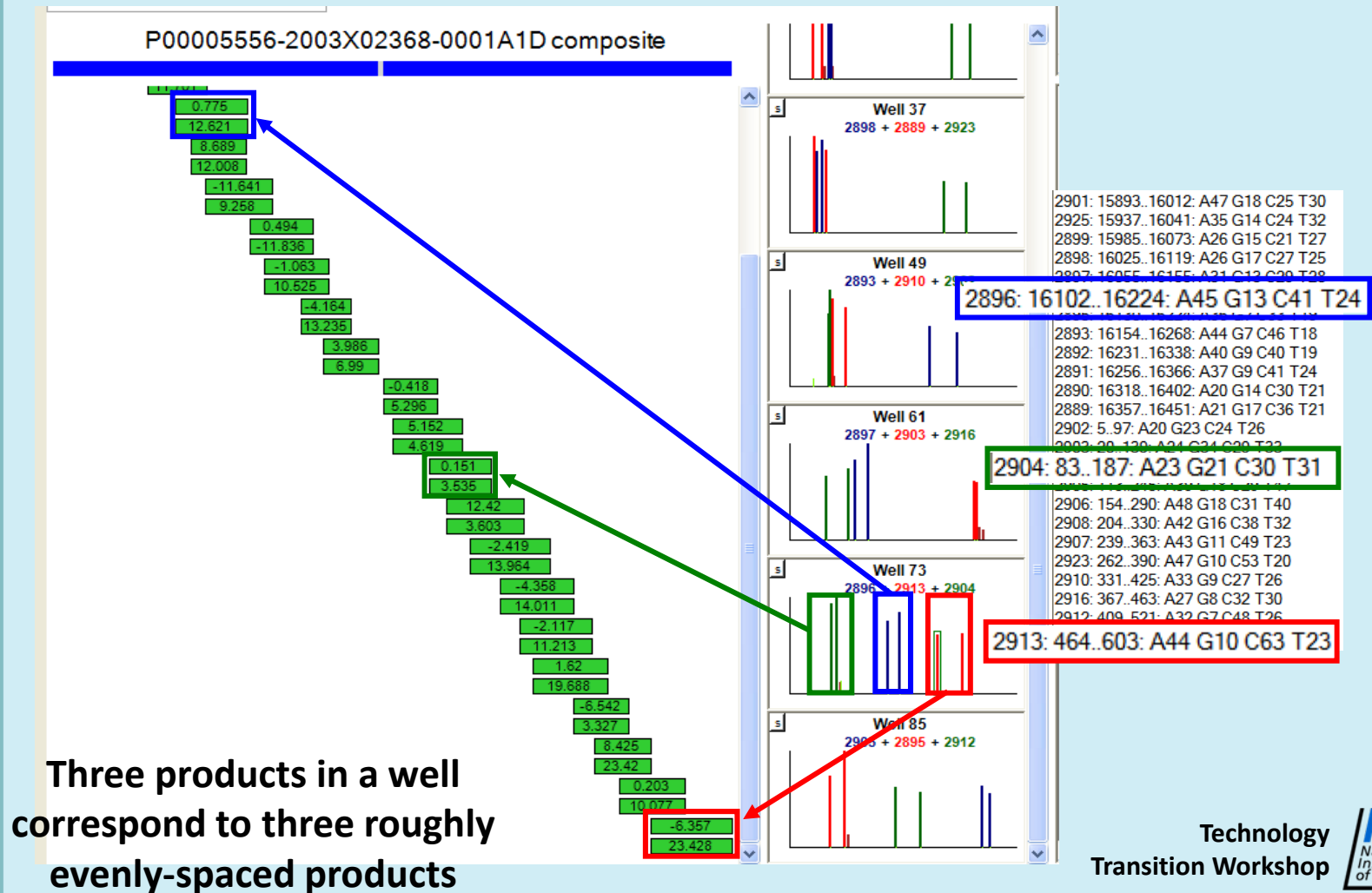
Comments for analysis report

Tasks-Analyze mtDNA

Single Sample Analysis – mtDNA

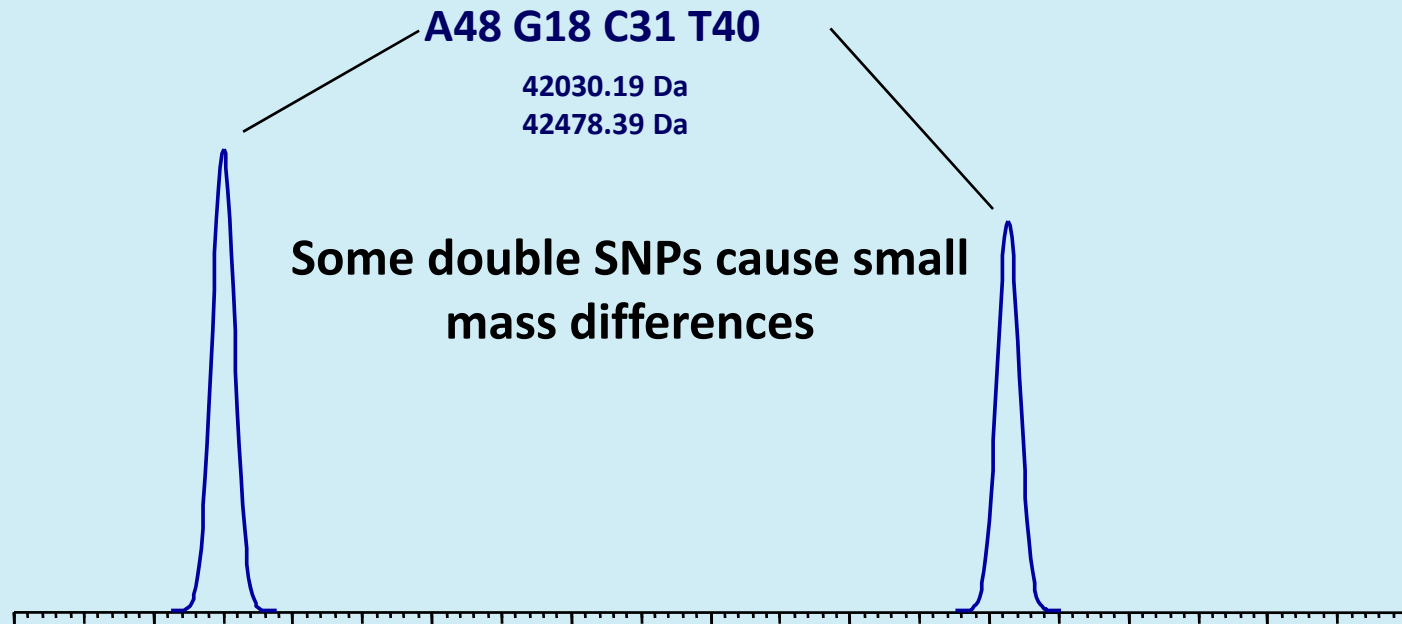
The screenshot shows the IbisTrack software interface for mtDNA analysis. The main window displays a grid of analysis results for a plate (P00005556) and sample (1). The grid shows various scenarios (HUM2906, HUM2901, HUM2902, HUM2903) and their corresponding sample IDs. Below the grid, there are tabs for Analysis, Profiles, Database, Mass Data, Preferences, Scenarios, Monthly report, and Report archive. The Analysis tab is active, showing a spectrum view of the data. The spectrum view displays a chromatogram with peaks labeled with their retention times (e.g., -8.938, 18.564, 1.193, 5.547, 2.916, 0.926, -2.079, 12.22, -4.418, 0.749, 12.938, 8.879, 11.925, 11.658, 9.166, 11.47). A blue box highlights the peak at 0.749 minutes, with an annotation: "Single assignment – bottom strand". Another blue box highlights the peak at 12.938 minutes, with an annotation: "Single assignment – top strand". A third blue box highlights the peak at 8.879 minutes, with an annotation: "Product strand corresponds to a mass peak". On the right side of the interface, there is a "Profile record" section. It contains a table with columns for "Primer pair", "CRS coords", and "base count". The table shows the following data: "2896: 16102..16224: A45 G13 C41 T24". A blue box highlights this row, with an annotation: "Pair of masses corresponds to a double-stranded PCR product". Below the table, there is a section for "Amplified coordinates" and "Base count". The coordinates are "16124..16201" and the base count is "A45 G13 C41 T24". There are also several chromatograms displayed, labeled "Well 61 (F01)", "Well 73 (G01)", and "Well 85 (H01)". The "Well 61 (F01)" chromatogram shows peaks at 2897 and 2903 + 2916. The "Well 73 (G01)" chromatogram shows peaks at 2896 and 2904. The "Well 85 (H01)" chromatogram shows peaks at 2905 and 2895 + 2912. The interface also includes a "Tasks" panel on the left with sections for "Register Assays", "Manage Inventory", "View Plates", "mtDNA Analysis", and "STR Analysis". The "mtDNA Analysis" section includes tasks like "Analyze mtDNA", "Import Mass Data", "Add Database Items", "Remove Database Items", "Move Samples to Populations", "Rebuild Unique Products", and "Build Amplified BC Database". The "STR Analysis" section includes the task "Analyze STRs".

Single Sample Analysis – mtDNA



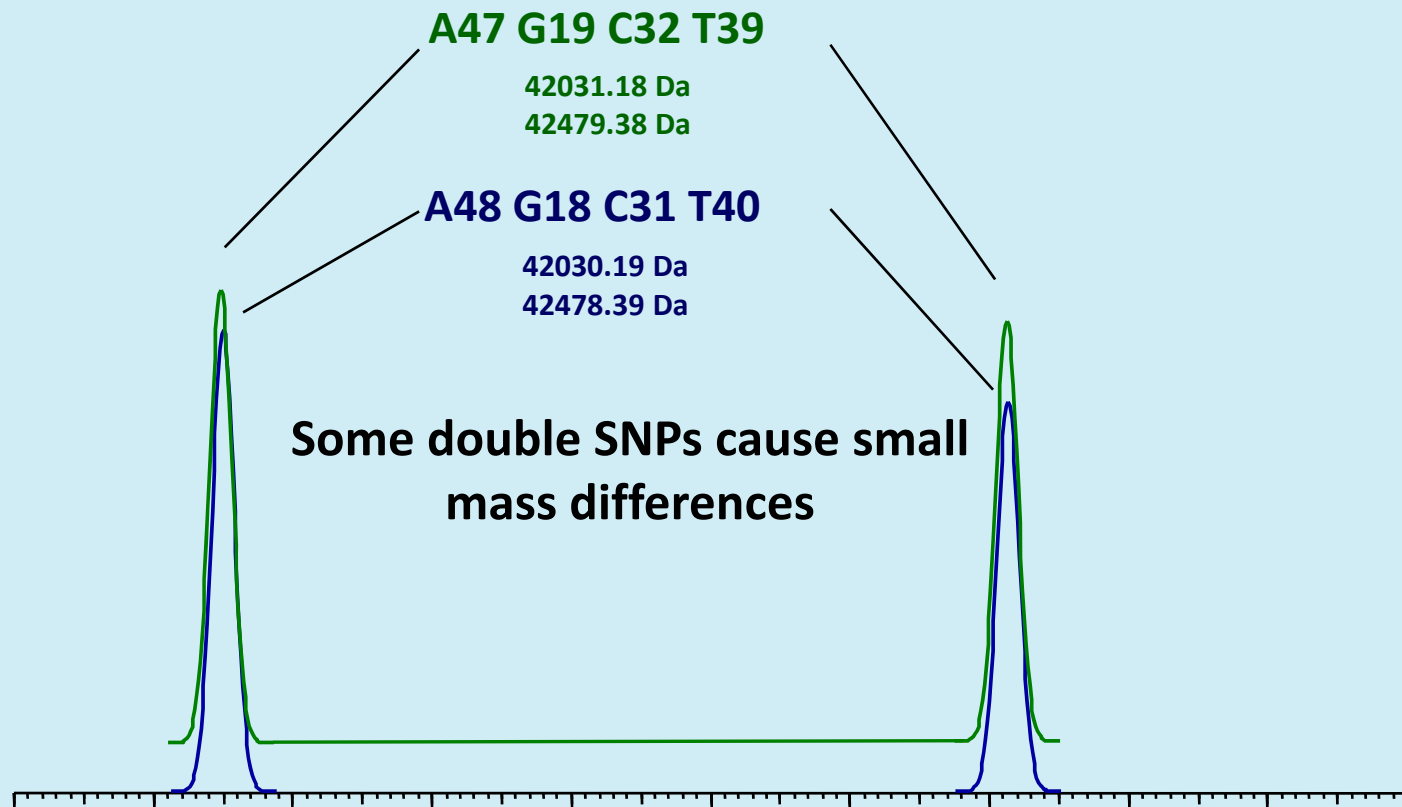
Use of a Mass Tag

High mass precision and mass tag combine to provide unambiguous base compositions in routine operation



Use of a Mass Tag

Without mass tag: Product strands differ by 1 Da for two products that differ by a G→A and C→T SNP at the same time

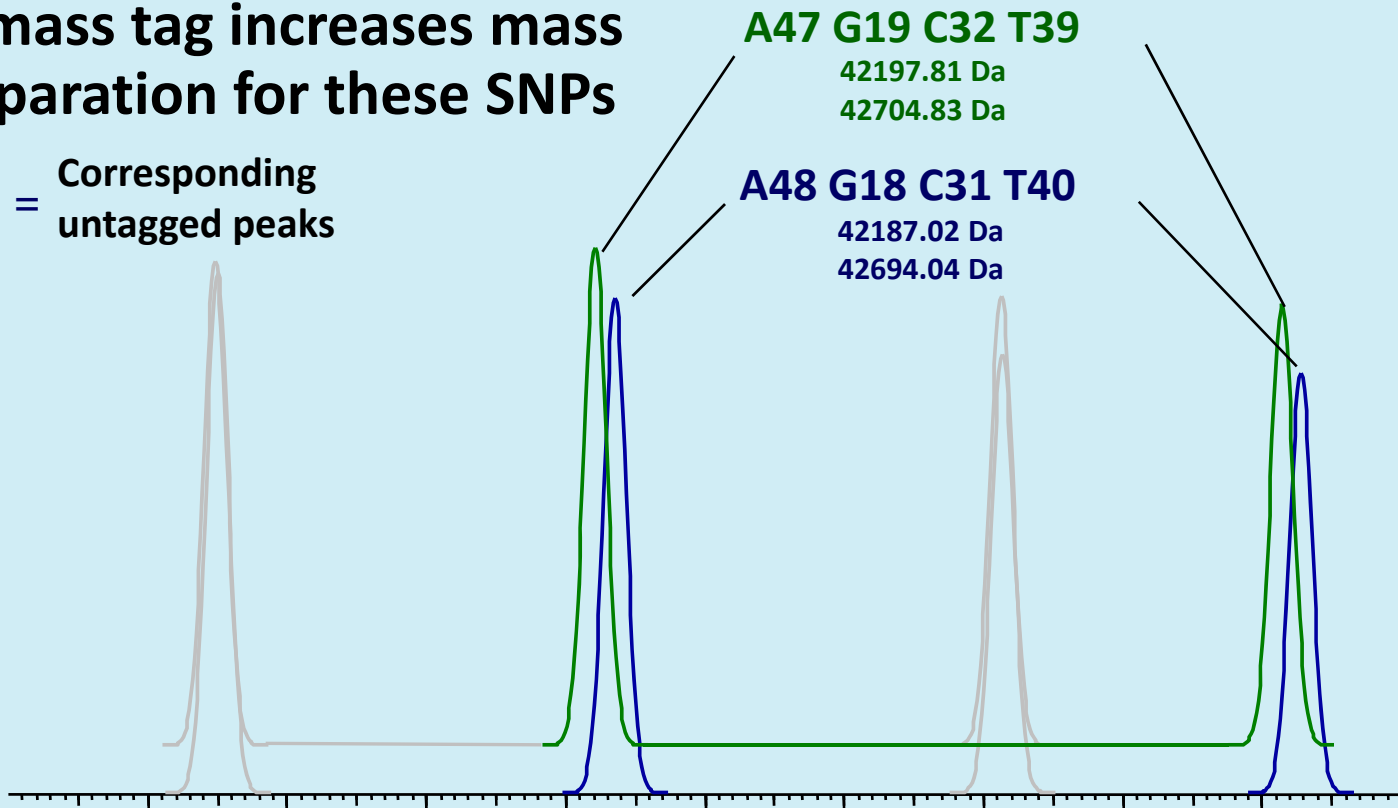


Use of a Mass Tag

With mass tag: With ^{13}C -dGTP, the mass separation increases to ~ 10 Da for each strand; this is about 300 ppm (we generally see errors ~ 10 ppm)

A mass tag increases mass separation for these SNPs

— = Corresponding untagged peaks



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Real Data with Mass Tag

Primer pair 2906 product from two representative samples (data for primer pair 2906 are overlaid)

Well A05: P00005582



A47 G19 C32 T39

42197.81 Da

42704.83 Da

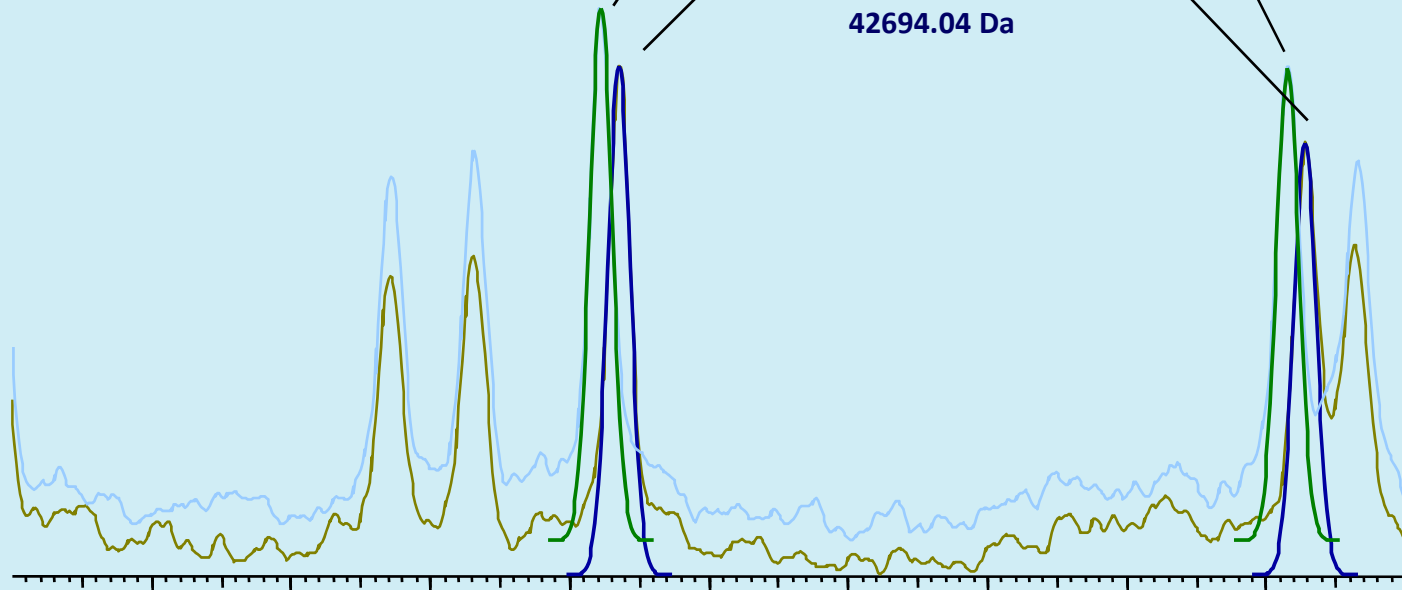
Well A01: P00005553



A48 G18 C31 T40

42187.02 Da

42694.04 Da



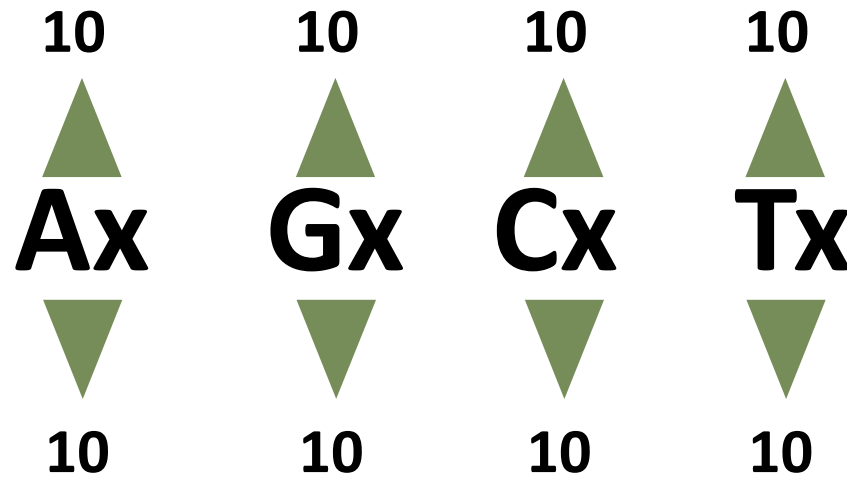
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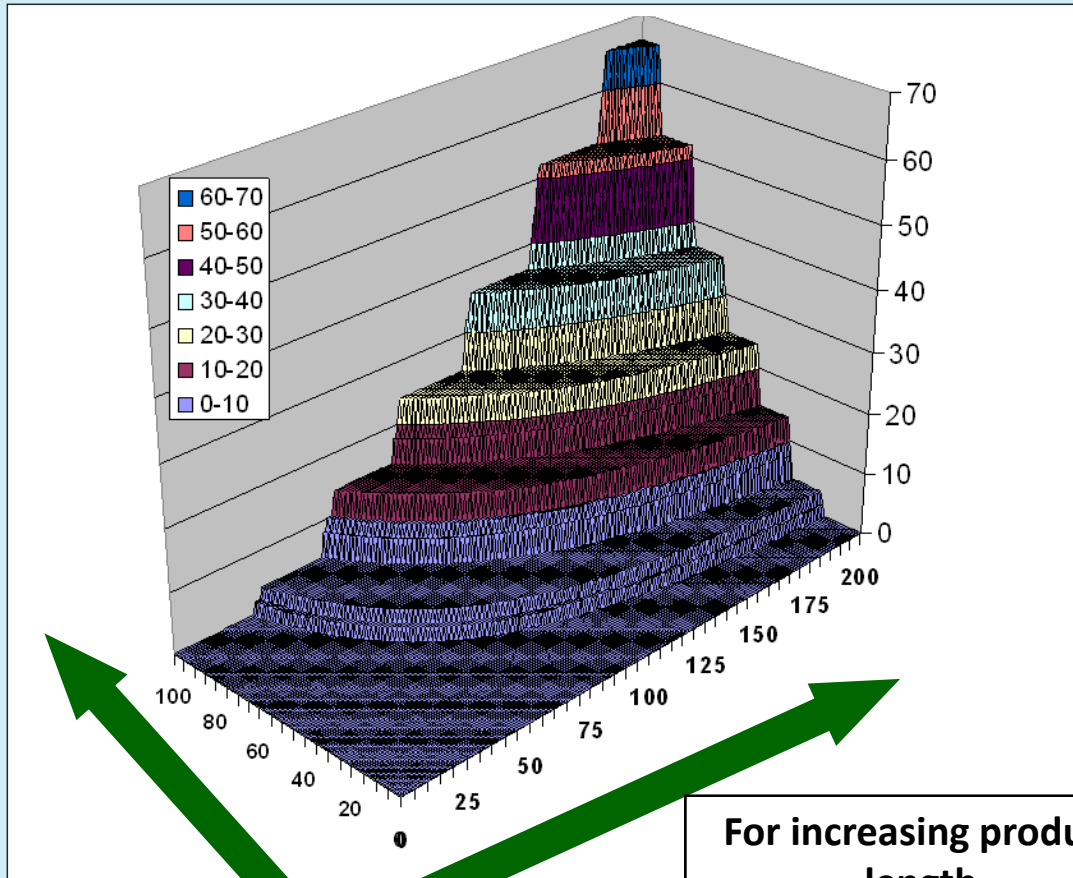
What Does Mass Tagging Mean?

For all
combinations of
base differences
plus or minus 10
A, G, C, T ...

For any base count



What Does Mass Tagging Mean?



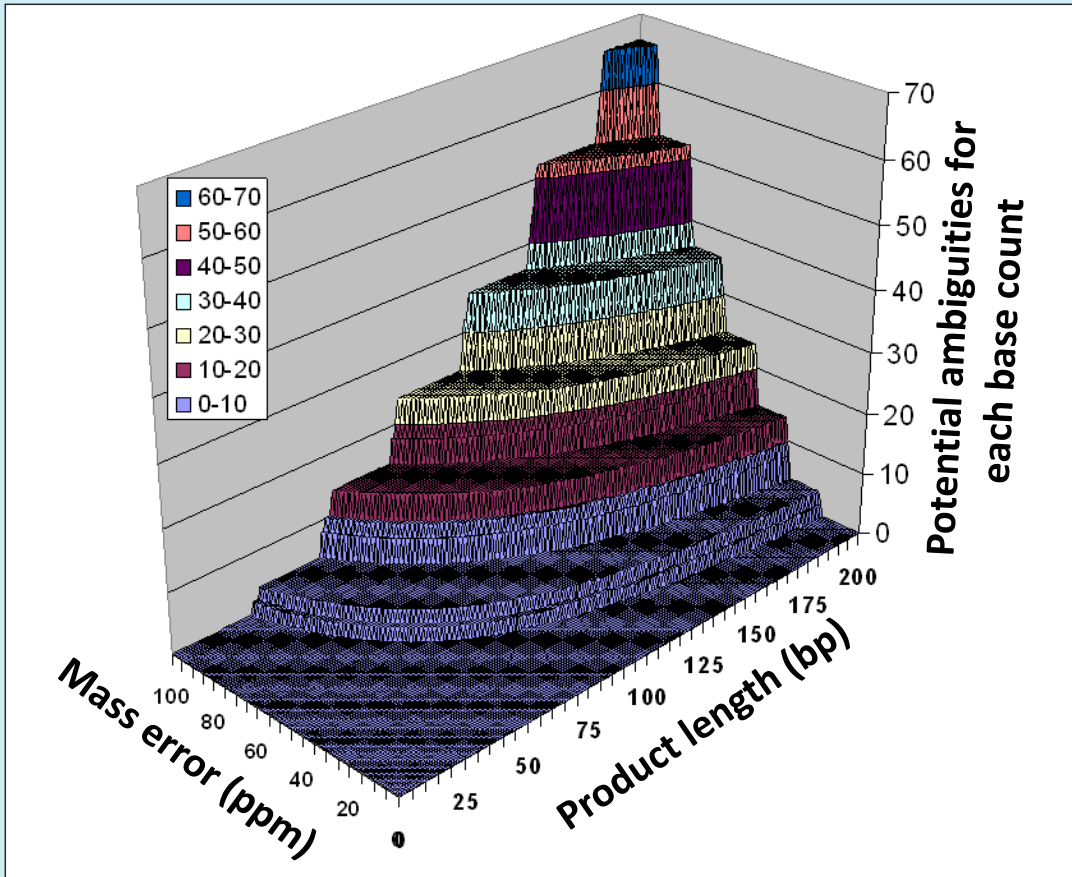
For all
combinations of
base differences
plus or minus 10
A, G, C, T ...

And increasing
measurement
error

For increasing product
length

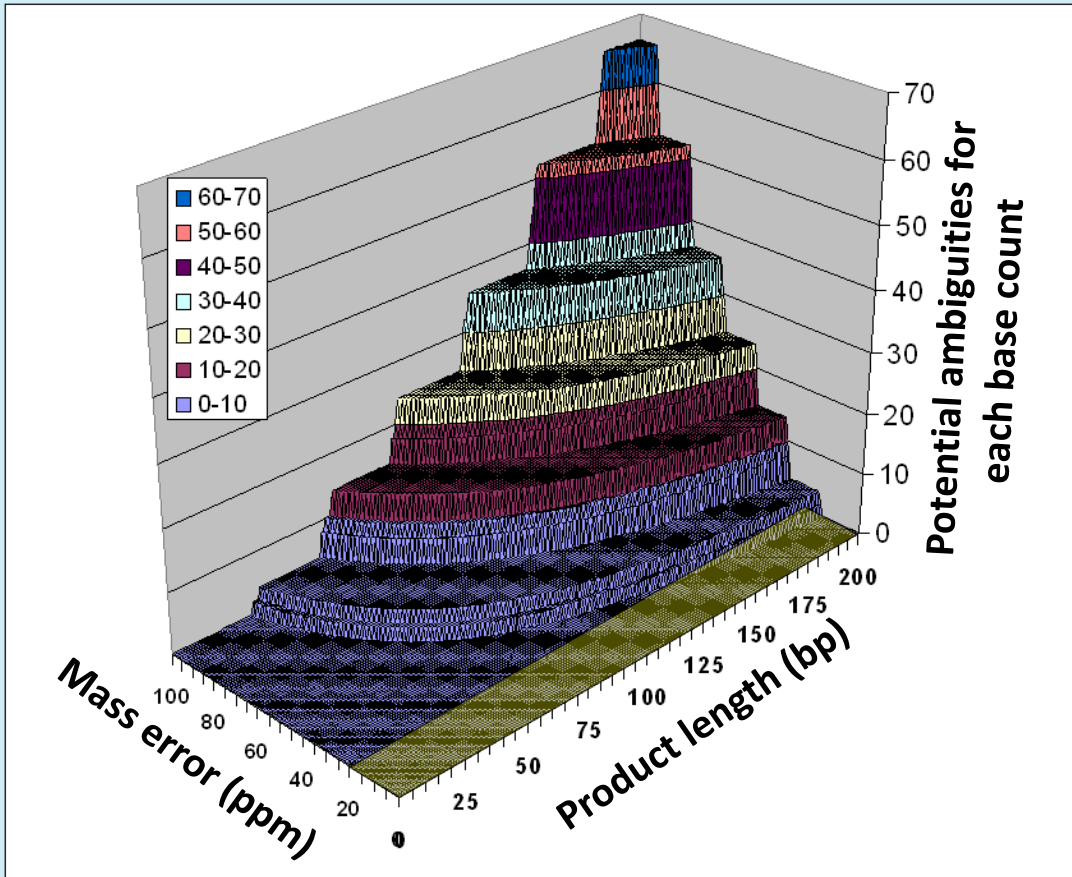
What Does Mass Tagging Mean?

Potential assignment ambiguities increase dramatically with measurement error and product size



What Does Mass Tagging Mean?

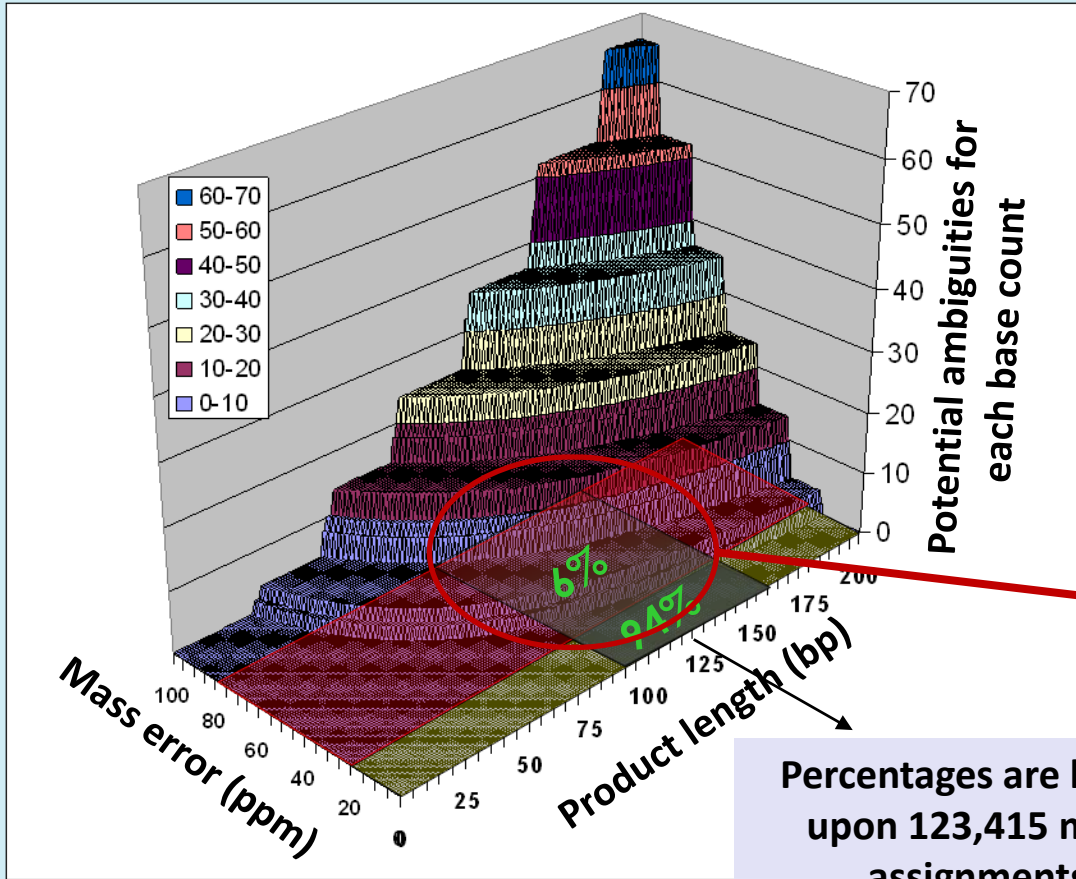
Ambiguous assignments not a problem in our normal working range of mass measurement



Working range for TOF (<20 ppm)

What Does Mass Tagging Mean?

Most assignments would be fine with natural nucleotides.
Some assignments fall outside of “normal” range.



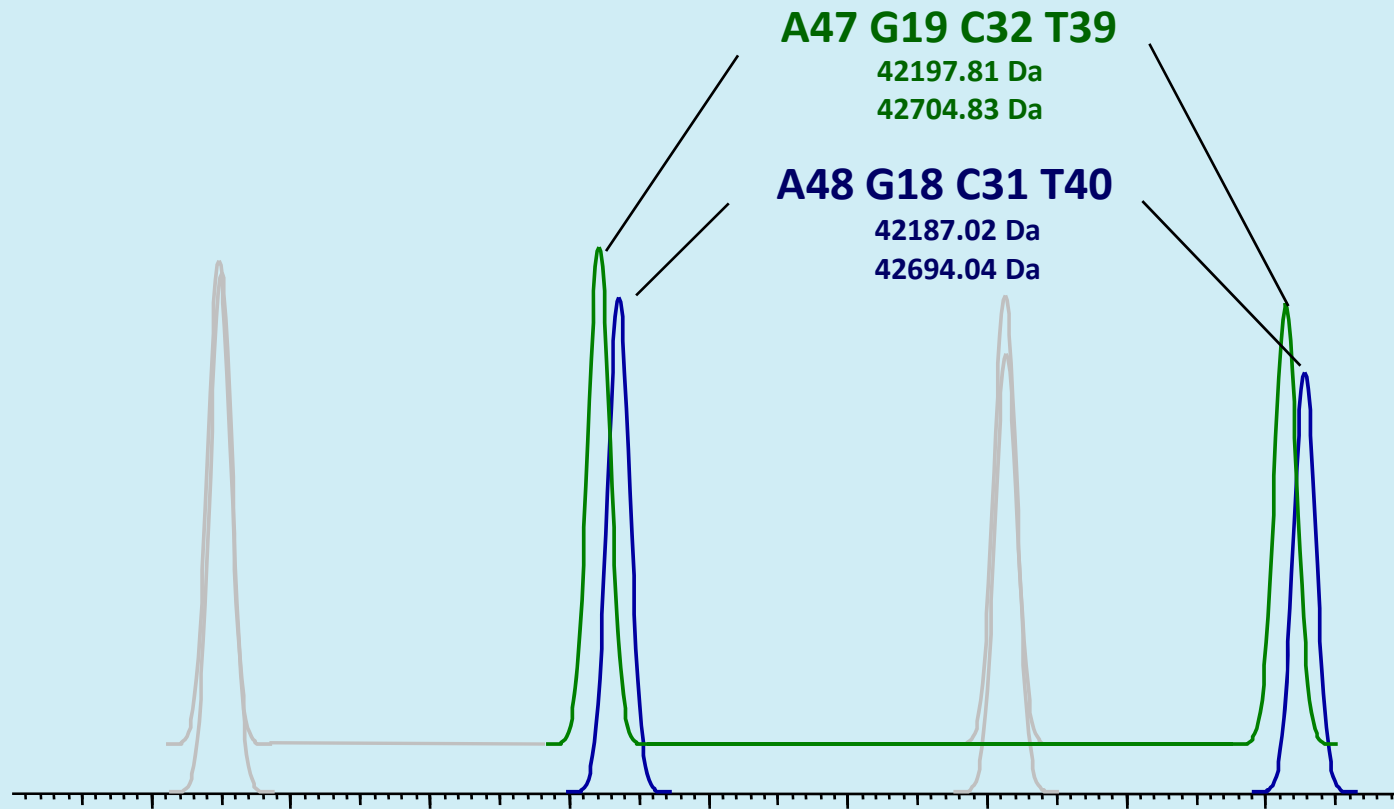
Working range for TOF (<20 ppm)

Which 6% of measurements are a problem?

Percentages are based upon 123,415 mass assignments

Mass Tag Changes Rules

With ^{13}C -dGTP, the mass separation increases to about 10 Da for each strand; this is about 300 ppm (we generally see errors about 10 ppm)

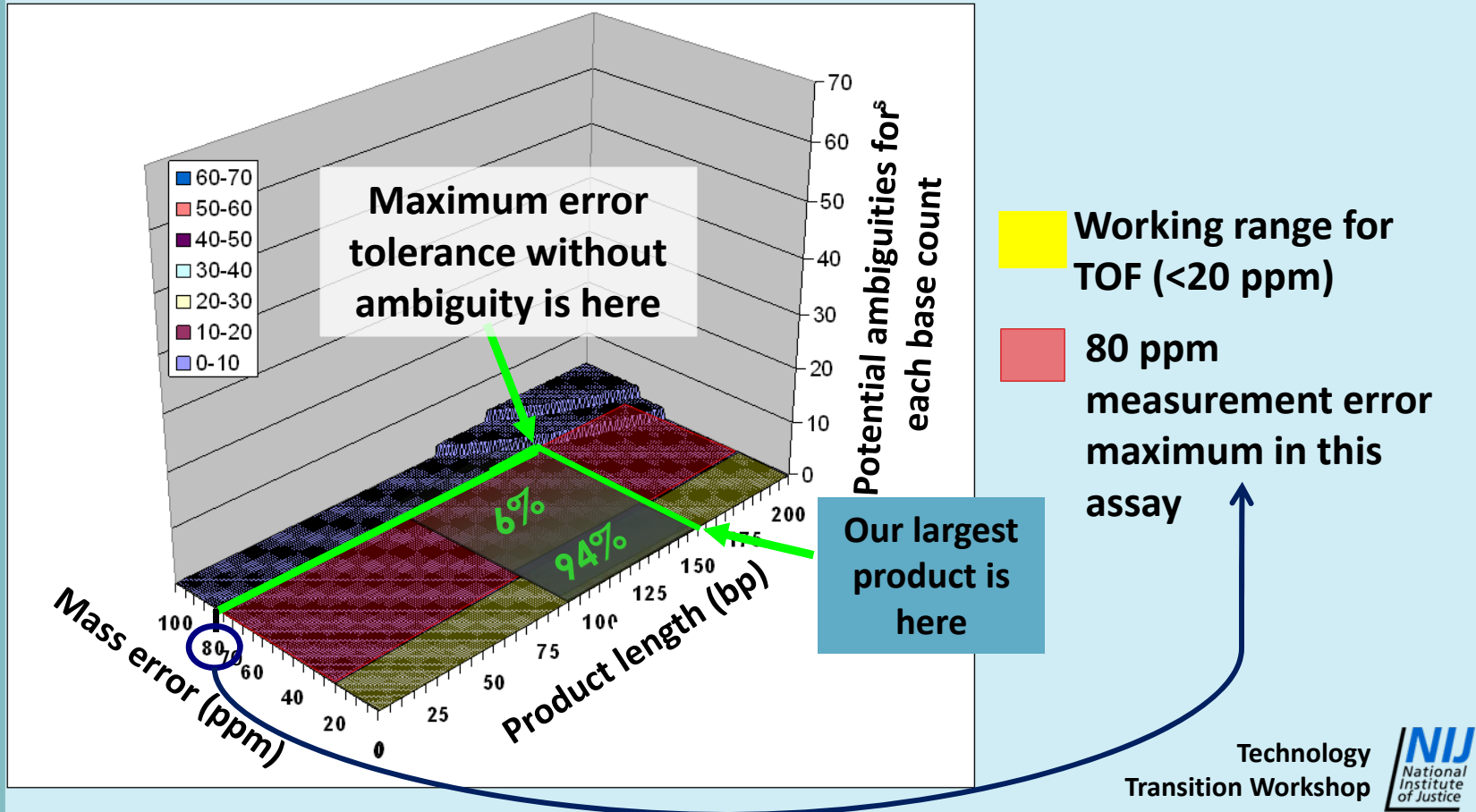


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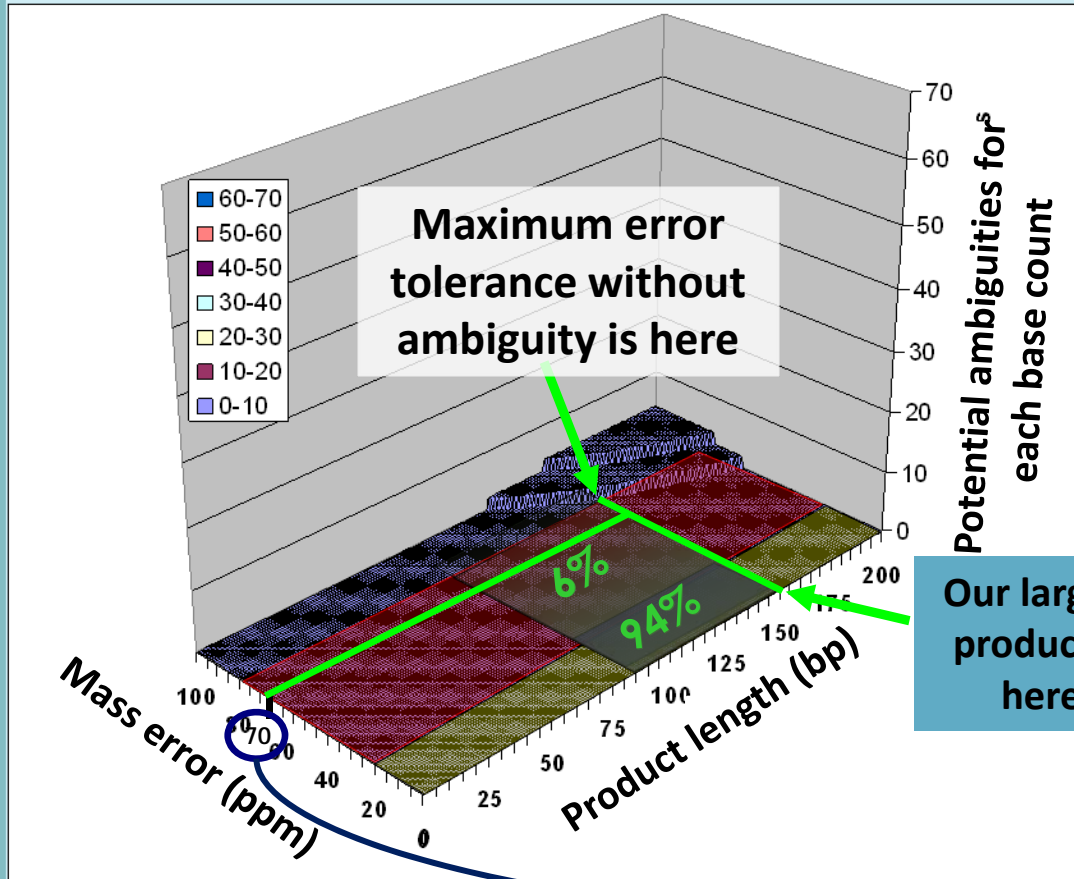
What Does Mass Tagging Mean?

Using ^{13}C -dGTP eliminates ambiguity with a wide margin around our working zone



What Does Mass Tagging Mean?

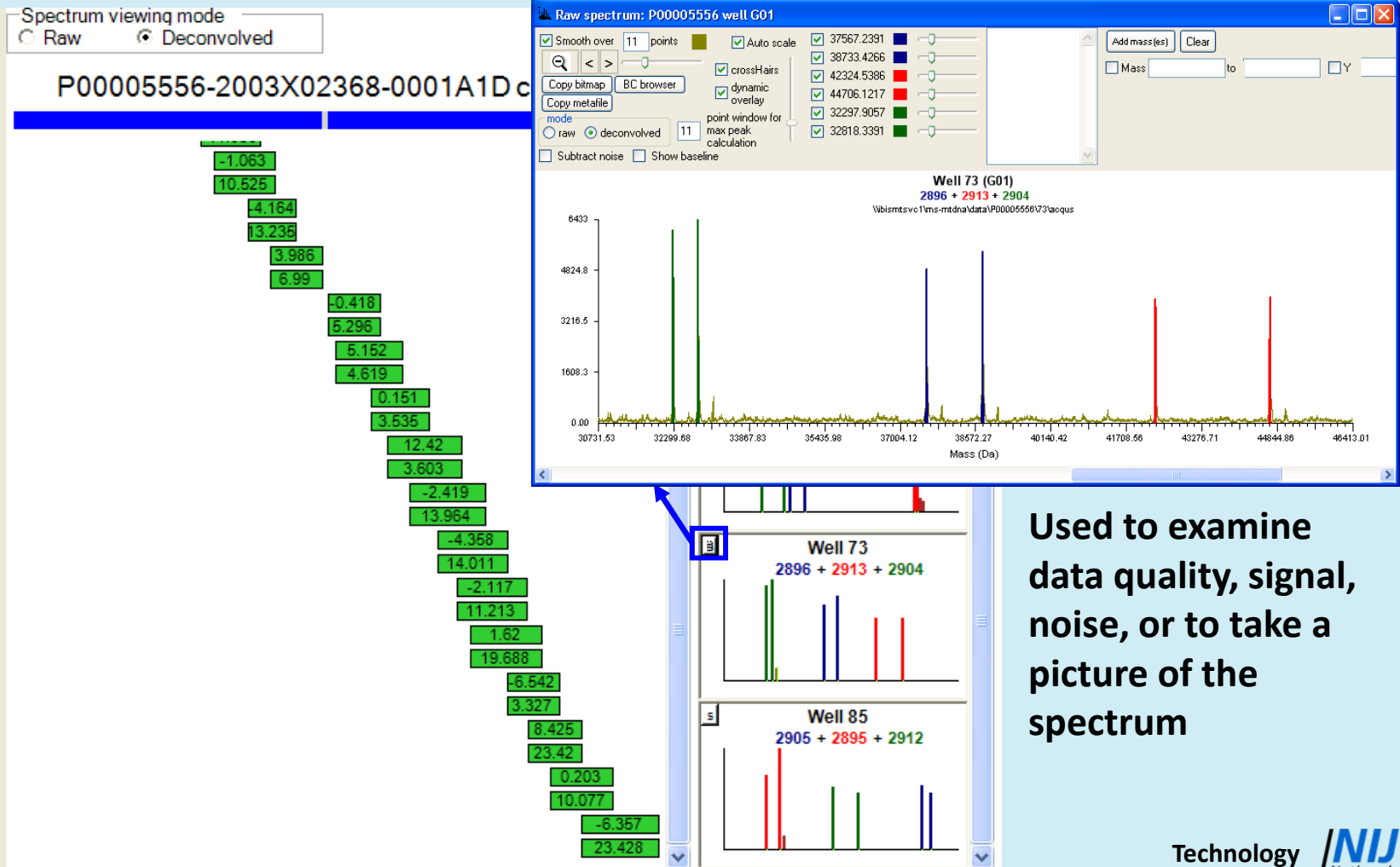
Using ^{13}C -dGTP eliminates ambiguity with a wide margin around our working zone



- Working range for TOF (<20 ppm)
- 80 ppm measurement error maximum in this assay
- Threshold at 70 ppm to be conservative

Our largest product is here

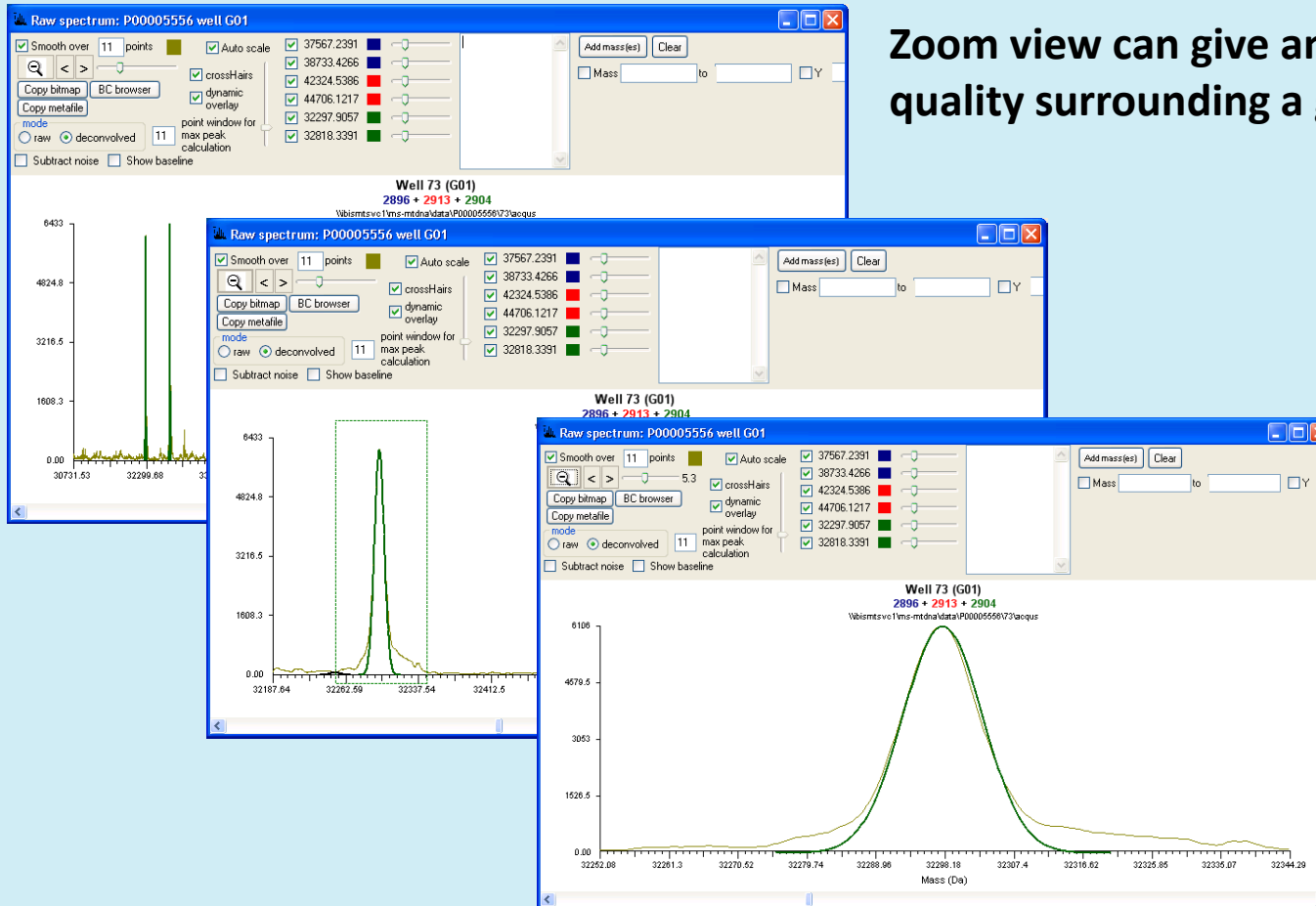
Spectral Viewer



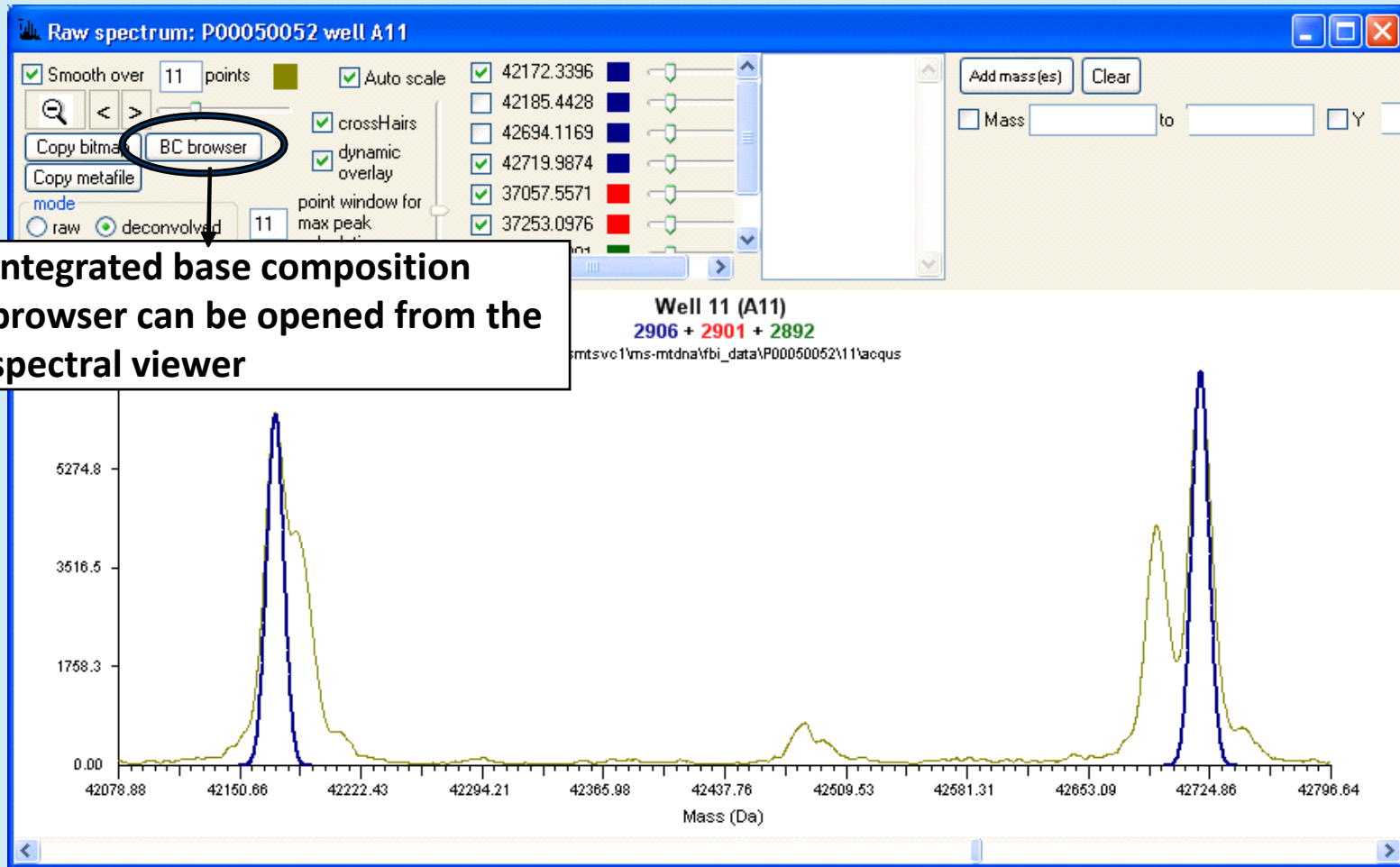
Used to examine data quality, signal, noise, or to take a picture of the spectrum

Spectral Viewer – Deconvolved

Zoom view can give an idea of data quality surrounding a given peak



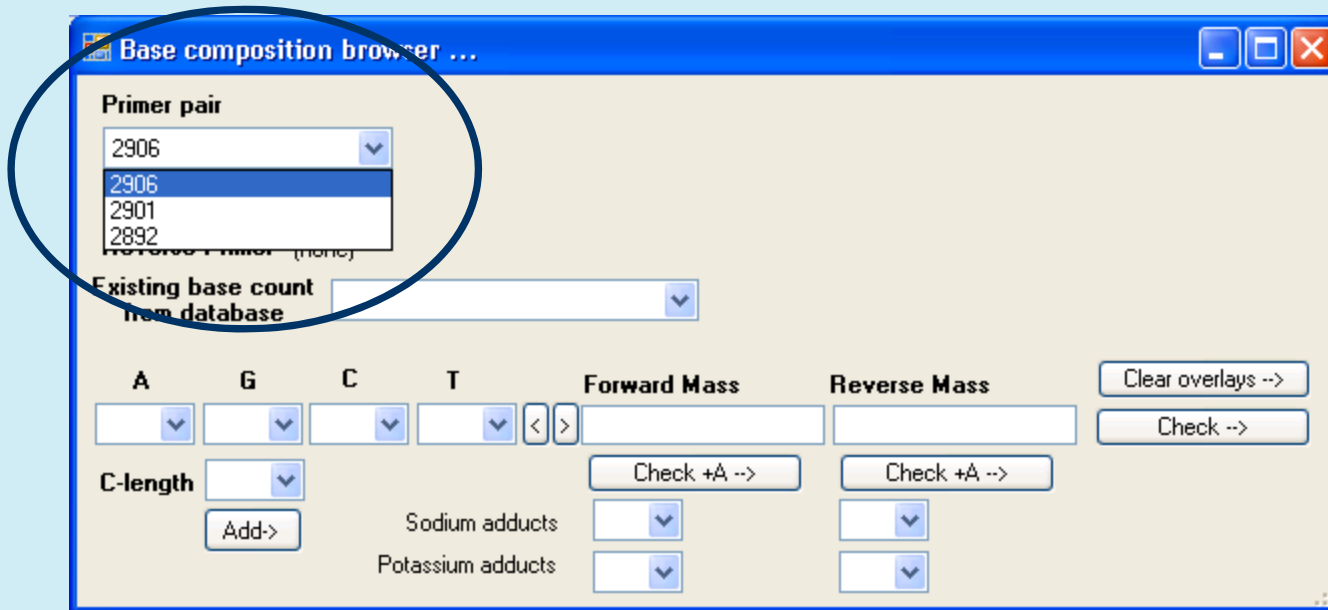
Base Composition Browser



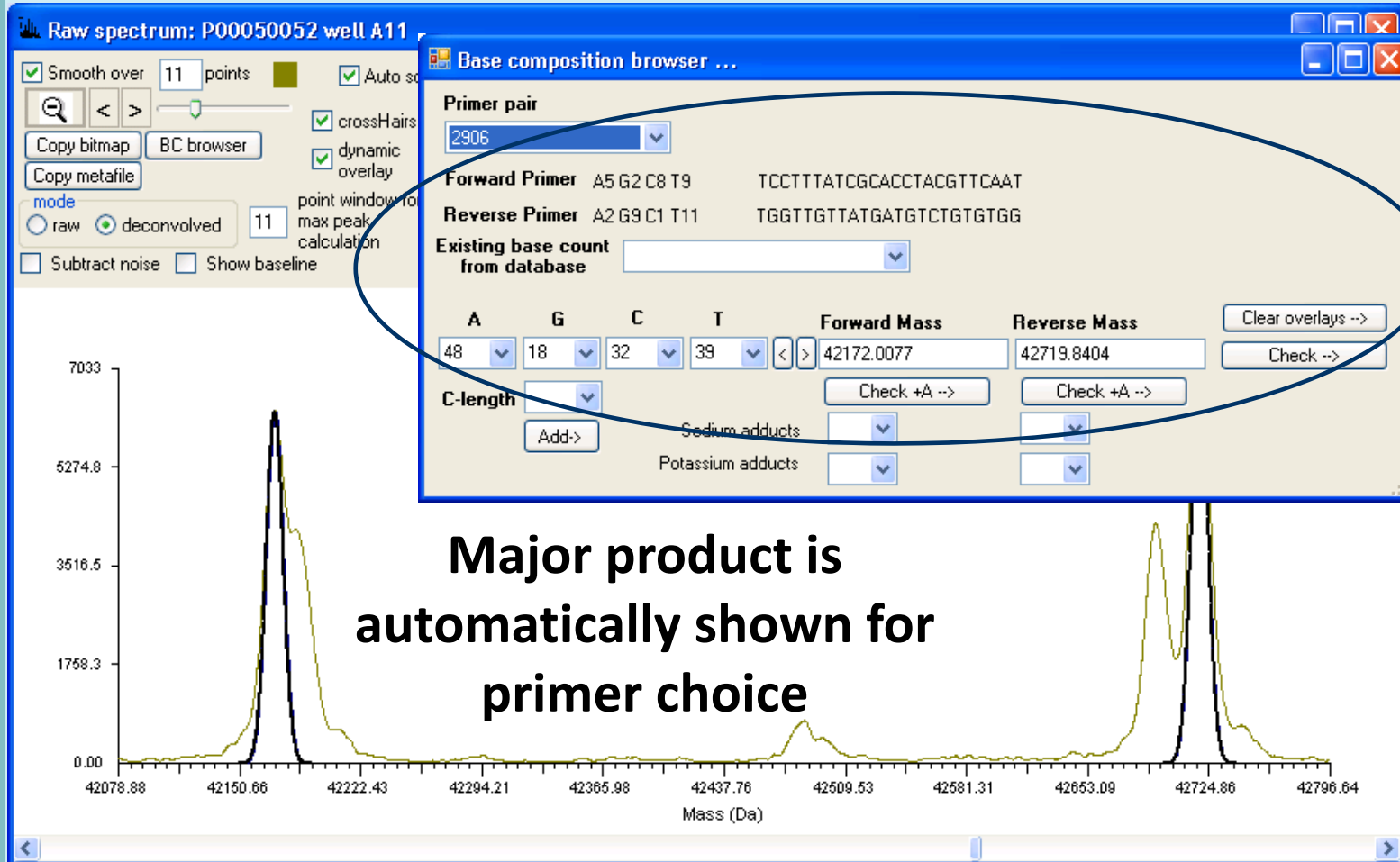
Integrated base composition browser can be opened from the spectral viewer

Base Composition Browser

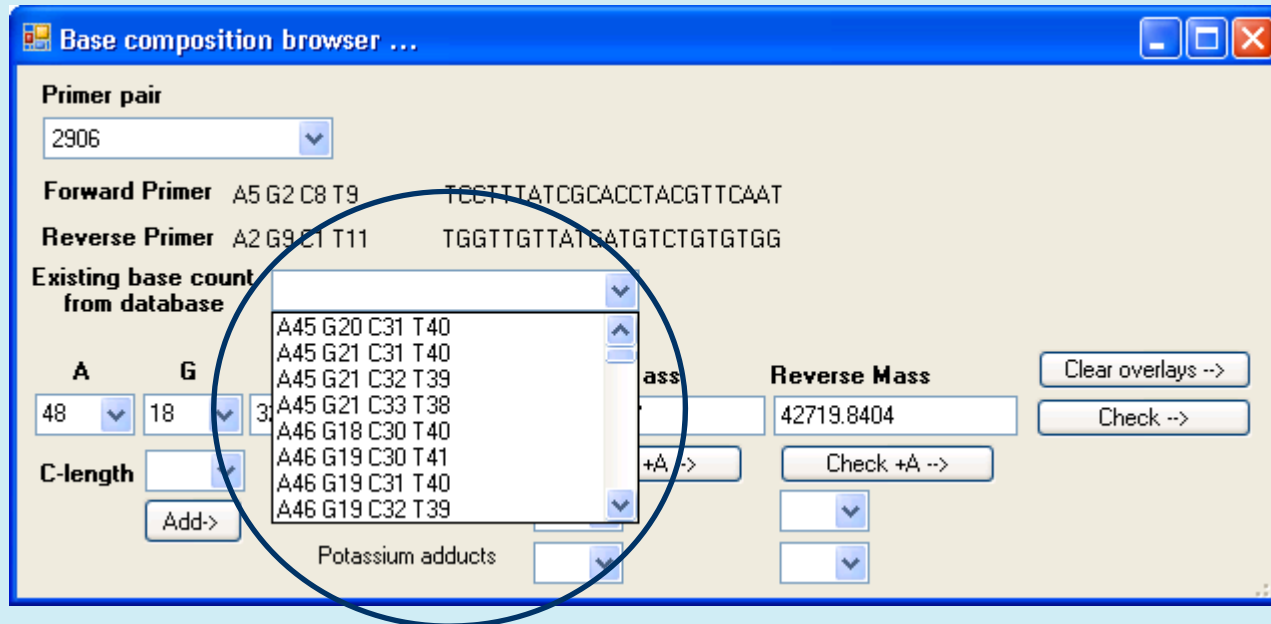
Primer pairs in current well are integrated to this view



Base Composition Browser

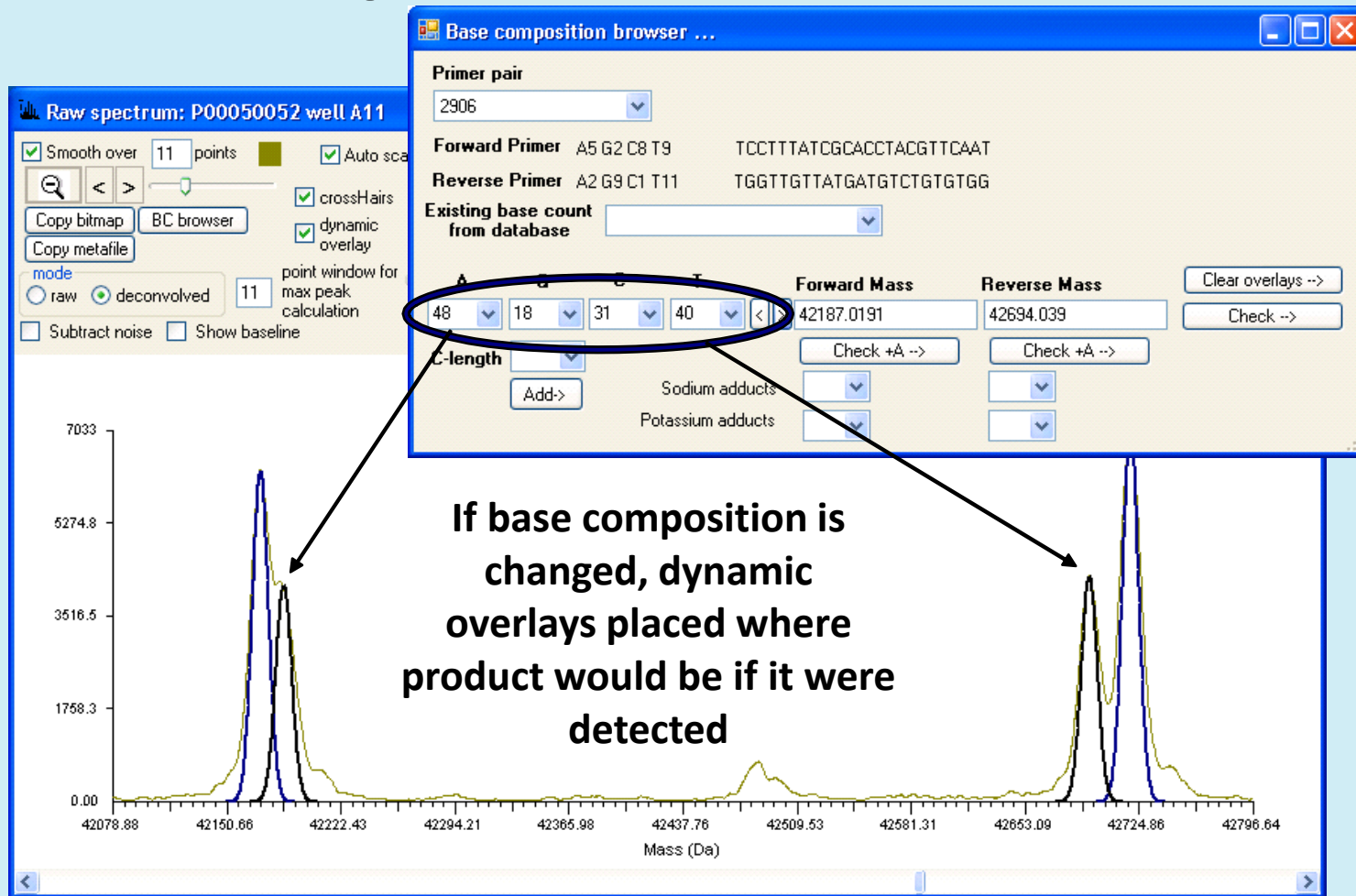


Base Composition Browser



All known products for selected primer pair are in this list

Base Composition Browser



Base Composition Browser

Base composition browser ...

Primer pair
2906

Forward Primer A5 G2 C8 T9 TCCTTTATCGCACCTACGTTCAAT
Reverse Primer A2 G9 C1 T11 TGGTTGTTATGATGTCTGTGTGG

Existing base count from database

A	G	C	T	Forward Mass	Reverse Mass
48	18	31	40	42187.0181	42854.099

C-length

Add->

Sodium adducts

Potassium adducts

Check +A -->

Check +A -->

Clear overlays -->

Check -->

Adenylation products, sodium adducts, and potassium adducts can also be looked for here

Search Database – mtDNA

The screenshot displays the IbisTrack software interface for mtDNA analysis. The main window shows a 'P00005556-2003X02368-0001A1D composite' profile with a ladder of peaks. A context menu is open over the profile, listing various actions such as 'Copy coverage map to Clipboard', 'Copy profile', and 'Search database with current profile'. The search menu is highlighted.

Tasks Panel:

- Register Assays
 - Register Casework Plates
 - Register New Plate for Database Population
 - Process Repeats for Database
 - Register Quality Control Plates
 - Generate Plate Setup Reports
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
- STR Analysis
 - Analyze STRs

Main Analysis Area:

Plate: P00005556 From: 18-Nov-2005 To: 02-Dec-2007

Sample: 1

Analysis Profiles: P00005556-2003X02368-0001A1D (1), P00050052-USA.FBI.000072.SAMPLE (11)

Database: P00005556, E01, P00005556, F01, P00005556, G01, P00005556, H01, P00005556-2003X02368-0001A1D composite

Options: Filter ambiguous assignments, Remove primers from profile, Raw, Deconvolved

Well 49 (E01): 2893 + 2910 + 2902

Well 61 (F01): 2893 + 2902 + 2896

Well: 73 (G01)
Scenario: 65, PP 2896 (HUMMTDNA_ASN_161(1))
Positions: 16102..16224
Amplified coordinates: 16124..16201
Base count: A45 G13 C41 T24

2901: 15893..16012: A47 G18 C25 T30
2925: 15937..16041: A35 G14 C24 T32
2899: 15985..16073: A26 G15 C21 T27
2898: 16025..16119: A26 G17 C27 T28
2897: 16055..16155: A31 G13 C29 T28
2896: 16102..16224: A45 G13 C41 T24

num error exp. mass obs. mass

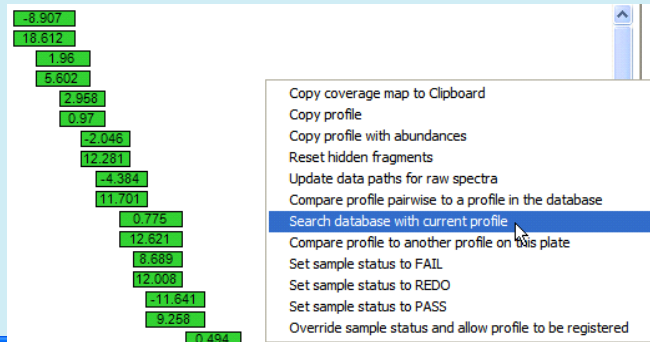
Search Database with current profile

- Copy coverage map to Clipboard
- Copy profile
- Copy profile with abundances
- Copy profile as table with average abundances
- Reset hidden fragments
- Update data paths for raw spectra
- Compare profile pairwise to a profile in the database
- Search database with current profile**
- Compare profile to another profile on this plate
- Register current sample as a contaminant profile
- Set sample status to PASS
- Set sample status to FAIL
- Set sample status to REDO
- Add sample to repeat list
- Remove from repeat list
- Re-evaluate controls and samples on plate
- Override sample status and allow profile to be registered
- Reanalyze current sample with all single SNP variants allowed
- Copy relative abundances of products in sample (per primer pair) to clipboard

Comments for analysis report

Tasks-Analyze mtDNA

Search Database – mtDNA



Profile comparison: P00005556-2003X02368-0001A1D (1)

Compare to another stored profile | Compare to another profile on the plate | Search database

Search Show profiles up to 5 differences

Ignore C-length in poly-C regions Use uniform query range in Preferences

Database	Population	Inc
AFDIL	(Select all)	<input type="checkbox"/>
AFDIL_QC	(Select all)	<input type="checkbox"/>
CONTAMINANTS	(Select all)	<input type="checkbox"/>
Fake Database	(Select all)	<input type="checkbox"/>
FBI	(Select all)	<input type="checkbox"/>
GENOMES	(Select all)	<input type="checkbox"/>
IBIS	(Select all)	<input type="checkbox"/>
MEASURED	(Select all)	<input type="checkbox"/>
NIST	(Select all)	<input type="checkbox"/>

Max number of differences to show in interface

Target databases

C-length heteroplasmy treatment

Search Database – mtDNA

Profile comparison: P00005556-2003X02368-0001A1D (1)

Compare to another stored profile | Compare to another profile on the plate | Search database

Search Show profiles up to 5 differences

Ignore C-length in poly-C regions Use uniform query range in Preferences

1 *	Database	Population	Inc	DB	Population	ID
<input type="checkbox"/>	AFDIL	(Select all)	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Turkmenistan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Uzbekistan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Vietnam	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	African American	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Hispanics	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Greece	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Budapest Hungary	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Russia	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Kyrgyzstan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Kazakhstan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Cyprus	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Asian	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Hungarian Romanies	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Caucasians	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Hong Kong Chinese	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Afghanistan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Egypt	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Nairobi Kenya	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Jordan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Indonesia	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL	Tajikstan	<input checked="" type="checkbox"/>			
<input type="checkbox"/>	AFDIL_QC	(Select all)	<input type="checkbox"/>			
<input type="checkbox"/>	CONTAMINANTS	(Select all)	<input type="checkbox"/>			
<input type="checkbox"/>	Fake Database	(Select all)	<input type="checkbox"/>			
<input type="checkbox"/>	FBI	(Select all)	<input type="checkbox"/>			
<input type="checkbox"/>	GENOMES	(Select all)	<input type="checkbox"/>			
<input type="checkbox"/>	IBIS	(Select all)	<input type="checkbox"/>			

Target populations choice

Target database

Target populations

Search Database - mtDNA

Profile comparison: P00005556-2003X02368-0001A1D (1)

Compare to another stored profile | Compare to another profile on the plate | Search database

Search Show profiles up to 5 differences

Ignore C-length in poly-C regions Minimum number of regions in targets 21

1 *	Database	Population	Inc
-	AFDIL	(Select all)	<input checked="" type="checkbox"/>
-	AFDIL	Afghanistan	<input checked="" type="checkbox"/>
-	AFDIL	African American	<input checked="" type="checkbox"/>
-	AFDIL	Asian	<input checked="" type="checkbox"/>
-	AFDIL	Budapest Hungary	<input checked="" type="checkbox"/>
-	AFDIL	Caucasians	<input checked="" type="checkbox"/>
-	AFDIL	Cyprus	<input checked="" type="checkbox"/>
-	AFDIL	Egypt	<input checked="" type="checkbox"/>
-	AFDIL	Greece	<input checked="" type="checkbox"/>
-	AFDIL	Hispanics	<input checked="" type="checkbox"/>
-	AFDIL	Hong Kong Chinese	<input checked="" type="checkbox"/>
-	AFDIL	Hungarian Romanies	<input checked="" type="checkbox"/>
-	AFDIL	Indonesia	<input checked="" type="checkbox"/>
-	AFDIL	Jordan	<input checked="" type="checkbox"/>
-	AFDIL	Kazakhstan	<input checked="" type="checkbox"/>
-	AFDIL	Kyrgyzstan	<input checked="" type="checkbox"/>
-	AFDIL	Nairobi Kenya	<input checked="" type="checkbox"/>
-	AFDIL	Russia	<input checked="" type="checkbox"/>
-	AFDIL	Tajikstan	<input checked="" type="checkbox"/>
-	AFDIL	Turkmenistan	<input checked="" type="checkbox"/>
-	AFDIL	Uzbekistan	<input checked="" type="checkbox"/>
-	AFDIL	Vietnam	<input checked="" type="checkbox"/>
+	AFDIL_QC	(Select all)	<input type="checkbox"/>
+	FBI	(Select all)	<input type="checkbox"/>

Report -> Comment This is just a test search

Summarize counts up to 5 differences

Detail profiles up to

1	2	3	4	* DB	Min Diff	
-	-	-	-	AFDIL	-	
-	-	-	-	+	5.697/-2.44	
-	-	-	-	+	1	
-	-	-	-	+	2	
-	-	-	-	+	Afghanistan Afghan0042	2
-	-	-	-	+	Afghanistan Afghan0046	2
-	-	-	-	+	Afghanistan Afghan0050	2
-	-	-	-	+	Afghanistan Afghan0059	2
-	-	-	-	+	Afghanistan Afghan0060	2
-	-	-	-	+	Afghanistan Afghan0061	2
-	-	-	-	+	Afghanistan Afghan0063	2
-	-	-	-	+	Afghanistan Afghan0065	2
-	-	-	-	+	Afghanistan Afghan0067	2
-	-	-	-	+	Afghanistan Afghan0069	2
-	-	-	-	+	Afghanistan Afghan0070	2
-	-	-	-	+	Afghanistan Afghan0086	2
-	-	-	-	+	Afghanistan Afghan0089	2
-	-	-	-	+	Afghanistan Afghan0006	3
-	-	-	-	+	Afghanistan Afghan0008	3

Ave min differences over entire population

Min differences between query and target

Search output

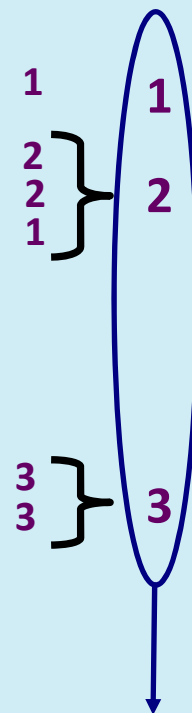
Comparing mtDNA Profiles

AF-2
 2901: 15893..16012: no data
 2925: 15937..16041: no data
 2899: 15985..16073: no data
 2898: 16048..16098: A15 G7 C17 T12
 2897: 16078..16129: A15 G8 C14 T15
 2896: 16124..16201: A27 G7 C27 T17
 2895: 16157..16201: A17 G1 C19 T8
 2893: 16182..16250: A24 G5 C28 T12
 2892: 16254..16305: A17 G4 C22 T8 N
 2891: 16283..16344: A23 G5 C18 T15 N
 2890: 16318..16402: no data
 2889: 16357..16451: no data
 2902: 5..97: no data
 2903: 20..139: no data
 2904: 103..162: A10 G10 C20 T20
 2905: 138..217: A23 G9 C21 T27
 2906: 178..267: A32 G15 C15 T28
 2908: 234..313: A30 G6 C30 T16
 2907: 263..340: A25 G6 C35 T14
 2923: 262..390: no data
 2910: 331..425: no data
 2916: 367..463: no data
 2912: 409..521: no data
 2913: 464..603: no data

USA.FBI.000070
 2901: 15893..16012: no data
 2925: 15937..16041: no data
 2899: 16015..16051: A7 G10 C5 T15
 2898: 16048..16098: A15 G7 C16 T13
 2897: 16078..16129: A15 G8 C14 T15
 2896: 16124..16201: A26 G7 C29 T16
 2895: 16157..16201: A16 G1 C21 T7
 2893: 16182..16250: A23 G5 C29 T12
 2892: 16254..16305: A18 G4 C22 T8
 2891: 16283..16344: A24 G5 C19 T14
 2890: 16342..16381: A8 G5 C17 T10
 2889: 16377..16428: A12 G9 C20 T11
 2902: 31..76: A5 G15 C12 T15
 2903: 41..114: A12 G24 C21 T18
 2904: 103..162: A9 G11 C18 T22
 2905: 138..217: A22 G10 C19 T29
 2906: 178..267: A32 G15 C15 T28
 2908: 234..313: A30 G6 C31 T16
 2907: 263..340: A25 G6 C36 T14
 2923: 289..367: A27 G6 C37 T12
 2910: 355..401: A21 G3 C14 T9
 2916: 389..437: A11 G7 C12 T19
 2912: 431..501: A20 G1 C34 T16
 2913: 493..576: A27 G6 C46 T5



Accounting
diff for overlaps



Total minimum differences

6

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Profile Registration – mtDNA

- Analysis of a full plate exposes profile registration interface
 - Samples that pass auto-processing are checked by default
 - Controls are not checked by default
 - Samples that failed will be disabled
 - If positive or negative control fails, registration for entire plate will be disabled; disabled state can be overridden

The screenshot displays the mtDNA profile registration interface. It features a 6x4 grid of sample wells, each containing a sample ID and scenario information. A 'Register' button is located at the top right of the grid. Below the grid is a list of controls with checkboxes. A status dialog box is open, displaying the registration results.

	1	2	3	4
A	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70
B	HUM2925 Scenario: 86 HUM2891 Scenario: 60	HUM2925 Scenario: 86 HUM2891 Scenario: 60	HUM2925 Scenario: 86 HUM2891 Scenario: 60	HUM2925 Scenario: 86 HUM2891 Scenario: 60
C	HUM2899 Scenario: 68 HUM2890 Scenario: 59	HUM2899 Scenario: 68 HUM2890 Scenario: 59	HUM2899 Scenario: 68 HUM2890 Scenario: 59	HUM2899 Scenario: 68 HUM2890 Scenario: 59
D	HUM2898 Scenario: 67 HUM2889 Scenario: 58	HUM2898 Scenario: 67 HUM2889 Scenario: 58	HUM2898 Scenario: 67 HUM2889 Scenario: 58	HUM2898 Scenario: 67 HUM2889 Scenario: 58
E	HUM2893 Scenario: 62 HUM2910 Scenario: 79	HUM2893 Scenario: 62 HUM2910 Scenario: 79	HUM2893 Scenario: 62 HUM2910 Scenario: 79	HUM2893 Scenario: 62 HUM2910 Scenario: 79
F	HUM2897 Scenario: 66 HUM2903 Scenario: 72	HUM2897 Scenario: 66 HUM2903 Scenario: 72	HUM2897 Scenario: 66 HUM2903 Scenario: 72	HUM2897 Scenario: 66 HUM2903 Scenario: 72

Register

- FBI-3
- FBI-9
- FBI-22
- FBI-28
- FBI-32
- FBI-33
- FBI-37
- FBI-47
- FBI-48
- FBI-49
- WATERCTRL
- WATERCTRL

Status [X]

532 products successfully registered.
0 failures.
0 products already registered.

OK

Report Generation – mtDNA

The screenshot displays the IbisTrack software interface for mtDNA analysis. The main window shows a grid of analysis results for plate P20000034, with columns for different scenarios (75, 70, 60, 59) and rows for different samples (A, B, C, D). A green box highlights the 'Generate report for P20000034' button, with an arrow pointing to it and the text 'Click to generate a report'. Below the grid, there are sections for 'Register' (listing AF-12 through AF-19) and 'Comments for analysis report' (providing details about a calculation mishap on 2/7/2006). A table shows 'Sample pg/rxn' values for AF-12 through AF-17. The bottom section shows 'Analysis Profiles' and 'Database' tabs, with a 'P20000034-AF-14 composite' profile selected. This section includes a chromatogram for 'Well 3 (A03)' and 'Well 15 (B03)', a table of peak data, and a 'Comments for analysis report' box containing the text: '85.6 pg per reaction used instead of 500 pg per reaction.' and a comparison to other profiles on plate P20000034.

Click to generate a report

Log general plate comments here

Log sample-specific comments here

Comments for analysis report

This plate was actually run on 2/7/2006. Tom somehow managed to mess up his calculation of DNA concentration after running the Quantifier assay. The target DNA concentration in all reactions was 500 pg. Because of the calculation mishap, the actual DNA concentrations used were:

Sample	pg/rxn
AF-12	85.6
AF-13	62.7
AF-14	46.4
AF-15	2.0
AF-16	120.5
AF-17	9.6

Comments for analysis report

85.6 pg per reaction used instead of 500 pg per reaction.

Comparison to other profiles on plate P20000034:

- 1: AF-12: 13 min differences.
- 2: AF-13: 11 min differences.
- 3: AF-14: 0 min differences.

mtDNA Plate Analysis Report – Page 1

- First page of report summarizes samples and controls on a plate
 - Quantity (or dilution) used
 - Status
 - Ave abundance (for controls)
 - Ave error (for positive)
 - Control status
 - Samples that have registered profiles
 - User comments

Mitochondrial DNA Plate Analysis Report

Plate: P00008859 (Mag = M00004214, PCR = C00014215) TTrack database: mtdna
Date: Sunday, May 27, 2007 9:19:56 PM mtDNA database: mtdna
User: thall
Experiment: NIST -SAMPLES

12 samples on plate P00008859:	Status
1. NIST-GT37869 (500.00 pg)	PASS
2. NIST-TT51399 (500.00 pg)	PASS
3. NIST-ZT80737 (500.00 pg)	PASS
4. NIST-ZT80870 (500.00 pg)	PASS
5. NIST-UT57317 (500.00 pg)	PASS
6. NIST-WT51359 (500.00 pg)	PASS
7. NIST-WA29584 (500.00 pg)	PASS
8. NIST-MT94875 (500.00 pg)	PASS
9. NIST-OT05896 (500.00 pg)	PASS
10. NIST-PT84222 (500.00 pg)	PASS
11. PDB (1.00 DF)	PASS
12. SC35495-10-POS (500.00 pg)	PASS

Positive control: 1
12: SC35495-10-POS (500.00 pg)
Average product abundance: 2698.771
Mean measurement error magnitude: 11.09 ppm
Status: PASS

Positive control status: PASS

Negative control: 1
11: PDB
Number of detected products: 0
Average product abundance: NaN
Ratio of average product abundance to corresponding positive control products: NaN
Status: PASS

Negative control status: PASS

10 samples, 1 positive, 1 negative.

Base counts are registered for NIST-GT37869, NIST-TT51399, NIST-ZT80737, NIST-ZT80870, NIST-UT57317, NIST-WT51359, NIST-WA29584, NIST-MT94875, NIST-OT05896, NIST-PT84222

User comments:
Plate #9 of NIST samples sent by John Butler.
Sample NIST-ZT80737 should be repeated to confirm the odd G-length heteroplasmy observed in overlapping primer pairs 2902 and 2903.

mtDNA Plate Analysis Report – Page 2

Second page of report summarizes analysis parameters used

Plate: P00008859 (Mag = M00004214, PCR = C00014215)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST-SAMPLES

TTrack database: mtdna
mtDNA database: mtdna

Analysis parameters for plate P00008859

Matching threshold: 70 ppm
Matching error delta threshold for double-stranded product: 80 ppm
Look for adenylations: OFF
Max ratio of strand abundance in double-stranded product: 2.5
Max negative to positive abundance ratio: 0.1
Min sample to positive abundance ratio: 0.25
Min fraction of ave peak abundance to report unmatched mass: 0.25
There is a filter in place to filter out minor SNP heteroplasmy assignments where the minor variant is less than 15% of the abundance of the major product.
There is a filter in place to filter out apparent +A artifacts where the minor variant is less than 30% of the abundance of the major product.

13C-enriched dGTP was used on plate P00008859:
Lot 4: 99.07% 13C enrichment

Criteria for passing the positive control:

All expected products for the positive control sample must be detected and the sample must match 100% to the expected positive control profile.

Criteria for passing the negative control:

If no positive control is present on the plate, the average abundance of any detected products in the negative control cannot exceed 10% of the average abundance of the corresponding products in all passed samples on the plate. If there is a positive control on the plate, the average abundance of any detected products in the negative control cannot exceed 10% of the average abundance of the corresponding products in the positive control.

Regardless of average abundance in the negative control, if identifiable products are observed in more than 1/2 of the primer pair regions, the negative control will be failed.

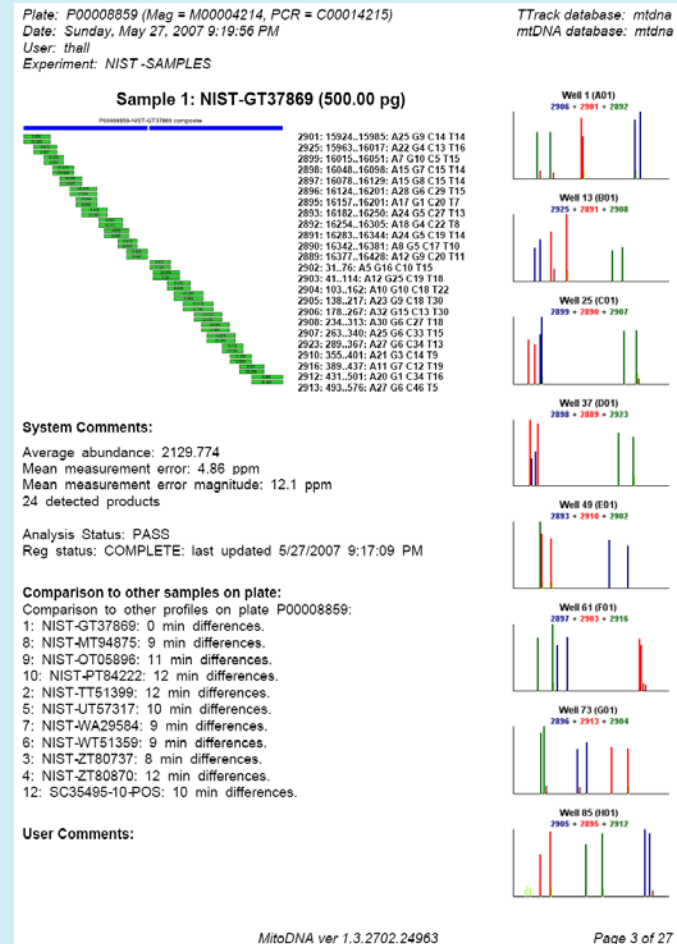
If either the negative or positive control fails, the plate must be rerun.

Criteria for passing a sample:

1. A double-stranded product must be detected for all primer pairs.
2. The average product abundance for the sample must equal or exceed 25% of the average for the positive control.

mtDNA Plate Analysis Report – Summary Page

- Each sample gets a summary page
 - Coverage map
 - Average abundance
 - Average error
 - Status
 - Comparison to other samples on the plate
 - Log of manual assignments and filtered assignments (if any)
 - User comments



mtDNA Plate Analysis Report – Assignment Report

- At the end of the report is a comprehensive raw mass-to-product assignment report in table format for the entire plate that serves as a raw data log
- Every report generated is automatically archived into the database

Plate: P00008859 (Mag = M00004214, PCR = C00014215)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST -SAMPLES

TTrack database: mtdna
mtDNA database: mtdna

Sample	Plate	Well	PP	CRS start	CRS end	Base string	Strand	Exp. mass	Obs. mass	Error (ppm)	Abundance	ratio	Arch. with
NIST-GT37889	P00000859	D01	2089	16327	16451	A21 G17 C26 T21	TOP	29026.419484	29030.402624	9.423	1645.525	0.0	
NIST-GT37889	P00000859	D01	2089	16327	16451	A21 G17 C26 T21	BOTTOM	29046.372861	29045.909050	15.367	1551.965	0.1	
NIST-GT37889	P00000859	C01	2080	16310	16402	A30 G14 C30 T21	TOP	25982.825414	25982.846691	-0.819	1946.62	1.0	
NIST-GT37889	P00000859	C01	2080	16310	16402	A21 G20 C14 T20	BOTTOM	26780.054038	26789.465042	-22.035	1763.427	1.1	
NIST-GT37889	P00000859	B01	2081	16296	16386	A37 G8 C24 T24	TOP	33175.586228	33175.742991	-4.832	2103.915	2.3	
NIST-GT37889	P00000859	B01	2081	16296	16386	A24 G41 C9 T37	BOTTOM	35125.012189	35124.862893	9.896	2633.053	2.0	
NIST-GT37889	P00000859	A01	2082	16231	16320	A40 G9 C29 T20	TOP	32089.899009	32079.880299	6.507	2032.839	3.2	
NIST-GT37889	P00000859	A01	2082	16231	16320	A20 C28 C9 T40	BOTTOM	34816.514842	34115.948437	18.172	2037.507	3.3	
NIST-GT37889	P00000859	E01	2093	16154	16200	A44 G7 C45 T19	TOP	34675.555204	34675.582199	-9.424	2343.952	4.2	
NIST-GT37889	P00000859	E01	2093	16154	16200	A19 G45 C7 T44	BOTTOM	36456.293531	36455.483468	22.302	2099.831	4.0	
NIST-GT37889	P00000859	H01	2095	16130	16224	A36 G7 C24 T18	TOP	28086.012028	28084.524924	16.694	1763.423	5.1	
NIST-GT37889	P00000859	H01	2095	16130	16224	A16 G42 C17 T36	BOTTOM	33008.388564	33009.303138	9.426	2731.649	5.0	
NIST-GT37889	P00000859	G01	2086	16102	16204	A46 G12 C43 T22	TOP	37511.721173	37512.474339	-20.078	2046.985	6.3	
NIST-GT37889	P00000859	G01	2086	16102	16204	A22 G43 C12 T46	BOTTOM	30001.638941	30000.909050	17.534	2370.70	8.0	
NIST-GT37889	P00000859	F01	2087	16056	16150	A21 G20 C13 T31	TOP	33624.070204	33623.206429	24.501	1646.214	7.2	
NIST-GT37889	P00000859	F01	2087	16056	16150	A27 G20 C13 T31	BOTTOM	31688.43279	31689.026993	10.67	1646.545	7.0	
NIST-GT37889	P00000859	D01	2088	16026	16110	A26 G17 C28 T26	TOP	28204.101132	28203.489503	22.073	690.890	8.1	
NIST-GT37889	P00000859	D01	2088	16026	16110	A26 G26 C17 T26	BOTTOM	29842.862817	29843.228427	-14.364	881.026	8.2	
NIST-GT37889	P00000859	C01	2089	15998	16073	A26 G15 C21 T27	TOP	27423.631953	27423.181146	16.420	2194.814	10.0	
NIST-GT37889	P00000859	C01	2089	15998	16073	A27 G21 C15 T26	BOTTOM	27672.791001	27672.889468	-3.862	2906.545	9.1	
NIST-GT37889	P00000859	A01	2081	15985	16012	A47 G18 C25 T30	TOP	31007.932675	31007.903059	1.069	2648.897	10.1	
NIST-GT37889	P00000859	A01	2081	15985	16012	A30 C25 C18 T47	BOTTOM	31263.764867	31263.180766	16.286	1849.174	10.0	
NIST-GT37889	P00000859	E01	2082	5	97	A19 G24 C24 T26	TOP	28885.725739	28885.464959	9.937	2428.451	11.0	
NIST-GT37889	P00000859	E01	2082	5	97	A26 G24 C24 T19	BOTTOM	28088.321145	28089.239973	3.121	3225.96	11.4	
NIST-GT37889	P00000859	F01	2083	20	139	A24 G24 C27 T33	TOP	31787.77867	31786.94949	20.994	1643.633	12.1	
NIST-GT37889	P00000859	F01	2083	20	139	A33 G29 C24 T24	BOTTOM	37198.616818	37199.340745	7.28	1804.11	12.4	
NIST-GT37889	P00000859	G01	2084	83	187	A23 G21 C29 T32	TOP	32313.353226	32313.303822	-0.232	2763.537	13.0	
NIST-GT37889	P00000859	G01	2084	83	187	A22 G29 C21 T23	BOTTOM	32760.331443	32763.476069	-4.426	3068.391	13.2	
NIST-GT37889	P00000859	H01	2085	113	248	A38 G18 C28 T48	TOP	40966.192738	40965.884906	-13.201	2893.871	14.2	
NIST-GT37889	P00000859	H01	2085	113	248	A40 G28 C15 T39	BOTTOM	41404.843150	41404.823955	-1.940	2875.047	14.2	
NIST-GT37889	P00000859	A01	2086	154	290	A43 G18 C20 T41	TOP	42232.524961	42233.287136	-17.174	2950.491	15.3	
NIST-GT37889	P00000859	A01	2086	154	290	A41 G20 C15 T40	BOTTOM	42668.366568	42669.913094	-6.744	2804.56	15.1	
NIST-GT37889	P00000859	C01	2087	239	363	A43 G11 C48 T24	TOP	38077.928333	38078.173332	-16.051	2330.849	16.1	
NIST-GT37889	P00000859	C01	2087	239	363	A24 G48 C14 T43	BOTTOM	39091.822206	39092.320996	-7.461	2330.214	16.0	
NIST-GT37889	P00000859	D01	2088	204	333	A22 G16 C28 T34	TOP	39271.87867	39271.87867	-19.127	1321.689	17.3	
NIST-GT37889	P00000859	D01	2088	204	333	A34 G36 C16 T42	BOTTOM	40126.806199	40126.981703	-1.133	1531.191	17.2	
NIST-GT37889	P00000859	B01	2010	331	429	A33 G9 C27 T26	TOP	29632.419383	29632.873643	-4.732	2864.078	18.1	
NIST-GT37889	P00000859	E01	2010	331	425	A28 G27 C9 T32	BOTTOM	29637.281148	29638.647267	-10.180	2424.782	18.0	
NIST-GT37889	P00000859	H01	2012	409	521	A32 G7 C48 T36	TOP	34874.631226	34874.880296	-2.911	2223.439	19.1	
NIST-GT37889	P00000859	H01	2012	409	521	A26 G48 C7 T32	BOTTOM	36015.536042	36014.233930	33.254	2669.327	19.0	
NIST-GT37889	P00000859	G01	2013	464	603	A44 G20 C33 T23	TOP	42324.573746	42324.202626	8.961	2164.881	20.2	
NIST-GT37889	P00000859	G01	2013	464	603	A22 G63 C14 T44	BOTTOM	44708.884416	44707.665697	31.987	2682.237	20.0	
NIST-GT37889	P00000859	F01	2018	367	463	A27 G8 C32 T30	TOP	29478.82045	29478.880432	-1.398	1896.365	21.0	
NIST-GT37889	P00000859	F01	2018	367	463	A36 C32 C8 T27	BOTTOM	30611.936489	30611.549736	12.634	2391.621	21.1	
NIST-GT37889	P00000859	D01	2023	262	380	A47 G10 C21 T21	TOP	33465.133843	33465.87376	-5.379	1335.642	22.1	
NIST-GT37889	P00000859	D01	2023	262	380	A21 G22 C10 T47	BOTTOM	41236.121999	41234.854051	25.308	1241.175	22.0	
NIST-GT37889	P00000859	B01	2026	19837	19848	A39 G14 C24 T32	TOP	32282.150028	32282.789819	-18.712	1472.833	23.1	
NIST-GT37889	P00000859	B01	2026	19837	19848	A32 G24 C14 T36	BOTTOM	32743.845361	32743.781624	2.957	1862.189	23.0	
NIST-TT51339	P00000859	D02	2089	16327	16451	A21 G17 C26 T21	TOP	29038.478484	29040.880296	9.423	2103.481	0.0	
NIST-TT51339	P00000859	D02	2089	16327	16451	A21 G17 C26 T21	BOTTOM	29046.372861	29045.909050	15.367	1827.045	0.1	
NIST-TT51339	P00000859	C02	2090	16318	16400	A20 G14 C31 T20	TOP	29687.814604	29687.227568	3.208	1763.537	1.0	
NIST-TT51339	P00000859	C02	2090	16318	16400	A20 G14 C31 T20	BOTTOM	29785.888465	29785.414618	17.451	1822.825	1.1	
NIST-TT51339	P00000859	C02	2091	16296	16386	A37 G9 C42 T23	TOP	33790.574818	33790.2872	8.532	2185.884	2.2	
NIST-TT51339	P00000859	C02	2091	16296	16386	A23 C42 C9 T37	BOTTOM	35150.842897	35150.533172	8.803	2943.299	2.0	
NIST-TT51339	P00000859	A02	2082	16231	16320	A41 G9 C40 T19	TOP	33229.055202	33233.945628	-9.844	2171.559	3.0	
NIST-TT51339	P00000859	A02	2082	16231	16320	A19 G42 C9 T44	BOTTOM	34157.355537	34157.056422	-7.793	2871.139	3.1	
NIST-TT51339	P00000859	E02	2083	16154	16200	A44 G7 C46 T18	TOP	34886.542114	34887.171026	-35.262	521.631	4.7	
NIST-TT51339	P00000859	E02	2083	16154	16200	A44 G7 C47 T18	TOP	35140.72508	35149.261212	-8.715	352.971	4.8	
NIST-TT51339	P00000859	E02	2083	16154	16200	A44 G7 C48 T18	TOP	36148.868848	36143.152382	21.881	448.164	4.9	
NIST-TT51339	P00000859	E02	2083	16154	16200	A18 G46 C7 T44	BOTTOM	36482.125839	36480.878957	39.699	388.527	4.0	
NIST-TT51339	P00000859	E02	2083	16154	16200	A18 G47 C7 T44	BOTTOM	36821.185656	36819.882091	49.272	301.491	4.1	
NIST-TT51339	P00000859	E02	2083	16154	16200	A18 G48 C7 T44	BOTTOM	37185.206074	37159.30909	22.703	427.664	4.2	
NIST-TT51339	P00000859	H02	2086	16130	16224	A36 G7 C24 T18	TOP	28088.012028	28088.200321	-44.418	605.243	5.6	
NIST-TT51339	P00000859	H02	2086	16130	16224	A36 G7 C25 T18	TOP	29154.201254	29153.563438	21.877	404.741	5.6	
NIST-TT51339	P00000859	H02	2086	16130	16224	A36 G7 C26 T18	TOP	29443.384422	29444.162258	-26.39	320.434	5.7	

SNP Sample Analysis

- **Data processing is automated and utilizes the same code as mtDNA data processing**
- **SNP analysis interface is similar to mtDNA interface**
- **Allele names displayed (as SNP identities) instead of base compositions**

SNP Sample Analysis

Highlighted allele assignment details

Well	Allele 1	Allele 2
1	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
2	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
3	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
4	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
5	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
6	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
7	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
8	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
9	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883
10	HUM4541 RS1058083 HUM4678 RS13182883	HUM4541 RS1058083 HUM4678 RS13182883

Homozygous (Well 1, 2, 3, 4, 5, 6, 7, 8, 9, 10)

Heterozygous (Well 13, 25, 37)

Allele assignment

Spectral thumbnails

Sample profile

Well 13 (B01) Profile:
 Well: 13 (B01), PP 4538 (HUMSNP_F
 Locus RS10488710
 Allele C
 Base count A10 G9 C10 T22
 Top strand
 Abundance: 3687.6495
 Predicted mass: 15656.6119
 Observed mass: 15656.6597
 Match error: -3.053 ppm

Locus	Allele	Allele
RS10092491	T	C
RS1019029	T	
RS10488710	C	
RS1058083	G	A
RS1109037	A	
RS12997453	G	
RS13134862	G	A
RS13182883	A	
RS13218440	G	A
RS1336071	G	A
RS1358856	C	
RS1410059	C	

SNP Sample Analysis – Plate Profile Summary

The screenshot shows the IbisTrack software interface. The main window displays a 'Plate Profile Summary' for plate P05015930. The data is organized into a grid with columns for wells (1-10) and rows for samples (A, B). Below the grid, there are tabs for 'Analysis', 'Plate summary', 'Profiles', 'Mass Data', and 'Preferences'. The 'Analysis' tab is active, showing 'Allele calls' and 'Assignment summary'. A 'Register' button is highlighted with a green circle and a callout box. Below the 'Register' button is a table of allele calls for various SNPs across different samples. A second callout box points to the table.

Profiles can be registered to the database here

Sample	RS1358856	RS1410059	RS1478829	RS1523537	RS1554472	RS1821380	RS2073383	RS214955	RS2272998	RS2503107
✓ N31774Q2	C, ---	C, ---	A, T	C, T	C, ---	C, G	C, T	A, ---	C, G	A, C
✓ N31774Q2	C, ---	C, ---	A, T	C, T	C, ---	C, G	C, T	A, ---	C, G	A, C
✓ SC35495-10	A, C	C, ---	A, T	C, T	C, T	C, G	C, ---	A, G	C, G	A, C
✓ SC35495-10	C	C, ---	A, T	C, T	C, T	C, G	C, ---	A, G	C, G	A, C
WATER_CONTROL	no data	no data	no data	no data	no data	no data	no data	no data	no data	no data
WATER_CONTROL	no data	no data	no data	no data	no data	no data	no data	no data	no data	no data

Profiles can be copied to the clipboard here

SNP Sample Analysis – Profile Query

Tasks

- Register Assays
 - Register Casework Plates
 - Register New Plate for Database Population
 - Process Repeats for Database
 - Register Quality Control Plates
 - Generate Plate Setup Reports
- Manage Inventory
- View Plates
- mtDNA Analysis
 - Analyze mtDNA
 - Import Mass Data
 - Add Database Items
 - Remove Database Items
 - Move Samples to Populations
 - Rebuild Unique Products
 - Build Amplified BC Database
 - Upload data to main server
 - Archive case/plate data
- STR Analysis
 - Analyze STRs
 - Analyze Y-STRs
- SNP Analysis
 - Analyze Autosomal SNPs

Analysis | Plate summary | Profiles | Mass Data | Preferences

Plate: P05015930 | From: 04-Oct-2007 | To: 18-Oct-2009 | Analyze

Sample: 1

Profile Query | Repeats | Status | Export XML

Database: IBIS | Population: UNKNOWN | Id: 55-24133 | Reaction set: Autosomal SNP reaction set 1

Sample	RS10092491	RS1019029	RS10488710	RS1058083	RS1109037	RS12997453	RS134862	RS13182883	RS13218440	RS1336071	RS1358856	RS1410055
55-24133	C	C	C	G	A	A	G	G	A	G	A	T
55-24137	C	C	C	A	A	A	A	A	A	A	A	T
55-24613	C	C	C	A	A	A	A	A	A	A	A	C
CS0001	C	C	C	A	A	A	A	A	A	A	A	C
CS0003	C	C	C	A	A	A	A	A	A	A	A	C
CS0008	C	C	C	A	A	A	A	A	A	A	A	T
CS0012	C	C	C	A	A	A	A	A	A	A	A	C
CS0031	C	C	C	A	A	A	A	A	A	A	A	C
CS0031	C	C	C	A	A	A	A	A	A	A	A	T

2.7.0530 | MTDNA | MTL0CAL2 | MTDNA

Summary

- **Data processing after MS is automated**
- **Processed data persist in database with registered sample and plate information**
- **Sample analysis is automated (triggered manually)**
- **Interface provides dynamic graphical functions to evaluate, QC, and adjust (if necessary) profile assignments**
- **Profiles can be registered a plate at a time**
- **Query profiles from database**
- **Automated comparison of profiles to database entries (mtDNA)**
- **Search database (mtDNA)**
- **Add sequences and convert to base compositions in the database (mtDNA)**

Questions?

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Note: All images and charts courtesy of Tom Hall, Ph.D.