National Institute of Justice *Technology Transition Workshop*

Analysis Software for the mtDNA Tiling Assay

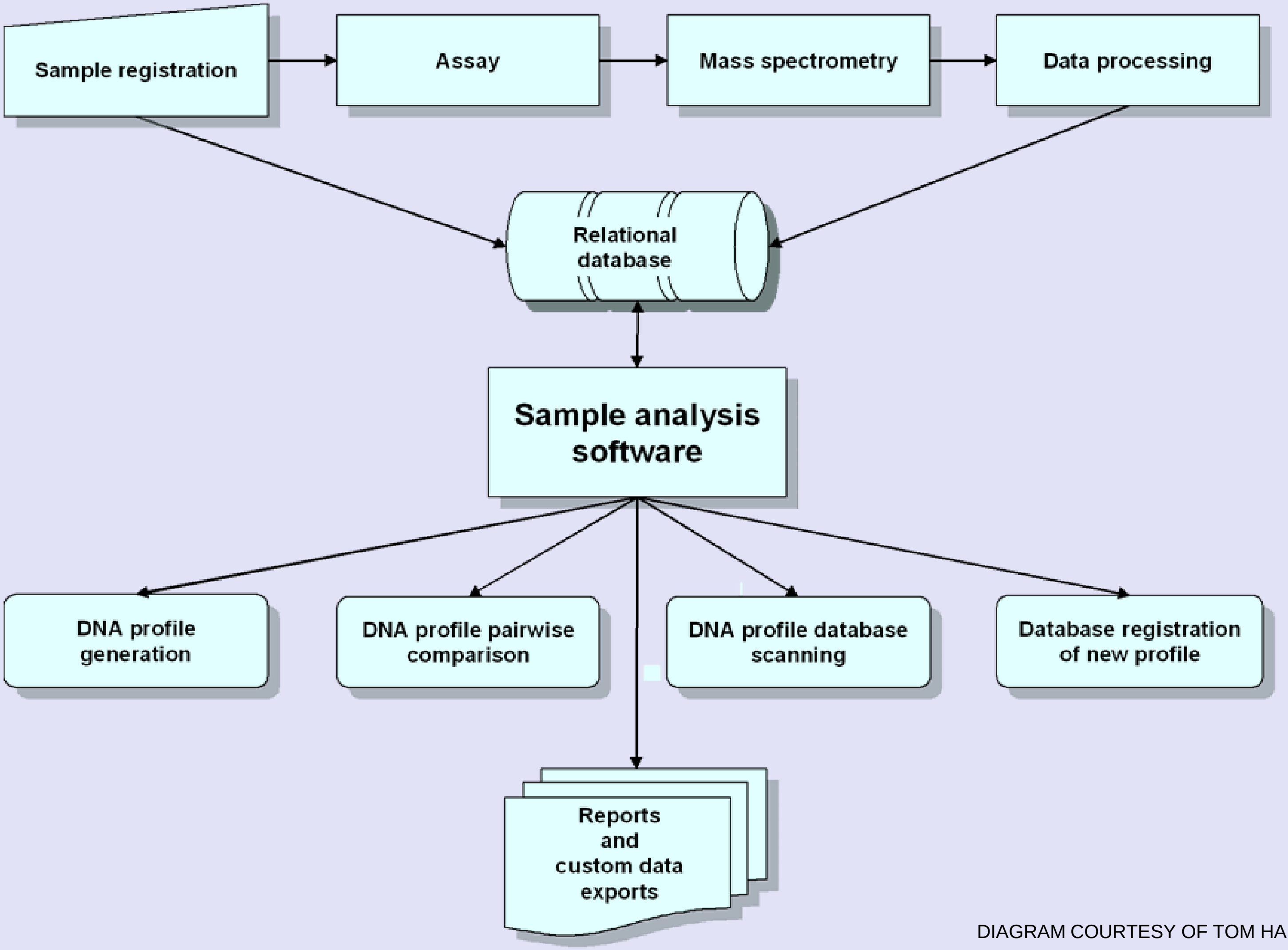
Tom Hall, Ph.D.

Ibis Biosciences, Inc.

Outline

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

mtDNA Analysis Software



Sample registration

Assay

Mass spectrometry

Data processing

Relational database

Sample analysis software

DNA profile generation

DNA profile pairwise comparison

DNA profile database scanning

Database registration of new profile

Reports and custom data exports

DIAGRAM COURTESY OF TOM HALL, PH.D.

Software Features

- ❑ **Leverages existing 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 mtDNA assay data and registration of profiles**
  - ➢ **Adding / removing databases, populations, sequence profiles, and base composition profiles**
  - ➢ **Automated conversion of sequence to base count profiles**
  - ➢ **Population-based searching and reporting**
  - ➢ **Plate-based analysis reporting**

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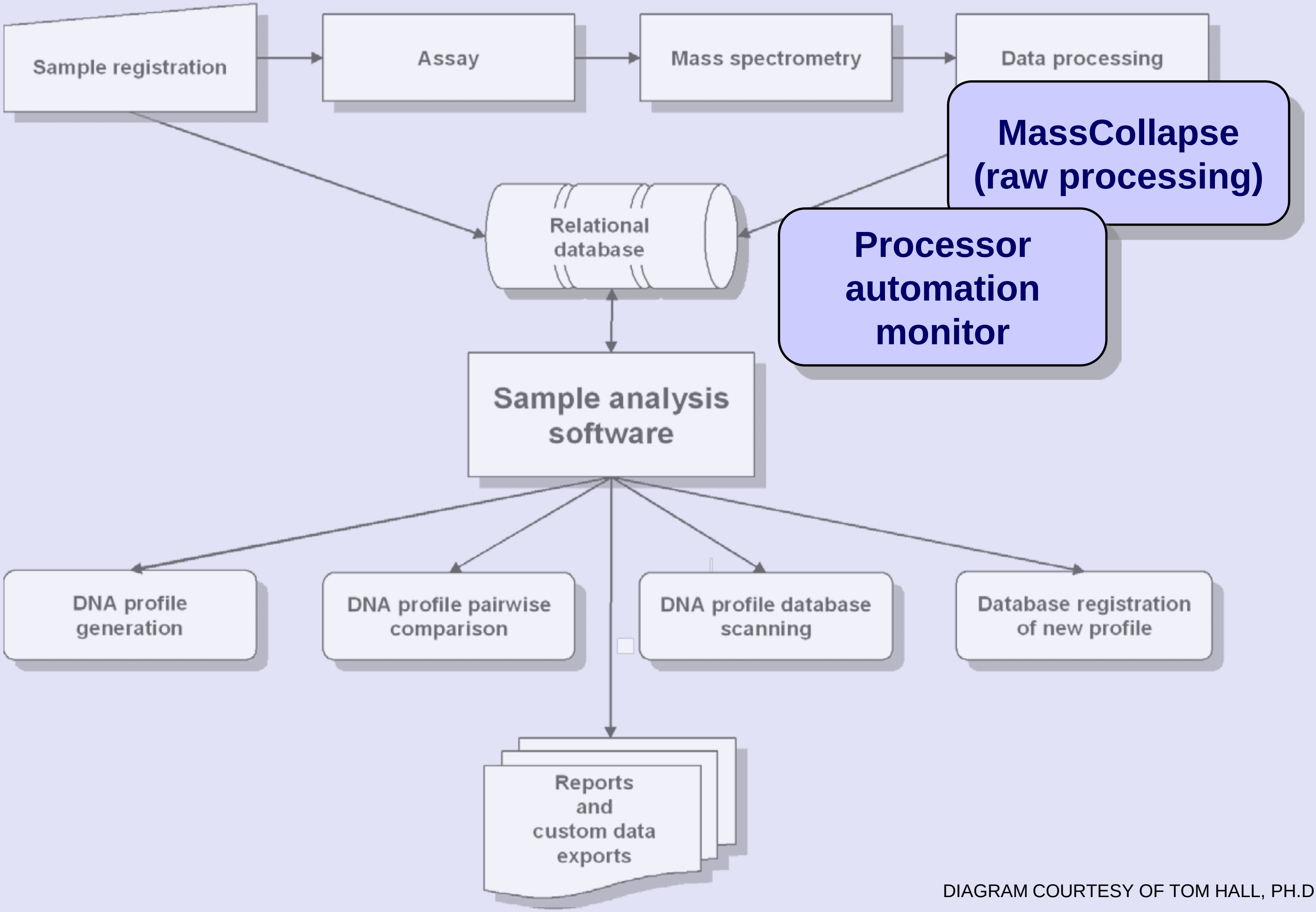
Data Processing



MassCollapse (raw processing)

Processor automation monitor

DIAGRAM COURTESY OF TOM HALL, PH.D.

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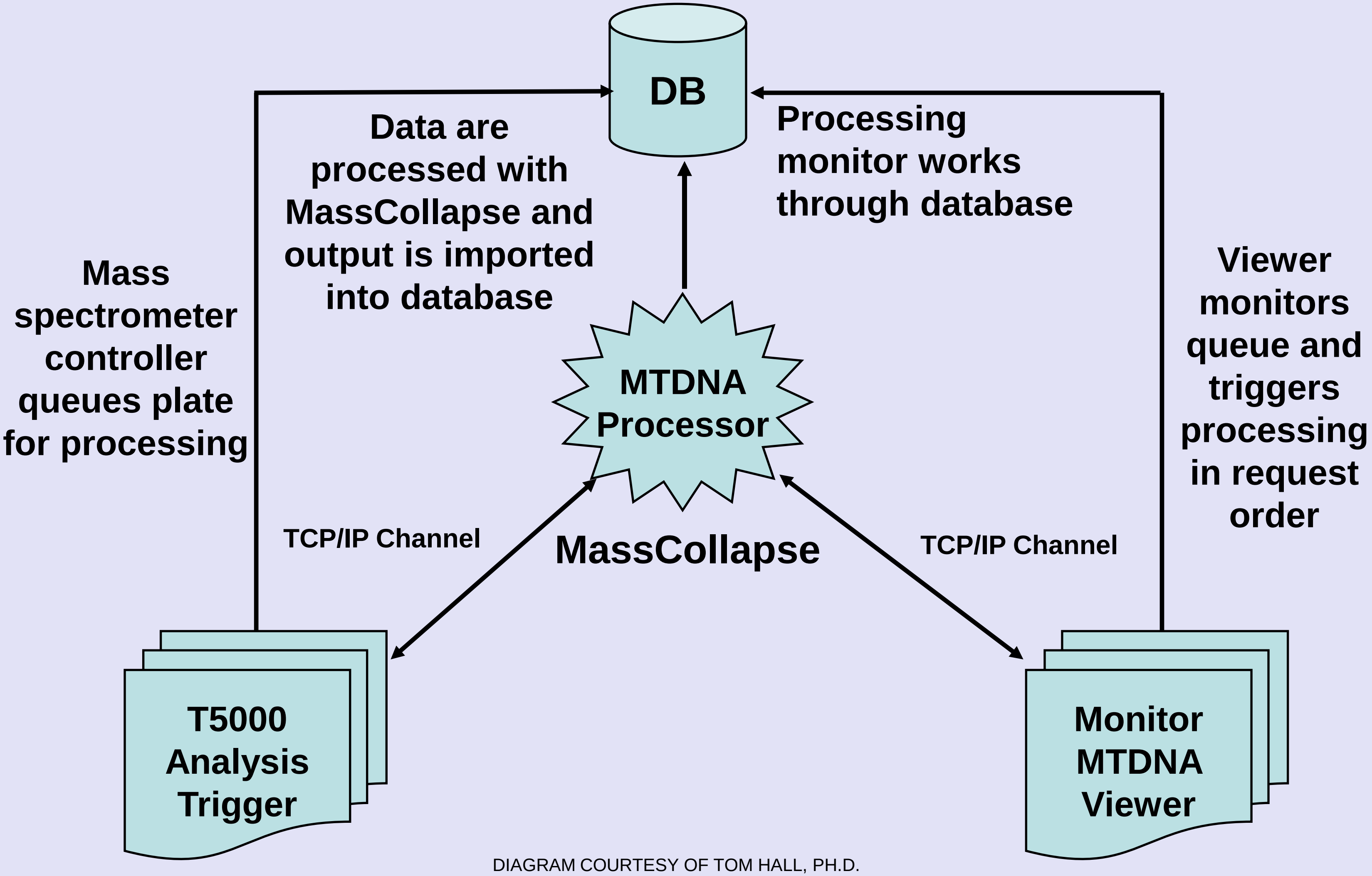
mtDNA Processing Monitor



DB

Data are processed with MassCollapse and output is imported into database

Processing monitor works through database

Mass spectrometer controller queues plate for processing

Viewer monitors queue and triggers processing in request order

MTDNA Processor

MassCollapse

TCP/IP Channel

TCP/IP Channel

T5000 Analysis Trigger

Monitor MTDNA Viewer

DIAGRAM COURTESY OF TOM HALL, PH.D.

MassCollapse Deconvolution

Raw spectrum

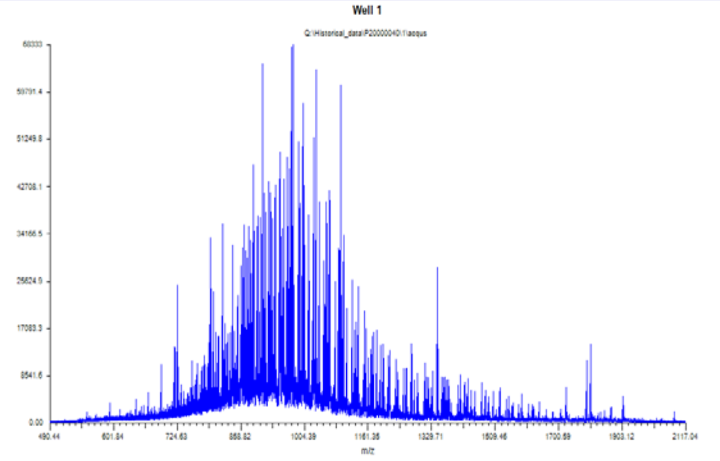


IMAGE COURTESY OF TOM HALL, PH.D.

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MassCollapse Deconvolution

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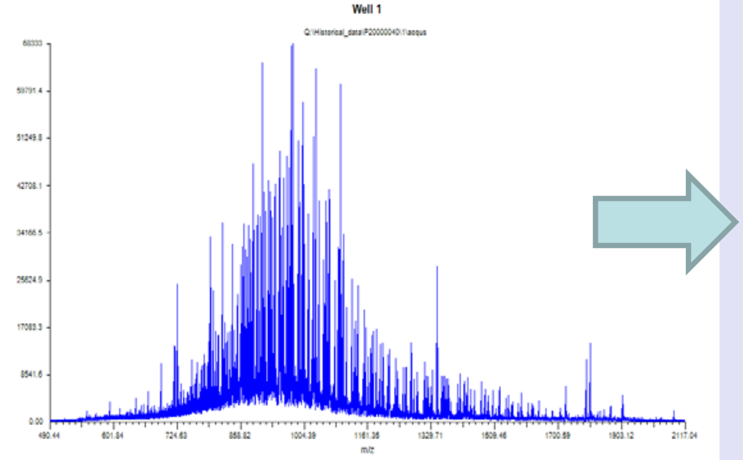
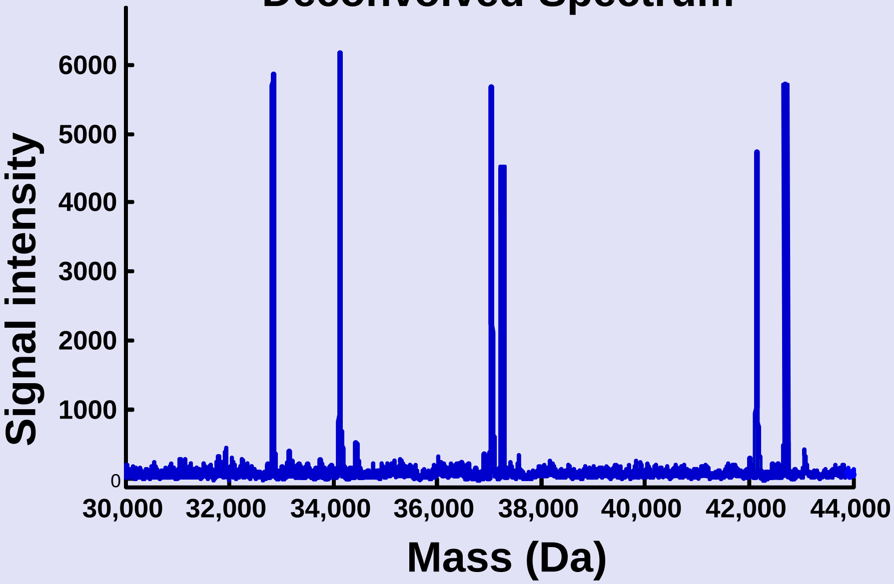


Deconvolved Spectrum



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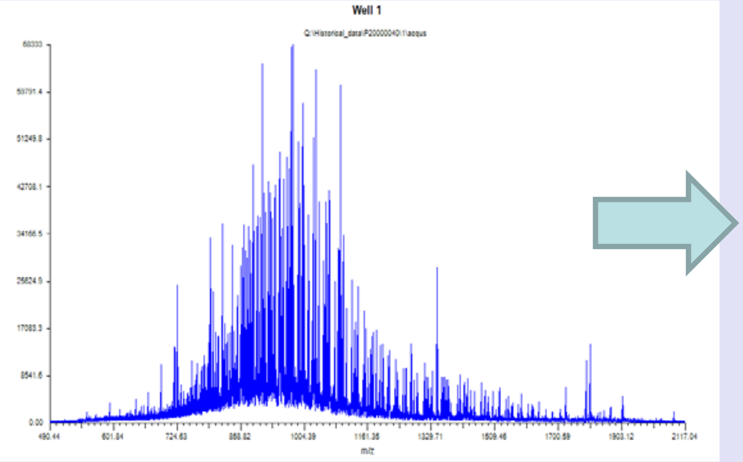
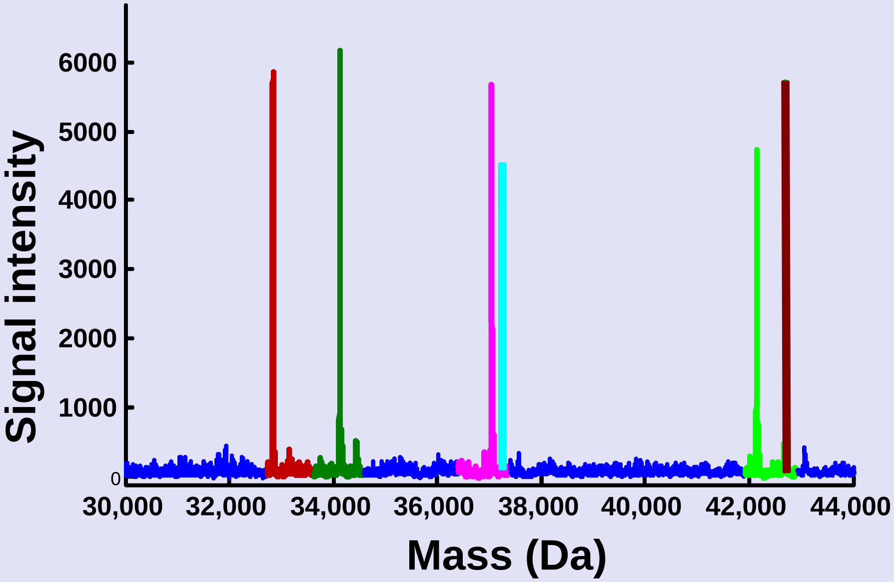
MassCollapse Deconvolution

Raw spectrum





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MassCollapse Deconvolution

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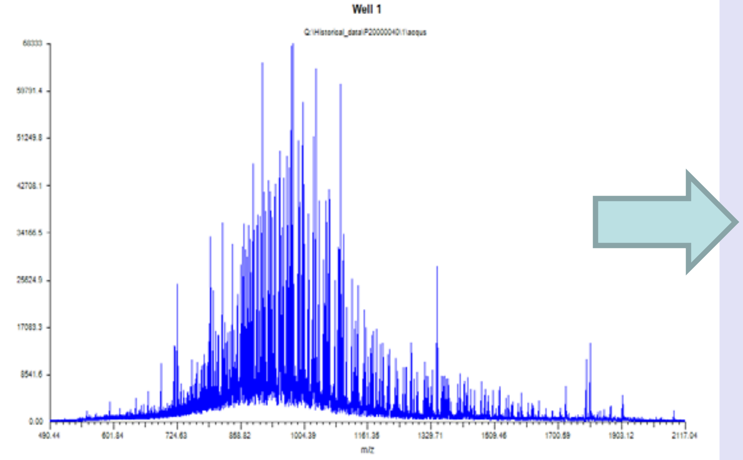

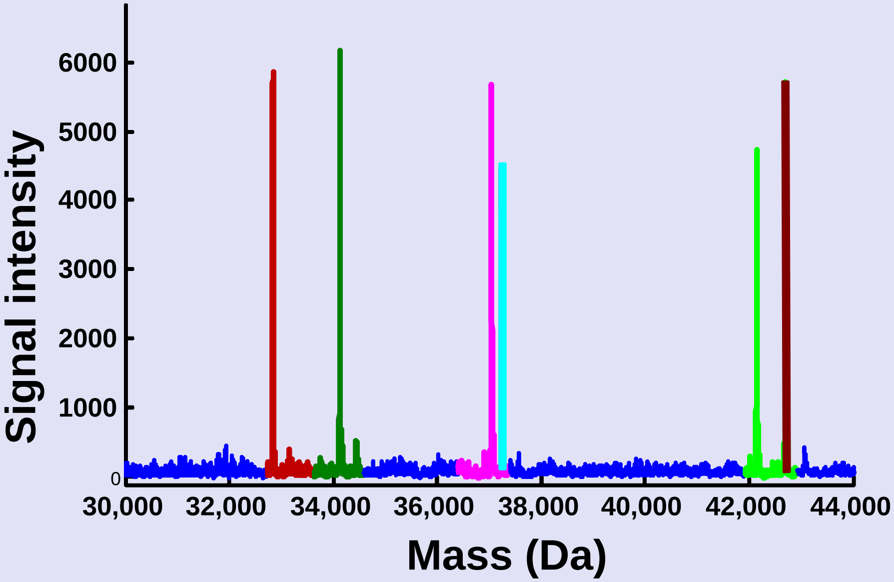

List of masses and intensities

32855.1 Da
34143.8 Da
37058.2 Da
37254.2 Da
42162.1 Da
42710.3 Da

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

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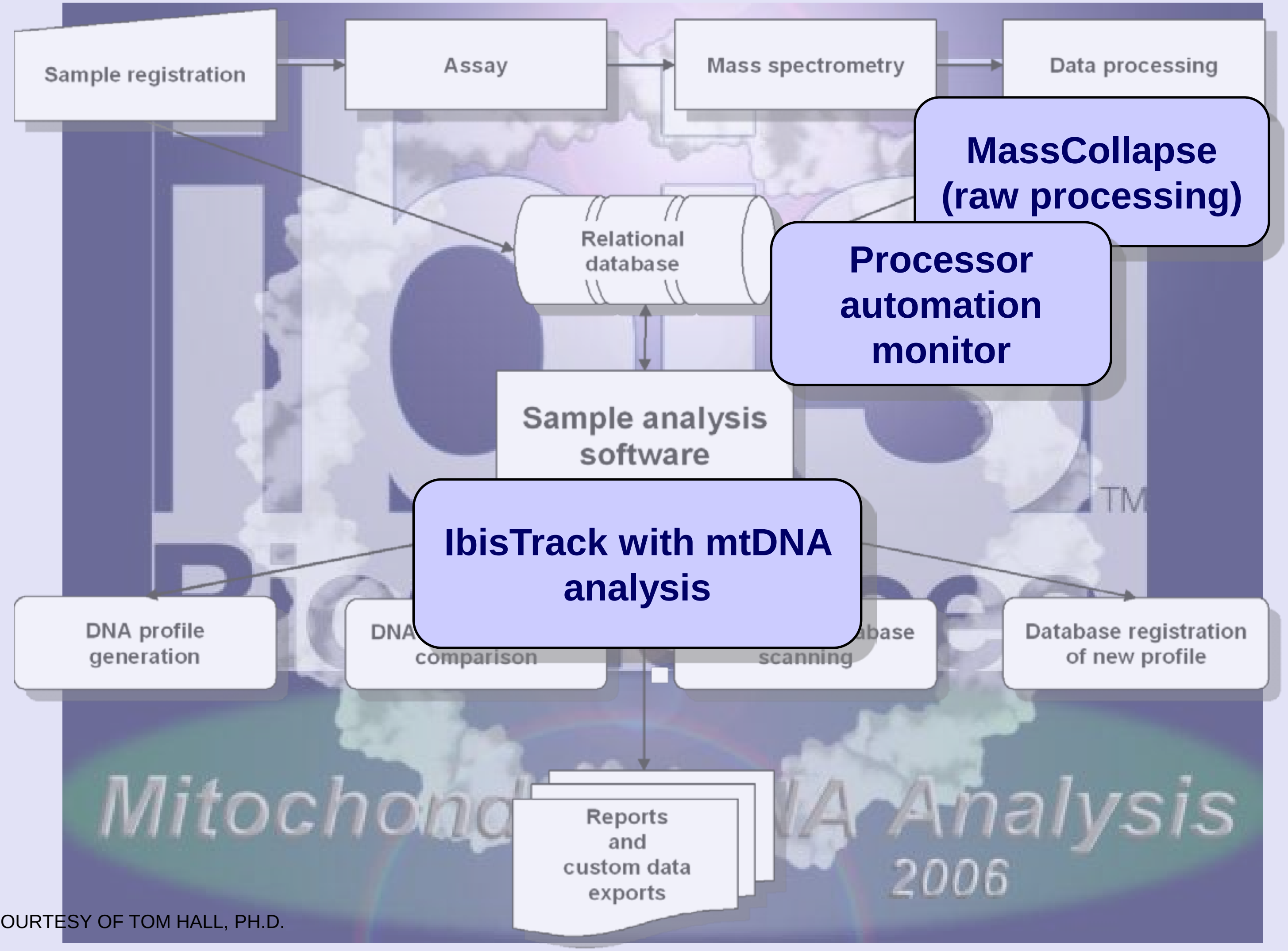
mtDNA Analysis Software



MassCollapse (raw processing)

Processor automation monitor

IbisTrack with mtDNA analysis

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Application Interface

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

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Analysis

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

IMAGE COURTESY OF TOM HALL, PH.D.

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Main IbisTrack program menu

IMAGE COURTESY OF TOM HALL, PH.D.

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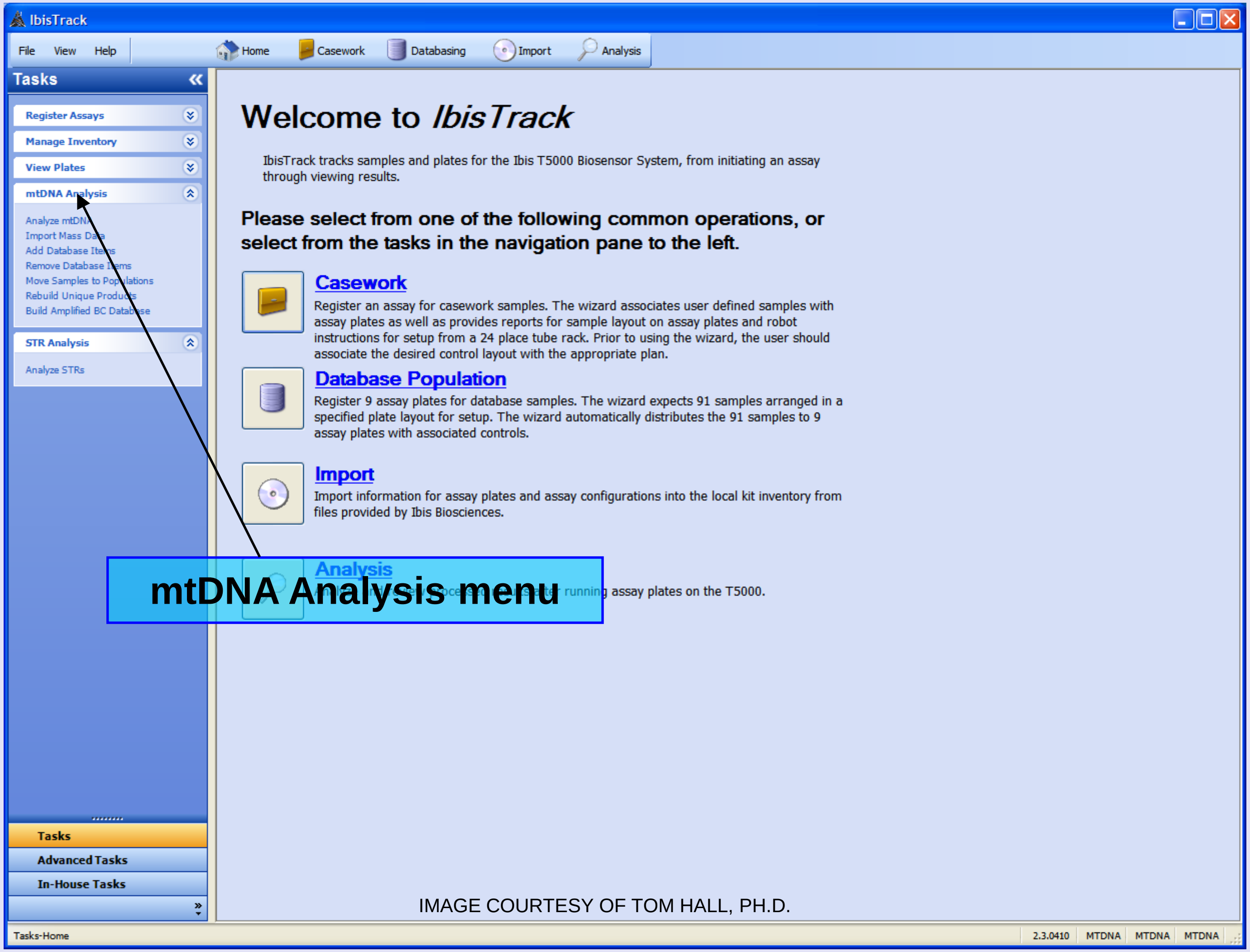

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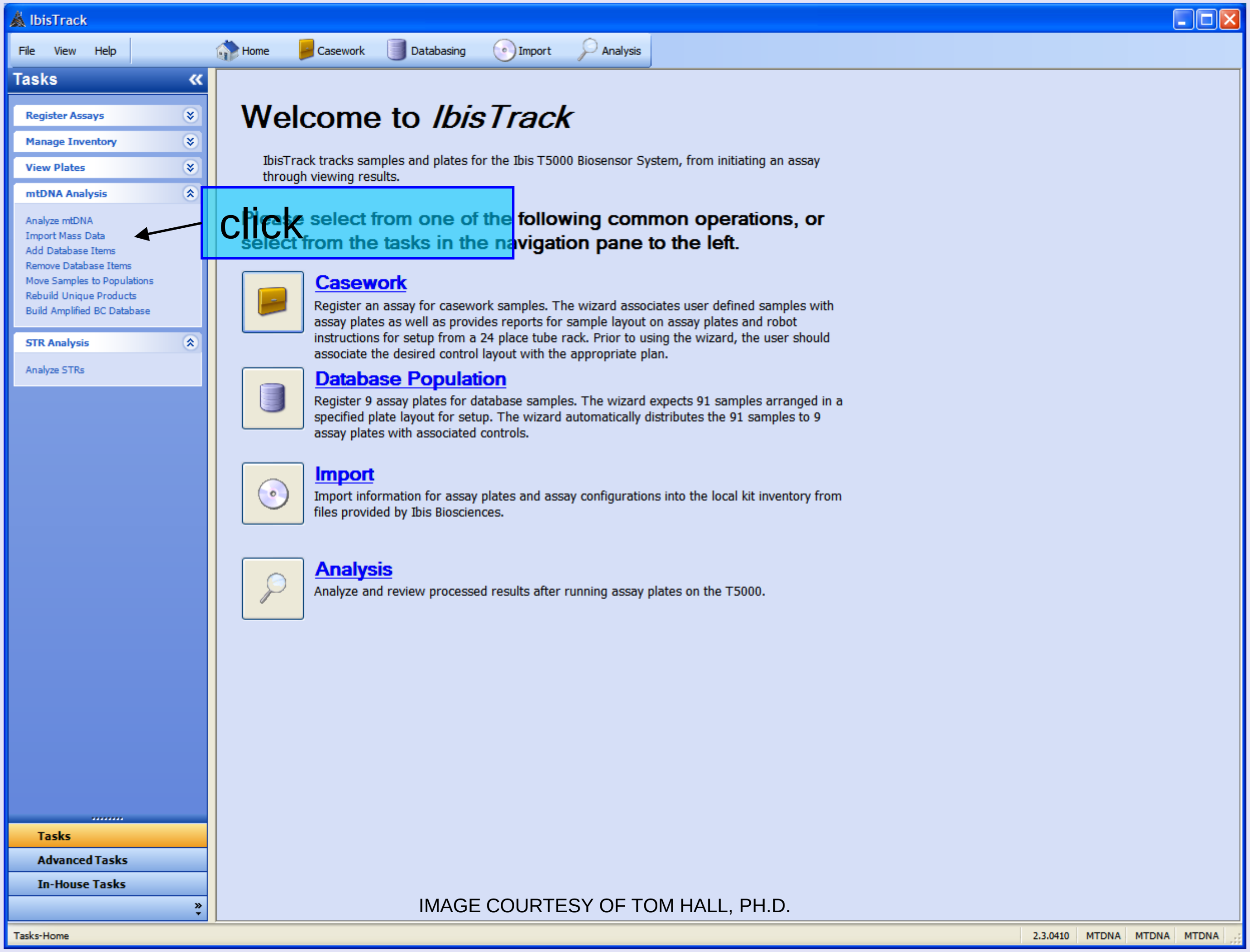
mtDNA Analysis menu

IMAGE COURTESY OF TOM HALL, PH.D.

Basic Application Interface



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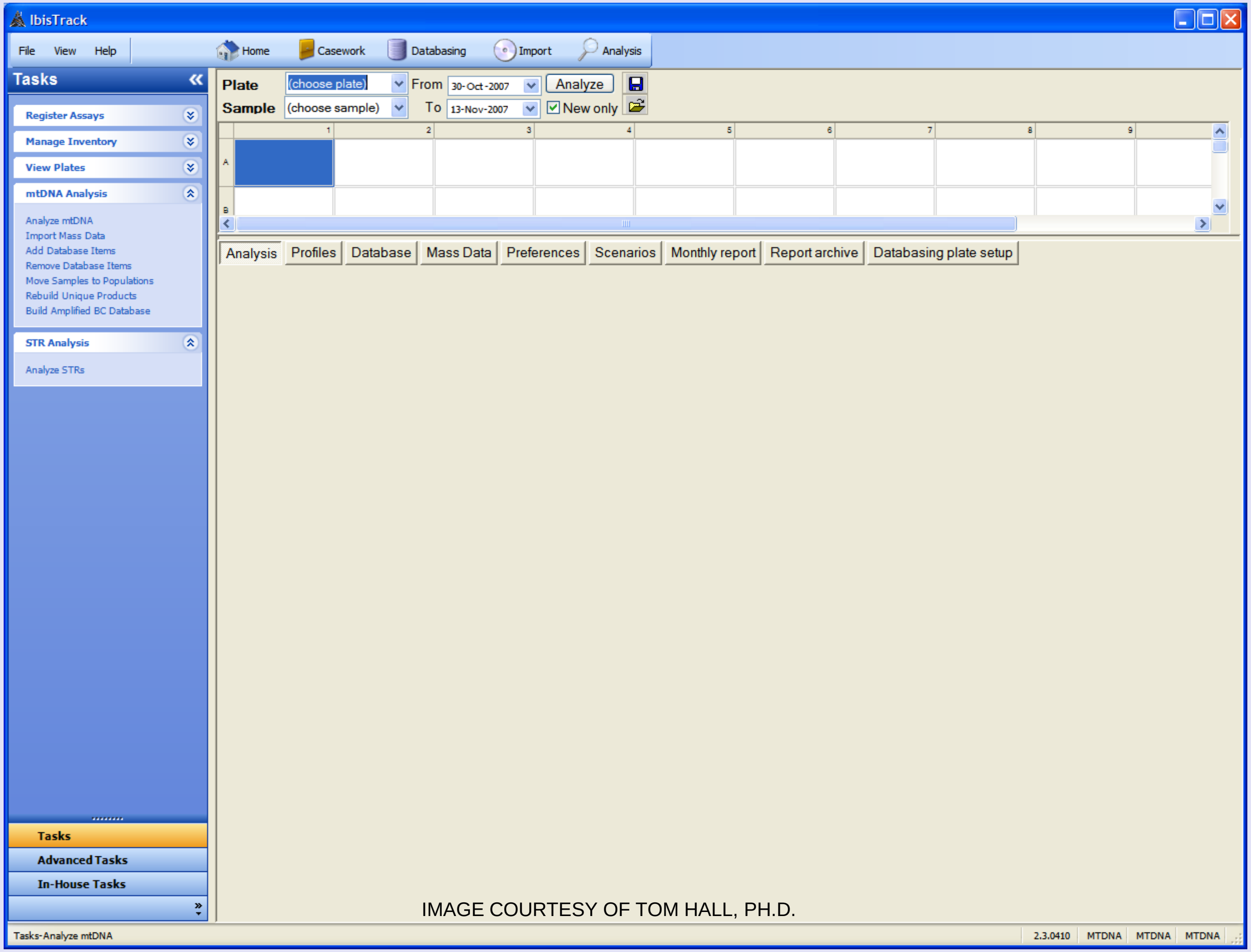

Plate (choose plate)
Sample (choose sample)
From 30-Oct-2007
To 13-Nov-2007
☑ New only

Tasks-Analyze mtDNA

2.3.0410 MTDNA MTDNA MTDNA

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Application Interface

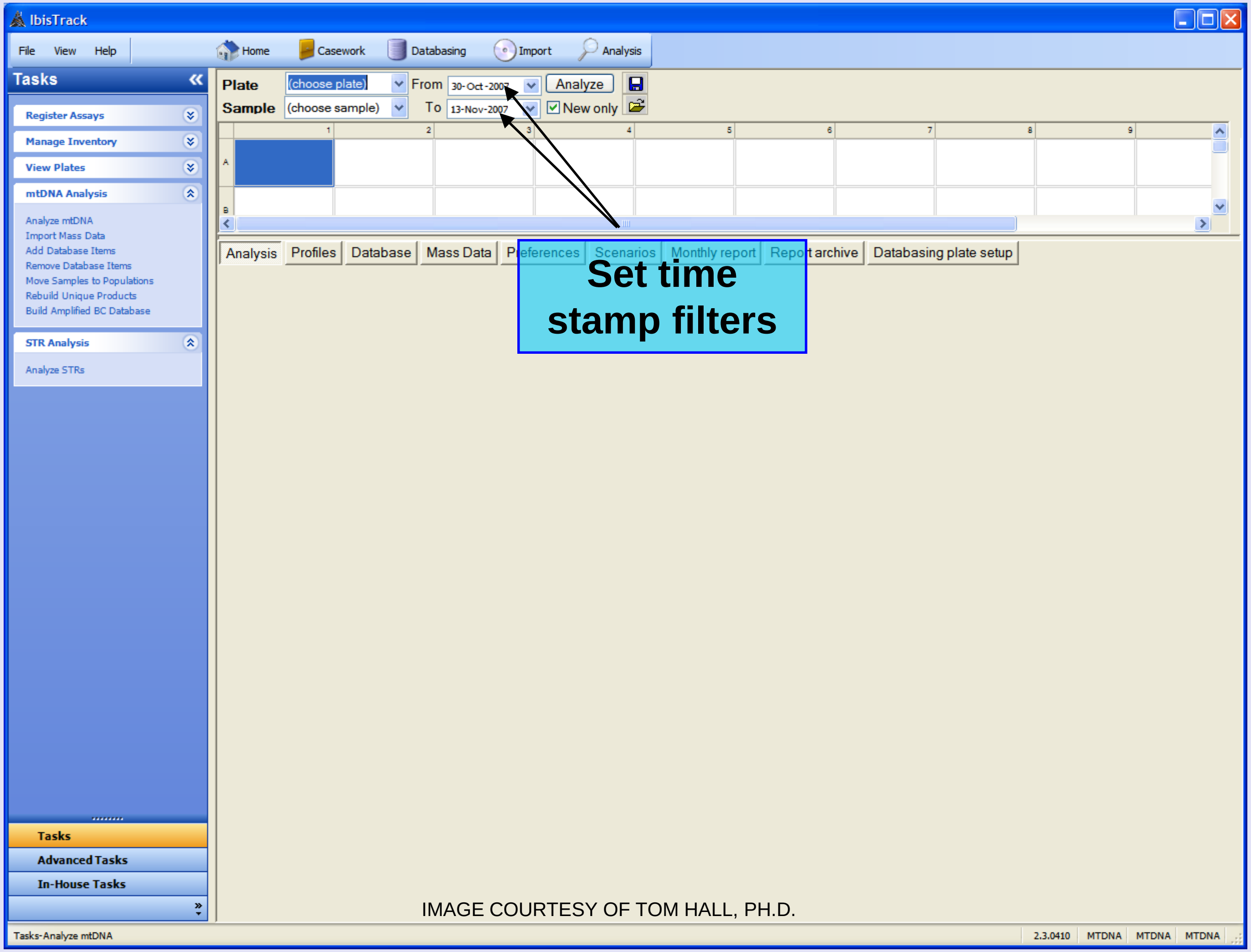

Plate (choose plate)
Sample (choose sample)
From 30-Oct-2007
To 13-Nov-2007
☑ New only

Tasks-Analyze mtDNA
2.3.0410 MTDNA MTDNA MTDNA

Set time stamp filters

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Application Interface

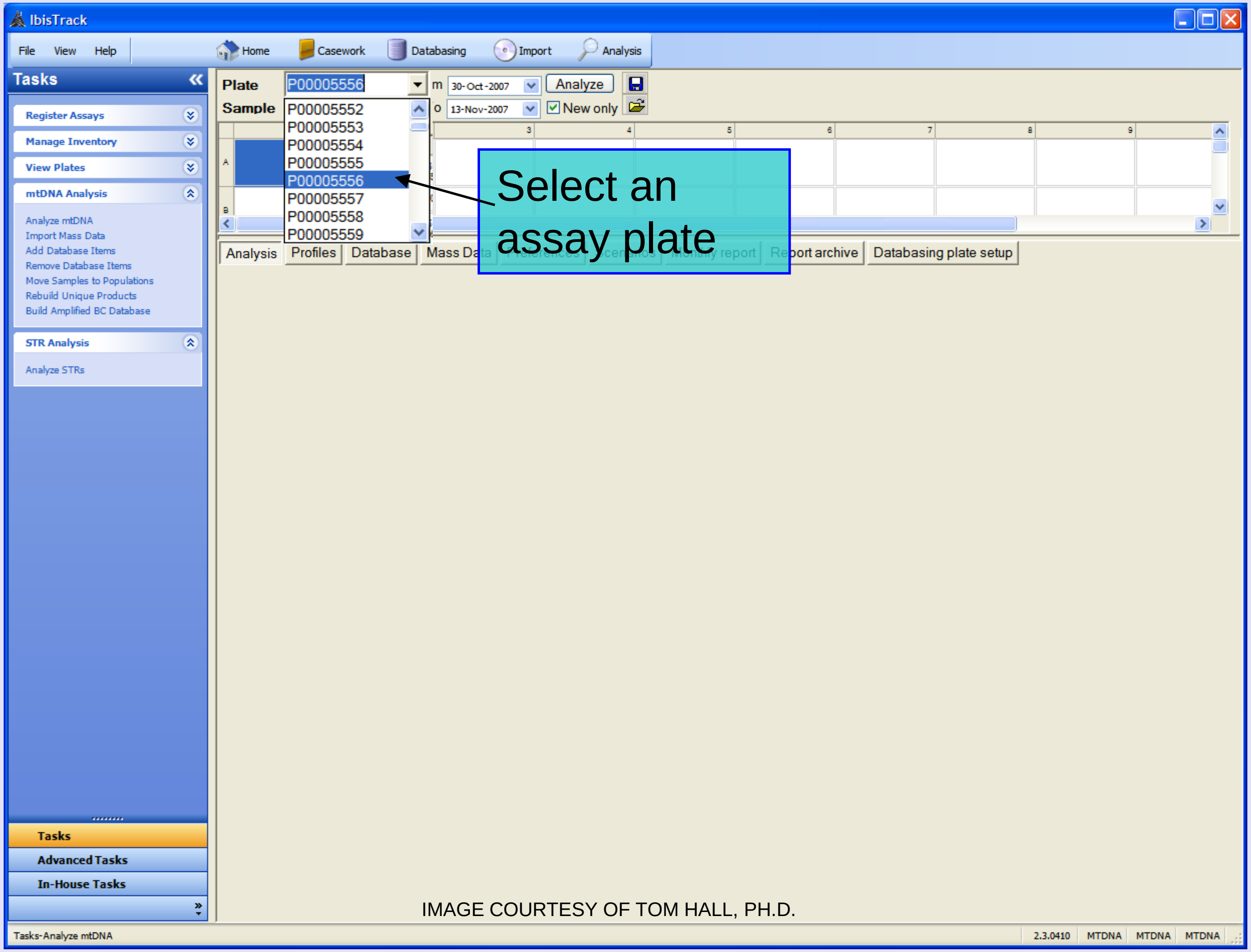

Plate: P00005556

Sample

m 30-Oct-2007

o 13-Nov-2007

☑ New only

Select an assay plate

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Application Interface

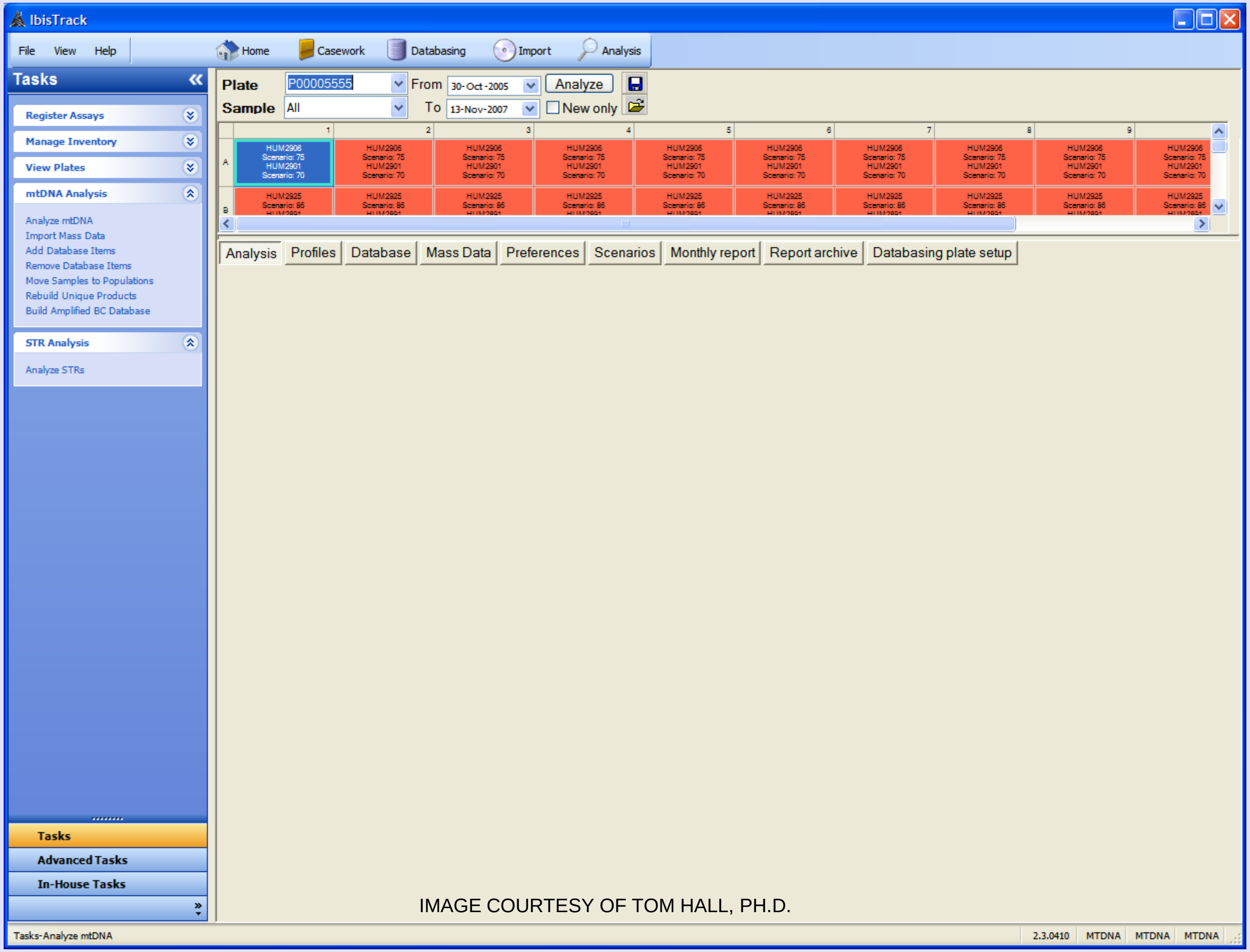

Plate P00005555 From 30-Oct-2005

Sample All To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86

Tasks-Analyze mtDNA | 2.3.0410 | MTDNA | MTDNA | MTDNA

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Application Interface

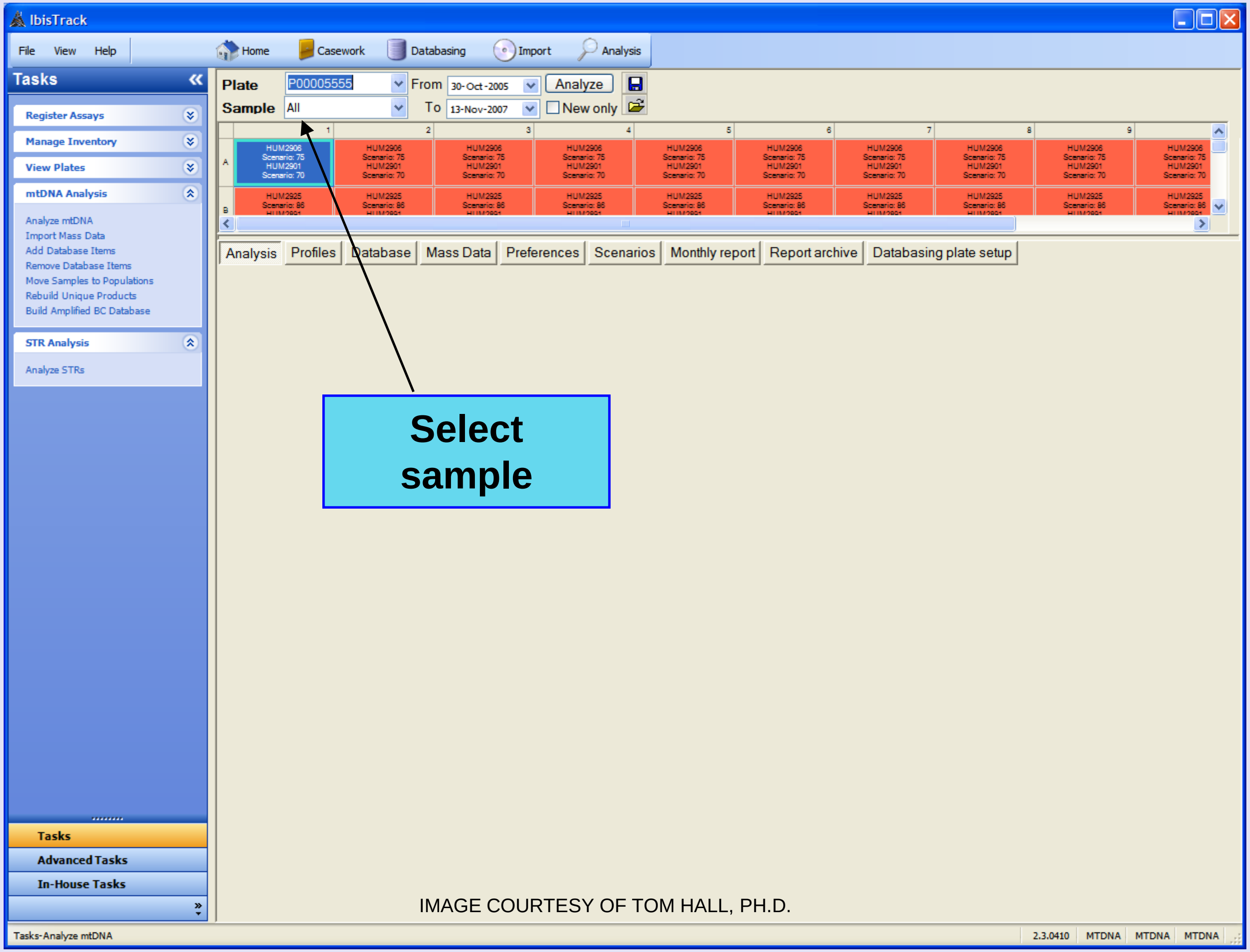

Plate P00005555 From 30-Oct-2005

Sample All To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86

Select sample

IMAGE COURTESY OF TOM HALL, PH.D.

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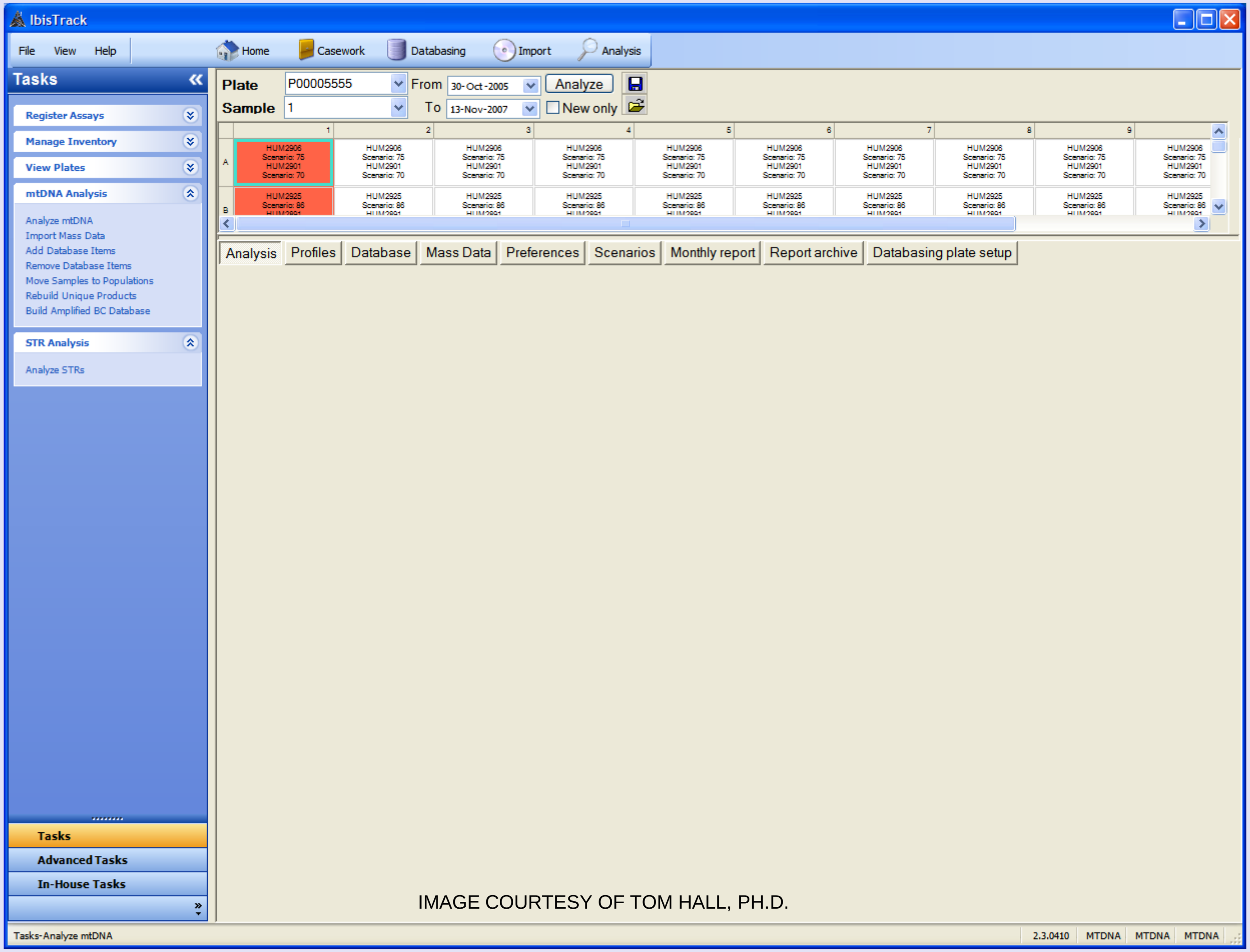

Plate P00005555 From 30-Oct-2005

Sample 1 To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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
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Tasks-Analyze mtDNA 2.3.0410 MTDNA MTDNA MTDNA

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Application Interface

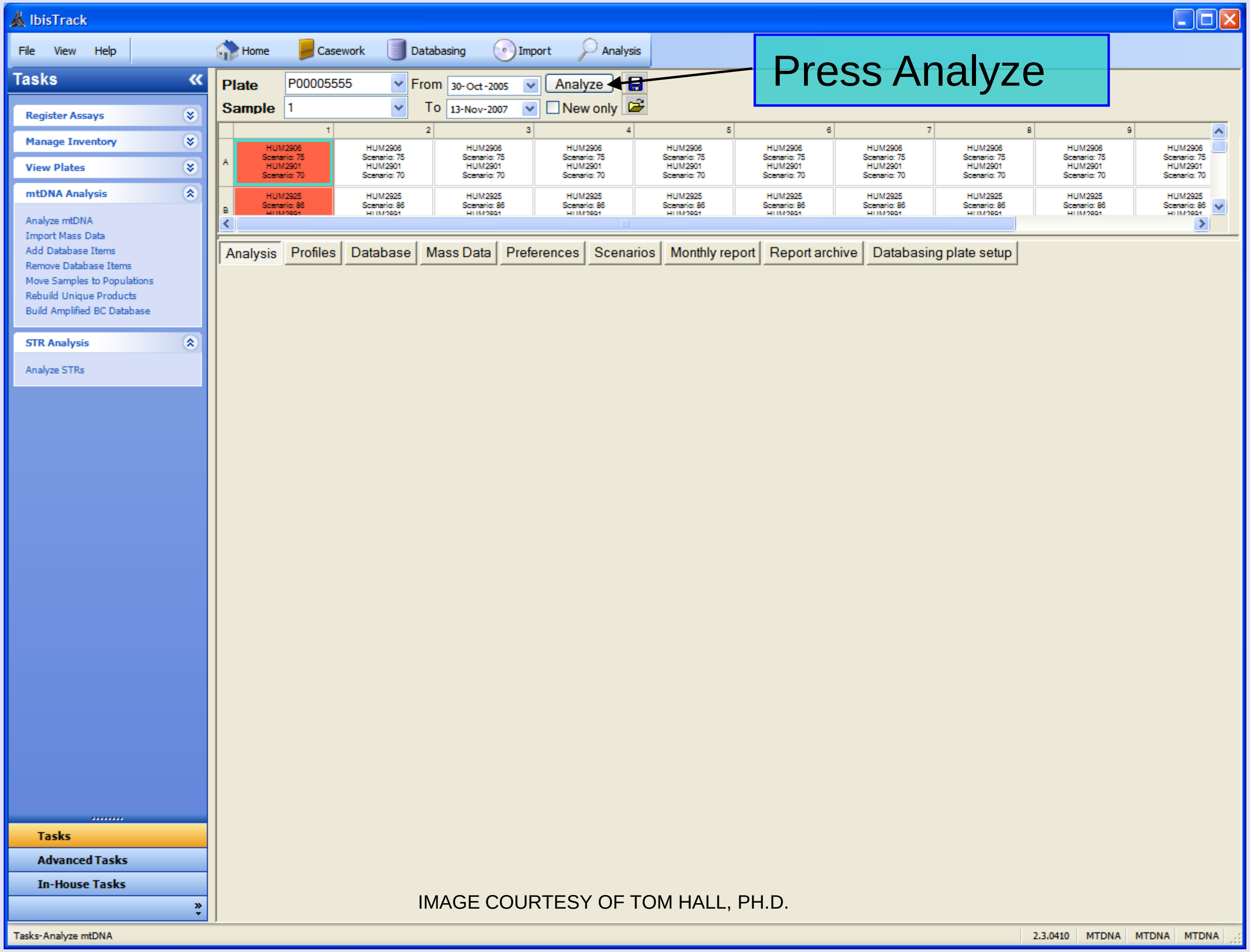

Plate P00005555 From 30-Oct-2005 Analyze

Sample 1 To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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
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Tasks-Analyze mtDNA

2.3.0410 MTDNA MTDNA MTDNA

Press Analyze

IMAGE COURTESY OF TOM HALL, PH.D.

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Basic Analysis Interface

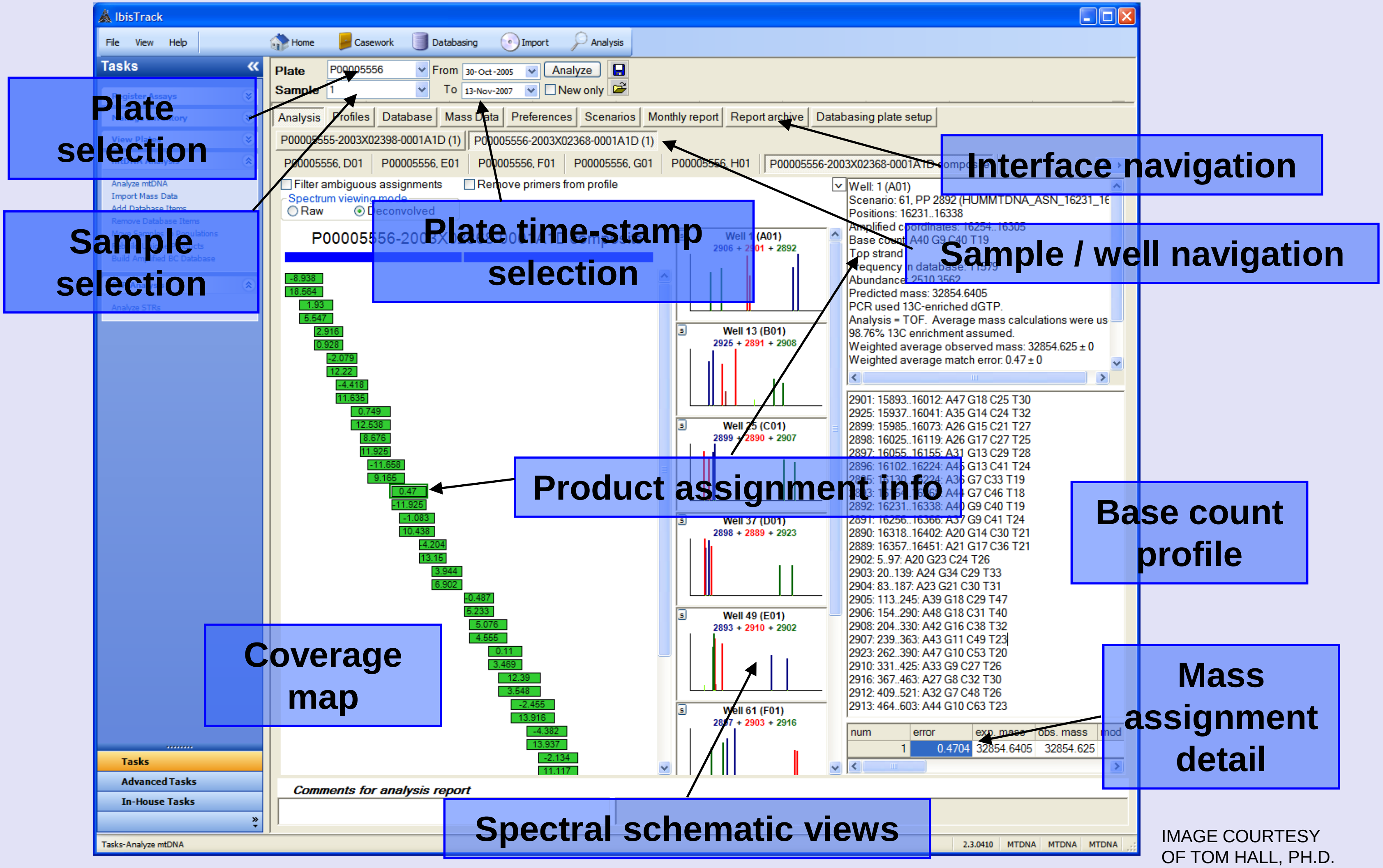

Plate P00005556 From 30-Oct-2005
Sample 1 To 13-Nov-2007 ☐ New only

P00005555-2003X02398-0001A1D (1) | P00005556-2003X02368-0001A1D (1)

P00005556, D01 | P00005556, E01 | P00005556, F01 | P00005556, G01 | P00005556, H01 | P00005556-2003X02368-0001A1D composite

☐ Filter ambiguous assignments ☐ Remove primers from profile

○ Raw ● Deconvolved

P00005556-2003X02368-0001A1D composite

```
Well: 1 (A01)
Scenario: 61, PP 2892 (HUMMTDNA_ASN_16231_16
Positions: 16231..16338
Amplified coordinates: 16254..16305
Base count: A40 G9 C40 T19
Top strand
Frequency in database: 11579
Abundance: 2510.3562
Predicted mass: 32854.6405
PCR used 13C-enriched dGTP.
Analysis = TOF.  Average mass calculations were us
98.76% 13C enrichment assumed.
Weighted average observed mass: 32854.625 ± 0
Weighted average match error: 0.47 ± 0
```

```
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 T25
2897: 16055..16155: A31 G13 C29 T28
2896: 16102..16224: A45 G13 C41 T24
2895: 16130..16224: A36 G7 C33 T19
2893: 16164..16268: A44 G7 C46 T18
2892: 16231..16338: A40 G9 C40 T19
2891: 16256..16366: A37 G9 C41 T24
2890: 16318..16402: A20 G14 C30 T21
2889: 16357..16451: A21 G17 C36 T21
2902: 5..97: A20 G23 C24 T26
2903: 20..139: A24 G34 C29 T33
2904: 83..187: A23 G21 C30 T31
2905: 113..245: A39 G18 C29 T47
2906: 154..290: A48 G18 C31 T40
2908: 204..330: A42 G16 C38 T32
2907: 239..363: A43 G11 C49 T23
2923: 262..390: A47 G10 C53 T20
2910: 331..425: A33 G9 C27 T26
2916: 367..463: A27 G8 C32 T30
2912: 409..521: A32 G7 C48 T26
2913: 464..603: A44 G10 C63 T23
```

num	error	exp. mass	obs. mass	mod
1	0.4704	32854.6405	32854.625	

Plate selection

Sample selection

Plate time-stamp selection

Interface navigation

Sample / well navigation

Product assignment info

Base count profile

Coverage map

Mass assignment detail

Spectral schematic views

IMAGE COURTESY
OF TOM HALL, PH.D.

Basic Utilities Interface

Click

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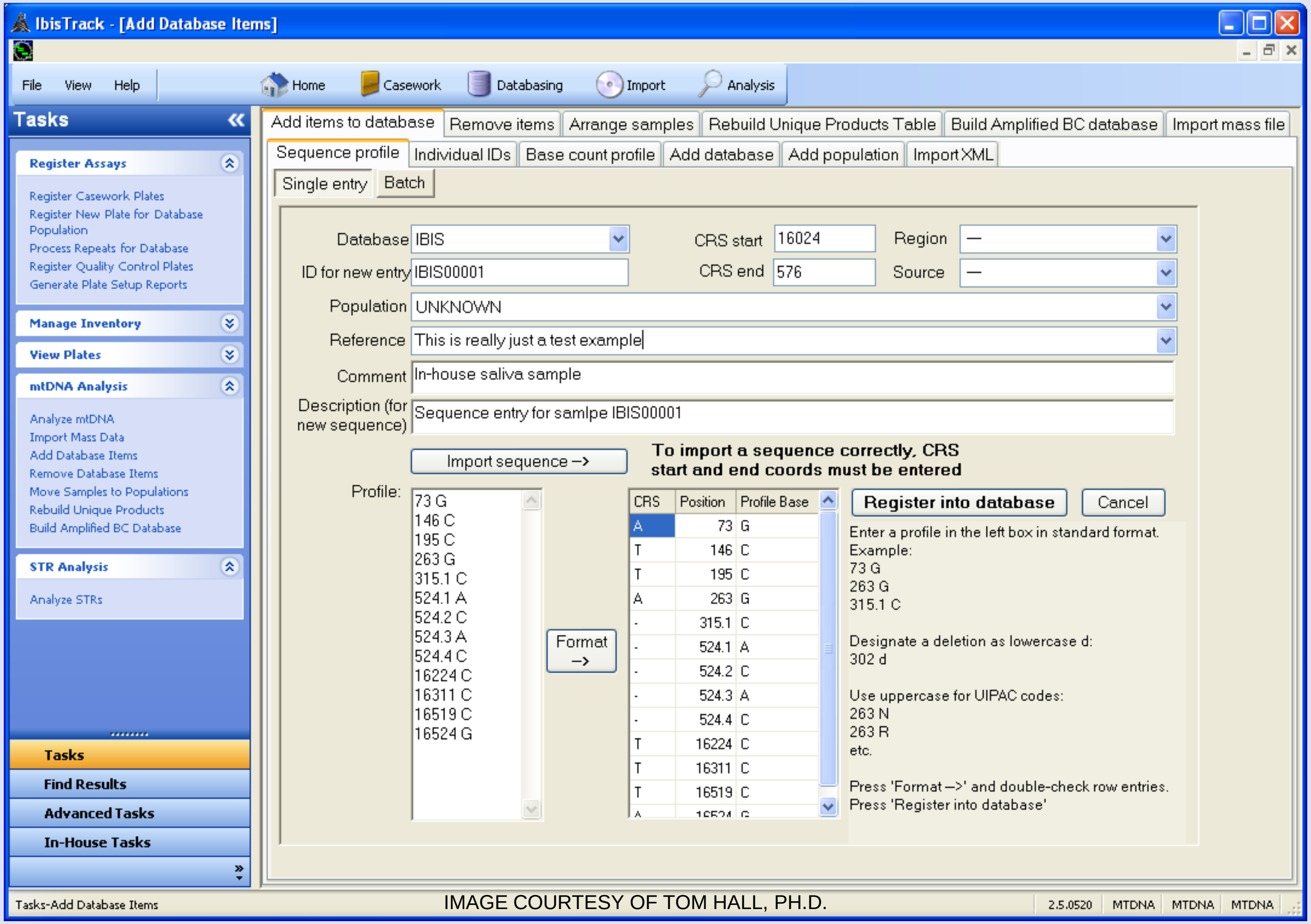

Database: IBIS

ID for new entry: IBIS00001

CRS start: 16024

CRS end: 576

Region: —

Source: —

Population: UNKNOWN

Reference: This is really just a test example

Comment: In-house saliva sample

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

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

Profile:

73 G
146 C
195 C
263 G
315.1 C
524.1 A
524.2 C
524.3 A
524.4 C
16224 C
16311 C
16519 C
16524 G

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

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'

IMAGE COURTESY OF TOM HALL, PH.D.

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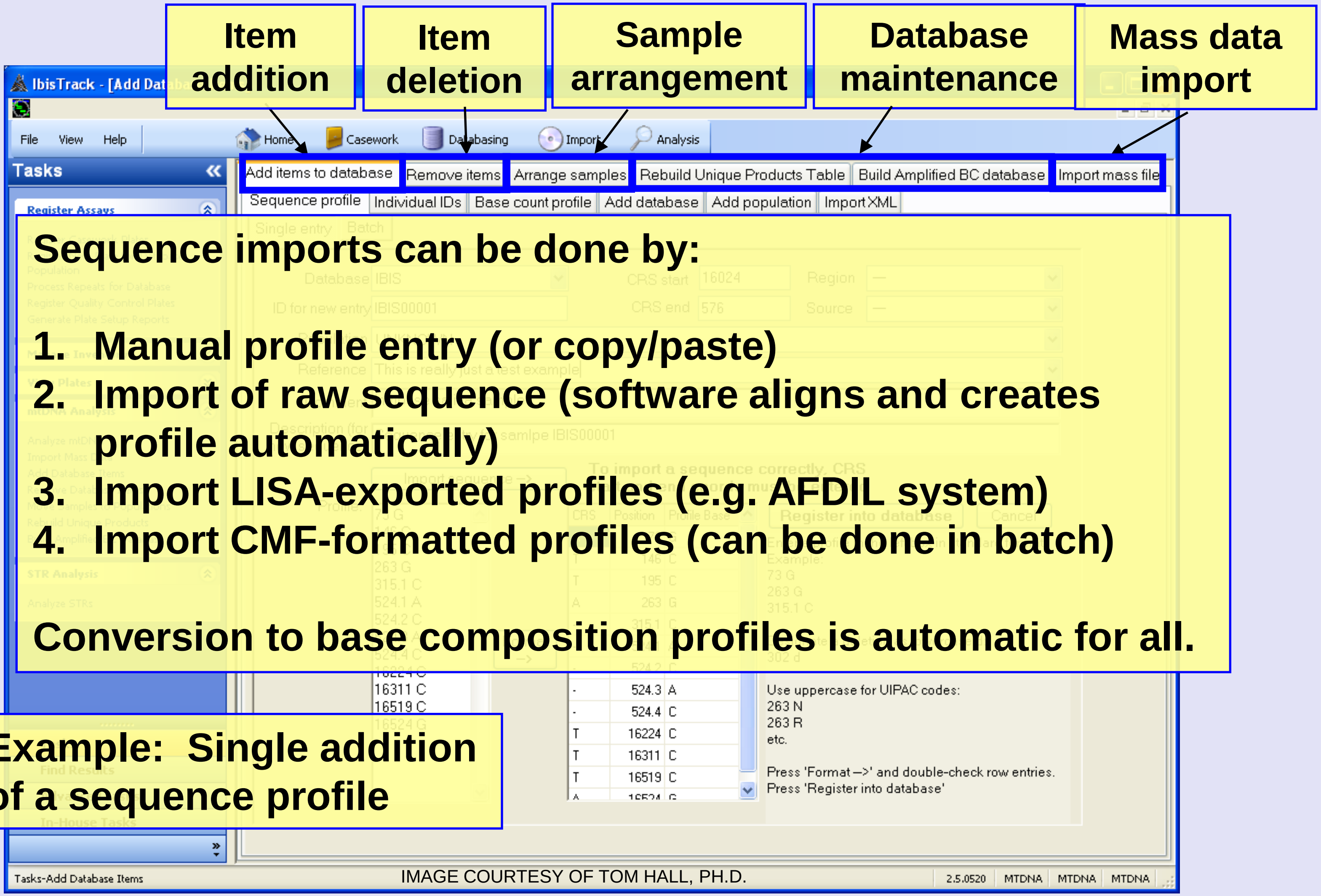
Basic Utilities Interface



Database IBIS

ID for new entry IBIS00001

CRS start 16024

CRS end 576

Reference This is really just a test example

-	524.3	A
-	524.4	C
T	16224	C
T	16311	C
T	16519	C

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

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

IMAGE COURTESY OF TOM HALL, PH.D.

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

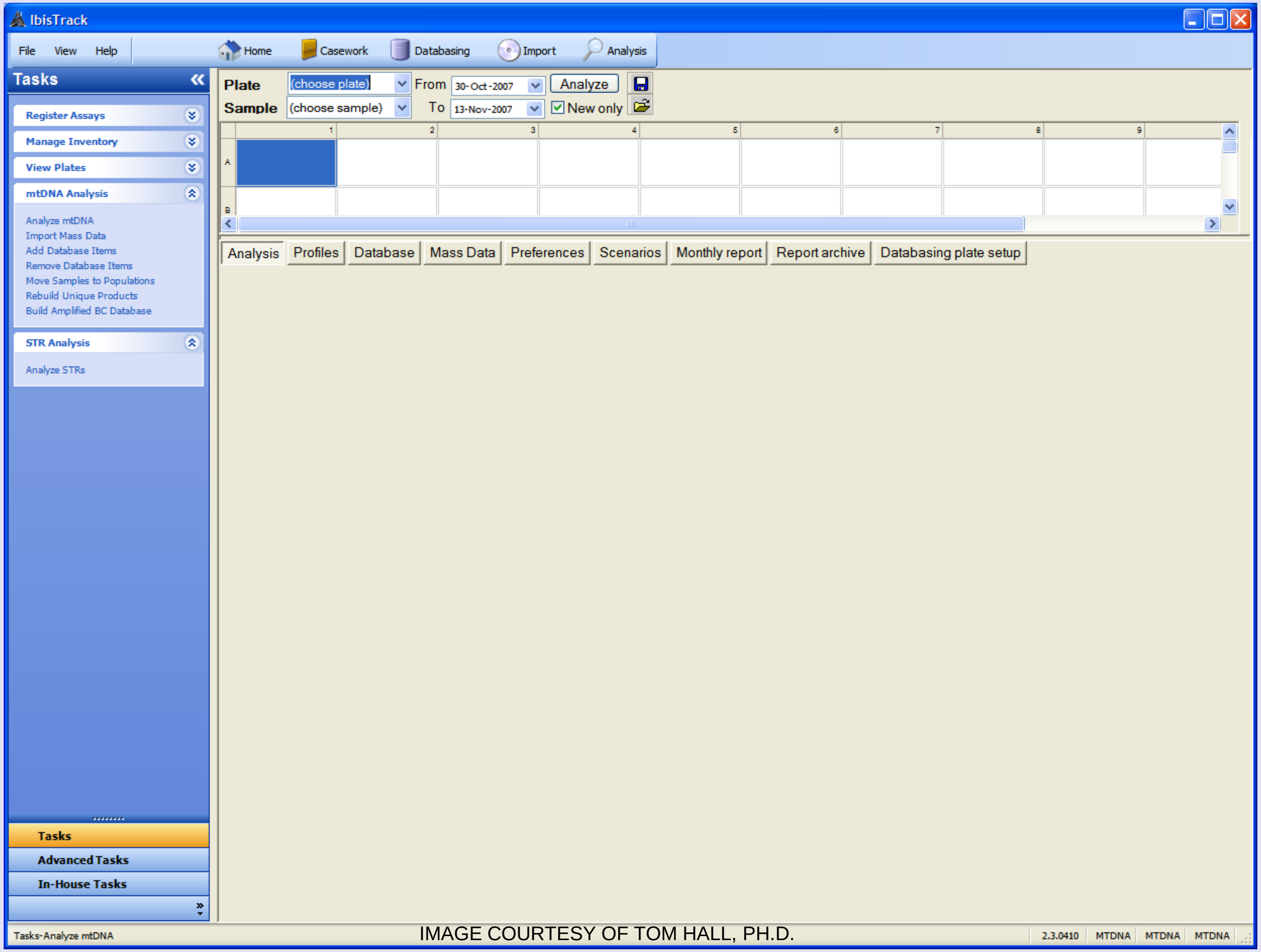


Plate (choose plate)
Sample (choose sample)
From 30-Oct-2007
To 13-Nov-2007
☑ New only

Tasks-Analyze mtDNA
2.3.0410 MTDNA MTDNA MTDNA

IMAGE COURTESY OF TOM HALL, PH.D.

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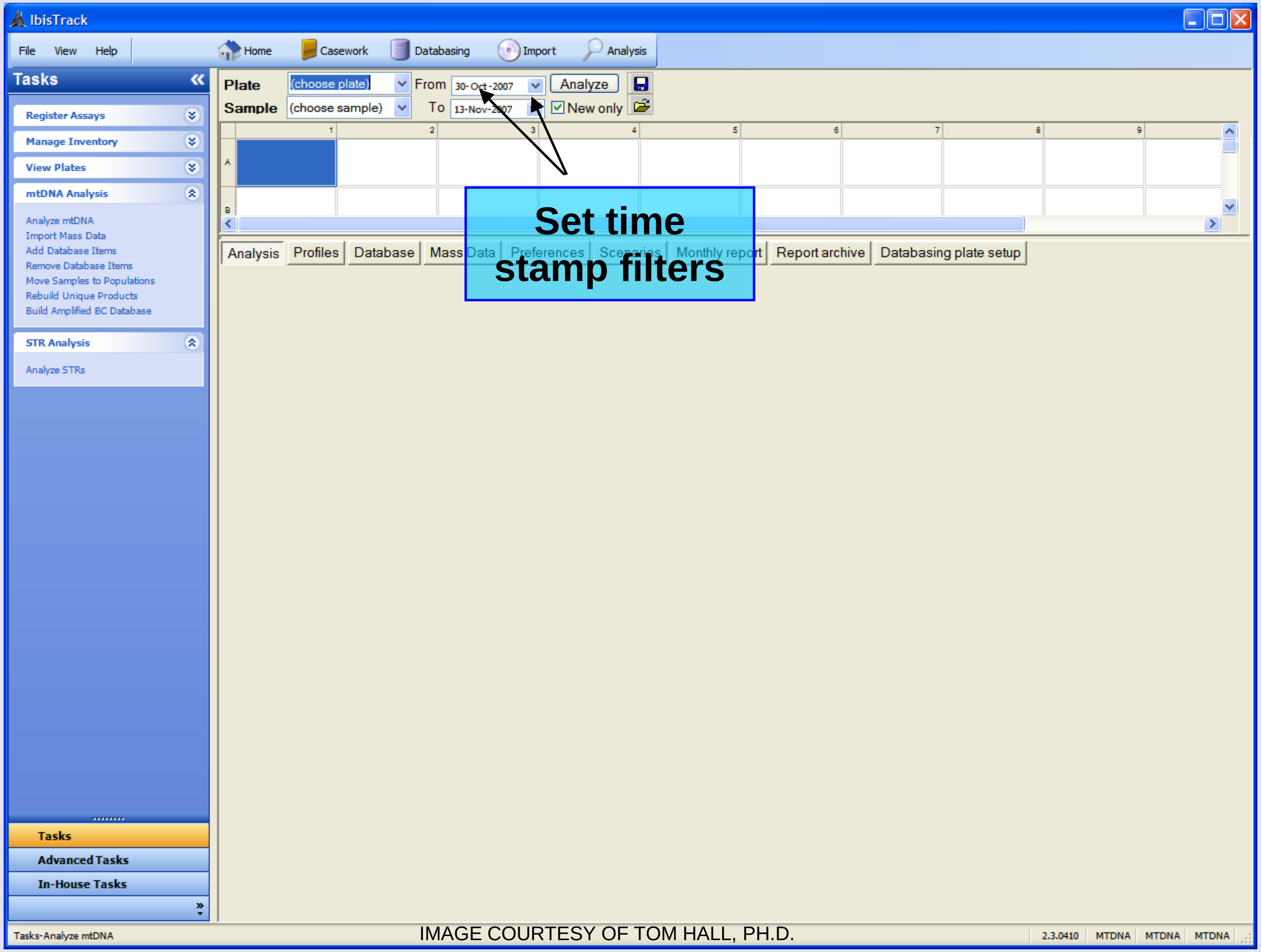

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☑ New only

Set time stamp filters

IMAGE COURTESY OF TOM HALL, PH.D.

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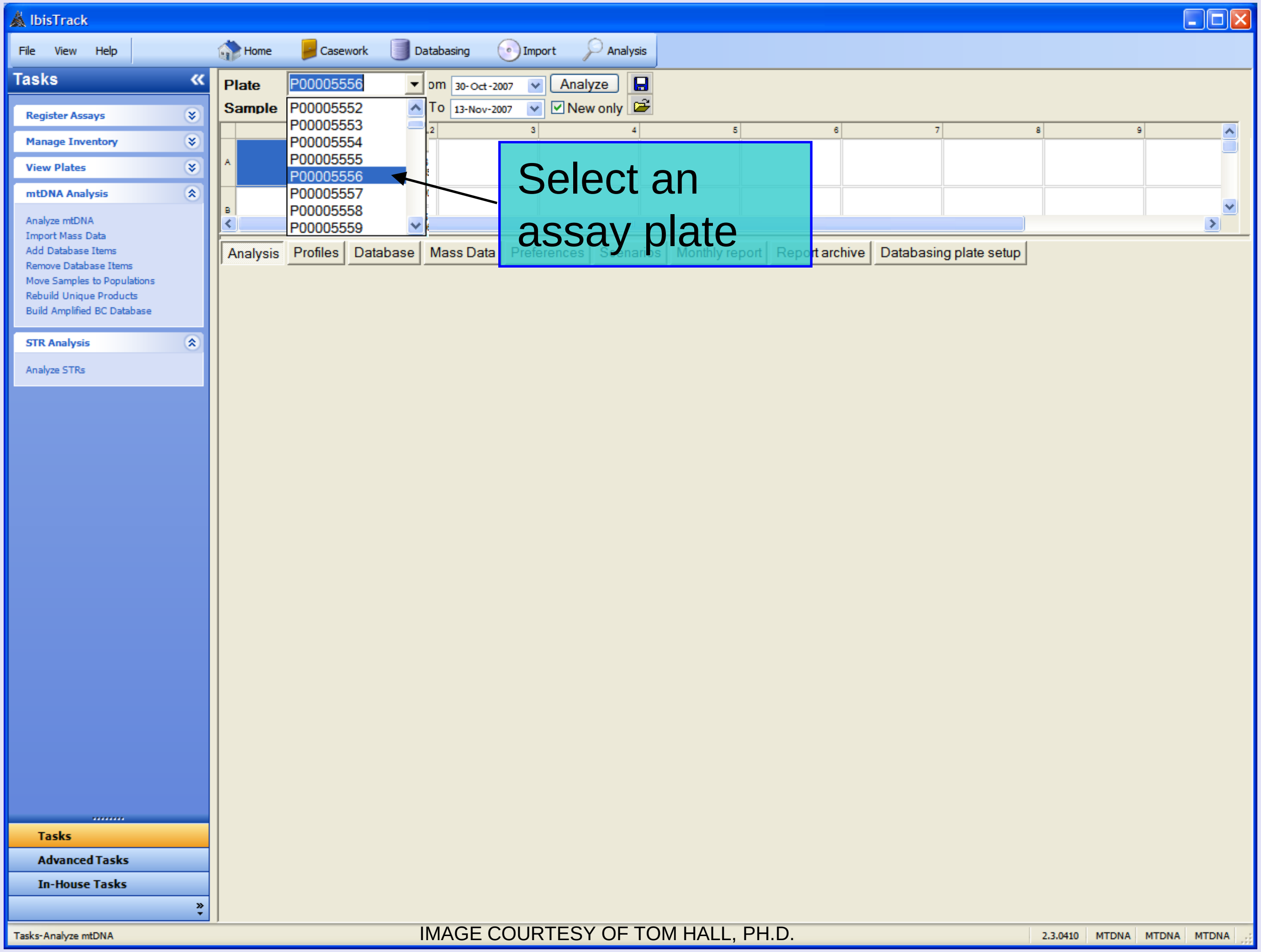

Plate: P00005556

From: 30-Oct-2007

To: 13-Nov-2007

☑ New only

Select an assay plate

IMAGE COURTESY OF TOM HALL, PH.D.

Technology Transition Workshop

Sample Analysis

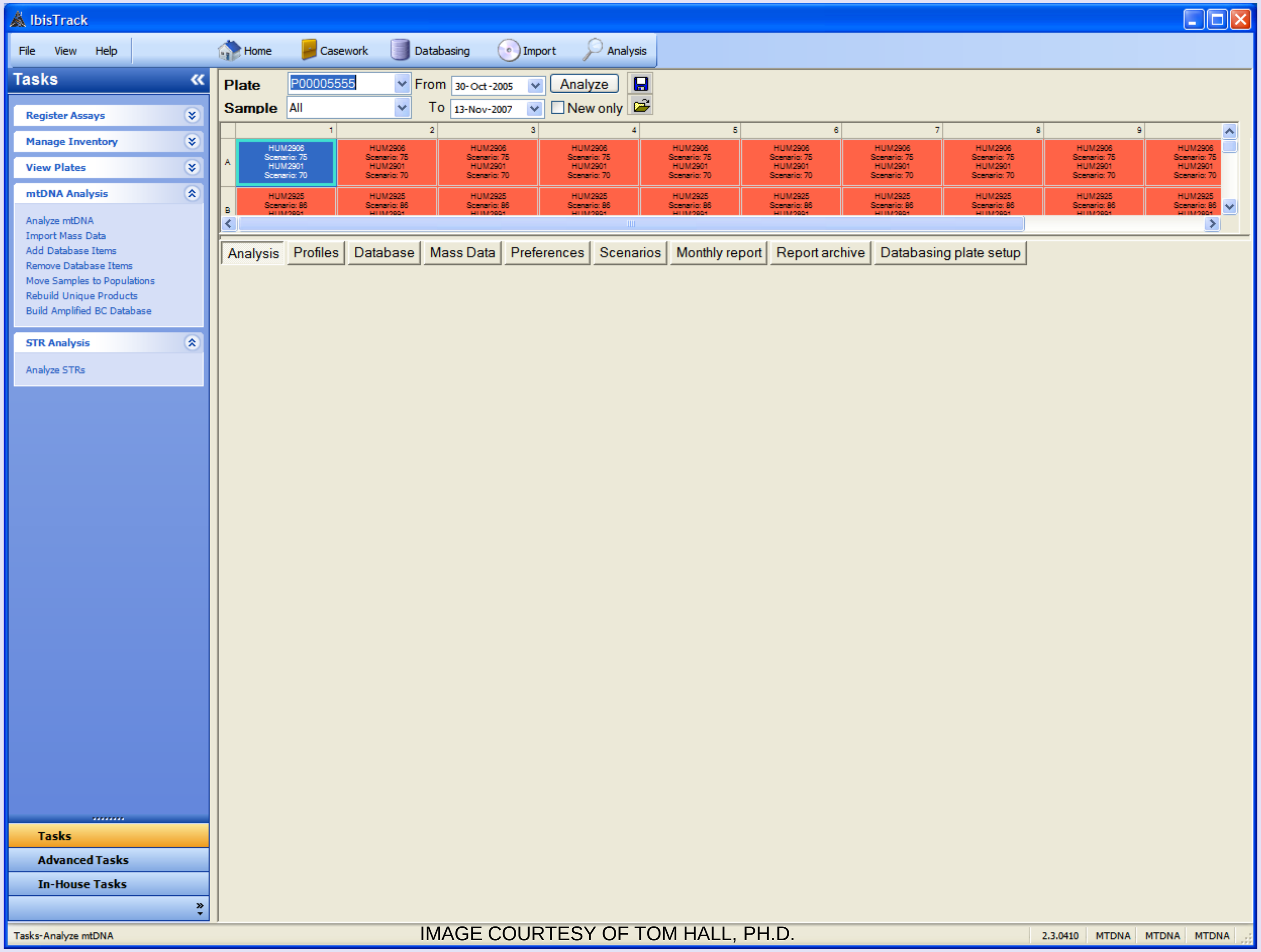

Plate P00005555 From 30-Oct-2005

Sample All To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86

Tasks-Analyze mtDNA

2.3.0410 MTDNA MTDNA MTDNA

IMAGE COURTESY OF TOM HALL, PH.D.

Technology Transition Workshop

Sample Analysis

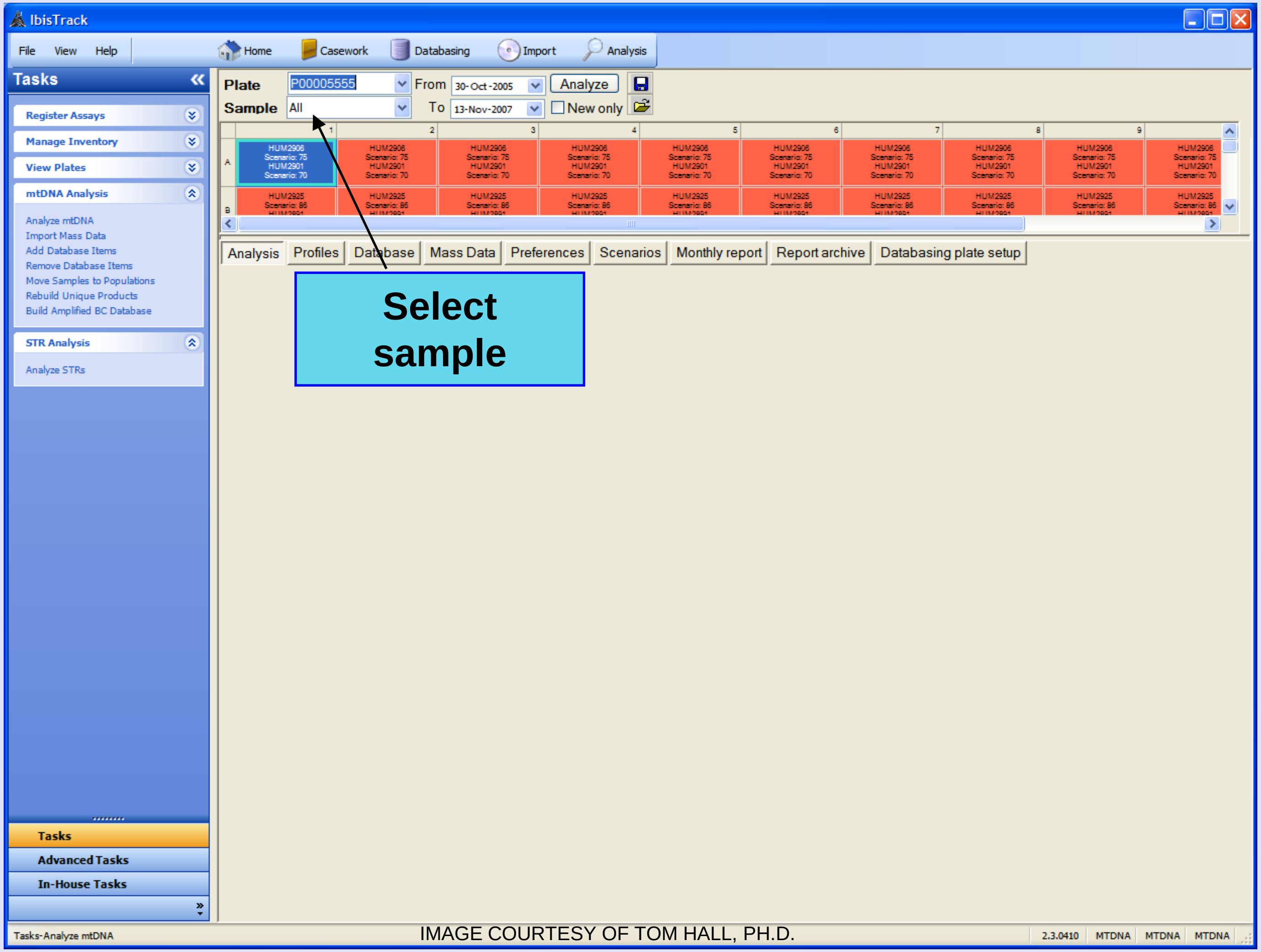

Plate P00005555 From 30-Oct-2005

Sample All To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86

Tasks-Analyze mtDNA

2.3.0410 MTDNA MTDNA MTDNA

Select sample

IMAGE COURTESY OF TOM HALL, PH.D.

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Sample Analysis

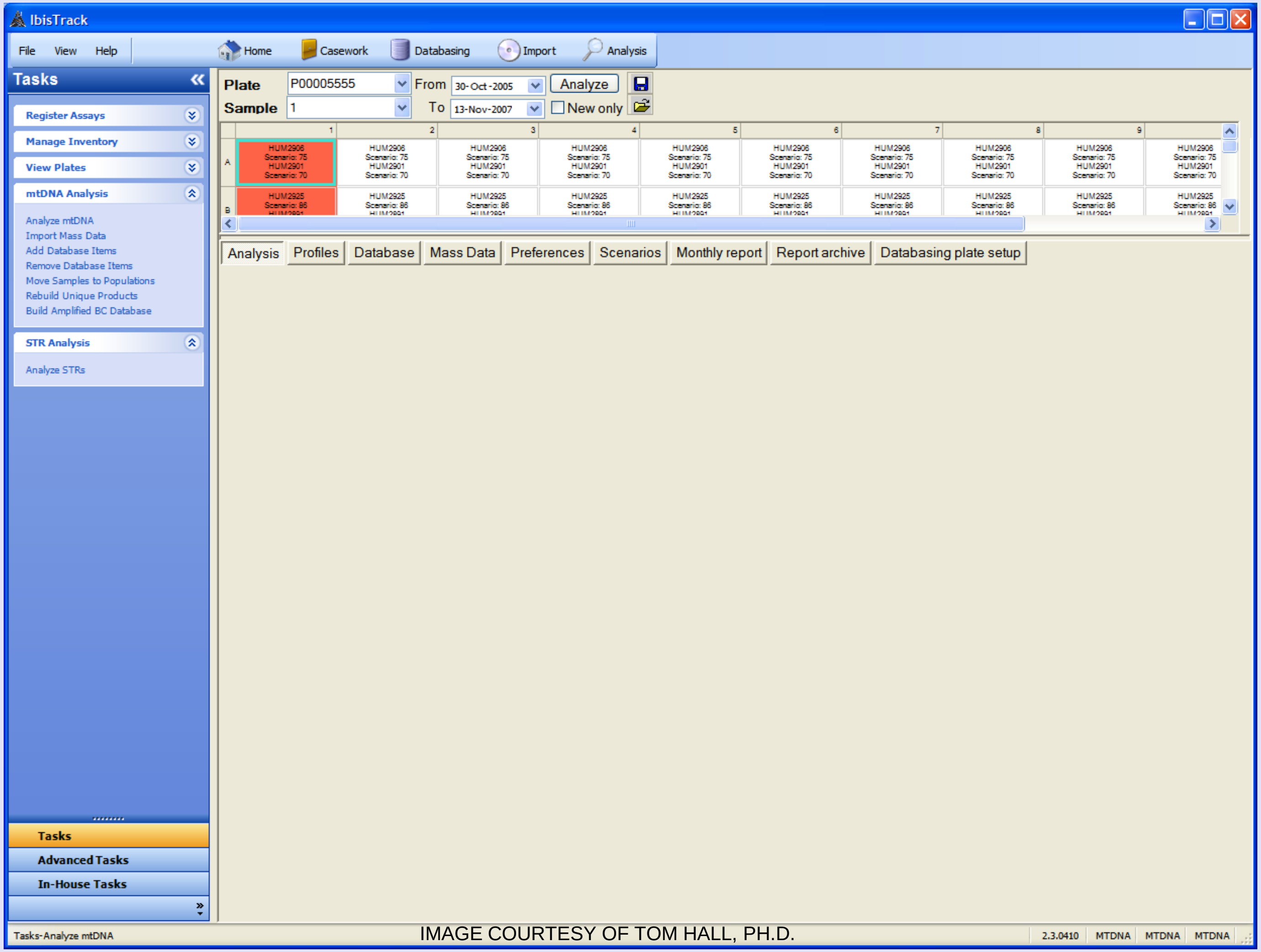

Plate P00005555
Sample 1
From 30-Oct-2005
To 13-Nov-2007
☐ New only

	1	2	3	4	5	6	7	8	9	
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	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86

Tasks-Analyze mtDNA

2.3.0410 MTDNA MTDNA MTDNA

IMAGE COURTESY OF TOM HALL, PH.D.

Sample Analysis

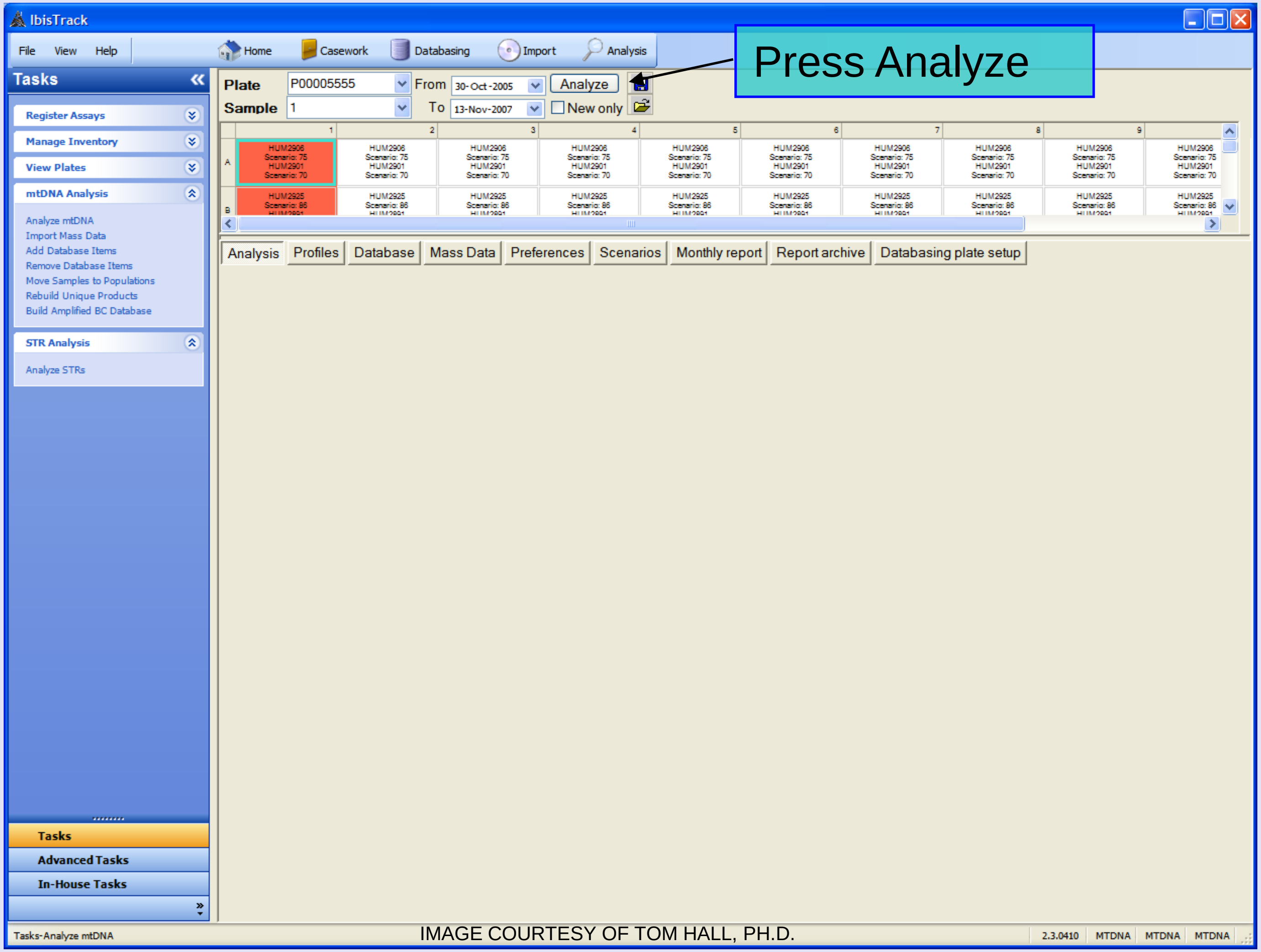

Plate P00005555 From 30-Oct-2005 Analyze

Sample 1 To 13-Nov-2007 ☐ New only

	1	2	3	4	5	6	7	8	9	
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	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86	HUM2925 Scenario: 86

Tasks-Analyze mtDNA 2.3.0410 MTDNA MTDNA MTDNA

Press Analyze

IMAGE COURTESY OF TOM HALL, PH.D.

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Single Sample Analysis

IMAGE COURTESY OF TOM HALL, PH.D.

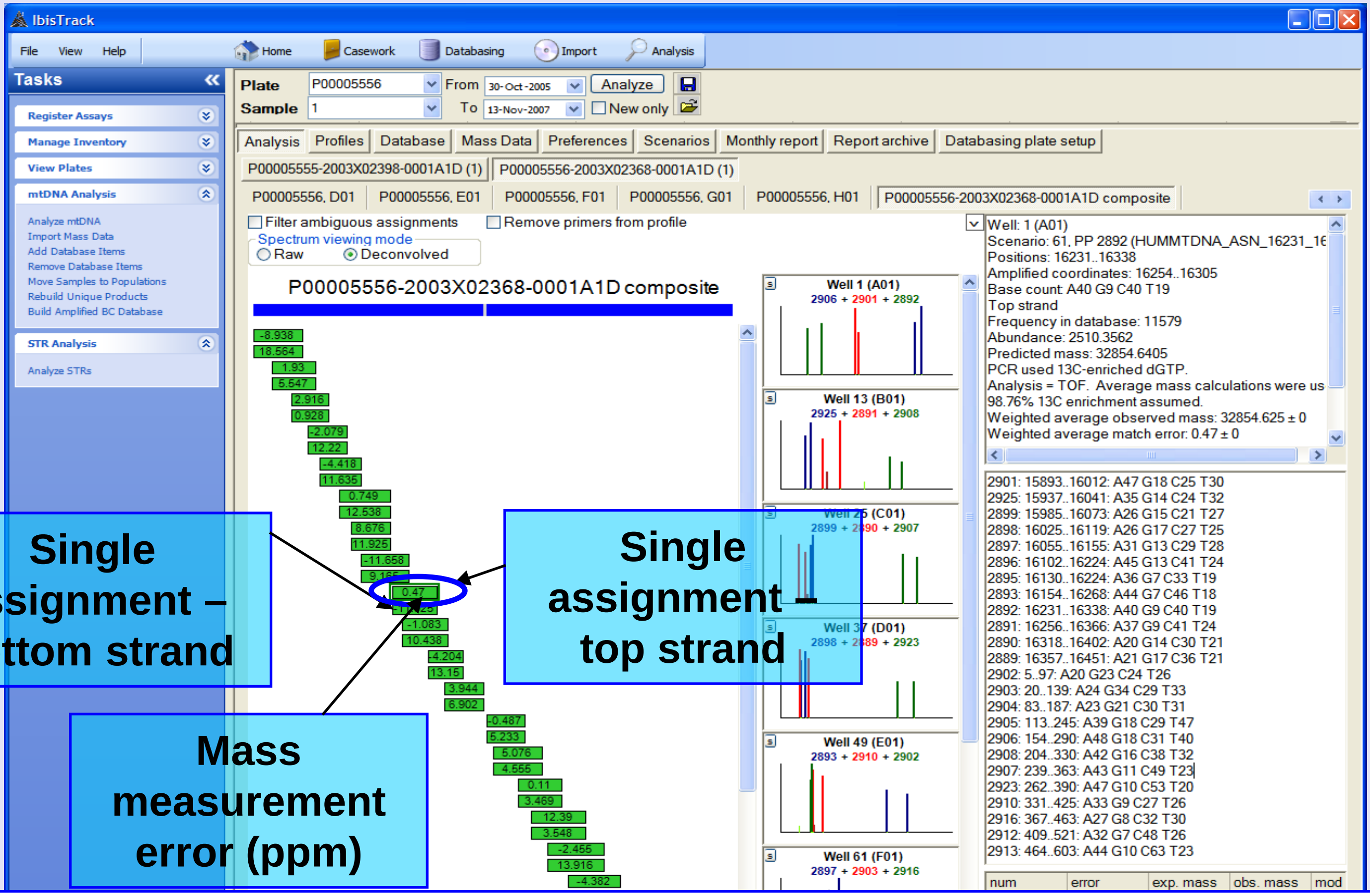

Plate: P00005556
Sample: 1
From: 30-Oct-2005
To: 13-Nov-2007
☐ New only
☐ Filter ambiguous assignments
☐ Remove primers from profile
Spectrum viewing mode: ○ Raw ● Deconvolved

Well: 1 (A01)
Scenario: 61, PP 2892 (HUMMTDNA_ASN_16231_16
Positions: 16231..16338
Amplified coordinates: 16254..16305
Base count A40 G9 C40 T19
Top strand
Frequency in database: 11579
Abundance: 2510.3562
Predicted mass: 32854.6405
PCR used 13C-enriched dGTP.
Analysis = TOF. Average mass calculations were us
98.76% 13C enrichment assumed.
Weighted average observed mass: 32854.625 ± 0
Weighted average match error: 0.47 ± 0

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 T25
2897: 16055..16155: A31 G13 C29 T28
2896: 16102..16224: A45 G13 C41 T24
2895: 16130..16224: A36 G7 C33 T19
2893: 16154..16268: A44 G7 C46 T18
2892: 16231..16338: A40 G9 C40 T19
2891: 16256..16366: A37 G9 C41 T24
2890: 16318..16402: A20 G14 C30 T21
2889: 16357..16451: A21 G17 C36 T21
2902: 5..97: A20 G23 C24 T26
2903: 20..139: A24 G34 C29 T33
2904: 83..187: A23 G21 C30 T31
2905: 113..245: A39 G18 C29 T47
2906: 154..290: A48 G18 C31 T40
2908: 204..330: A42 G16 C38 T32
2907: 239..363: A43 G11 C49 T23
2923: 262..390: A47 G10 C53 T20
2910: 331..425: A33 G9 C27 T26
2916: 367..463: A27 G8 C32 T30
2912: 409..521: A32 G7 C48 T26
2913: 464..603: A44 G10 C63 T23

Single assignment – bottom strand

Single assignment – top strand

Mass measurement error (ppm)

ppm = Parts per million: 1 ppm = expected mass / 1,000,000

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

Single Sample Analysis

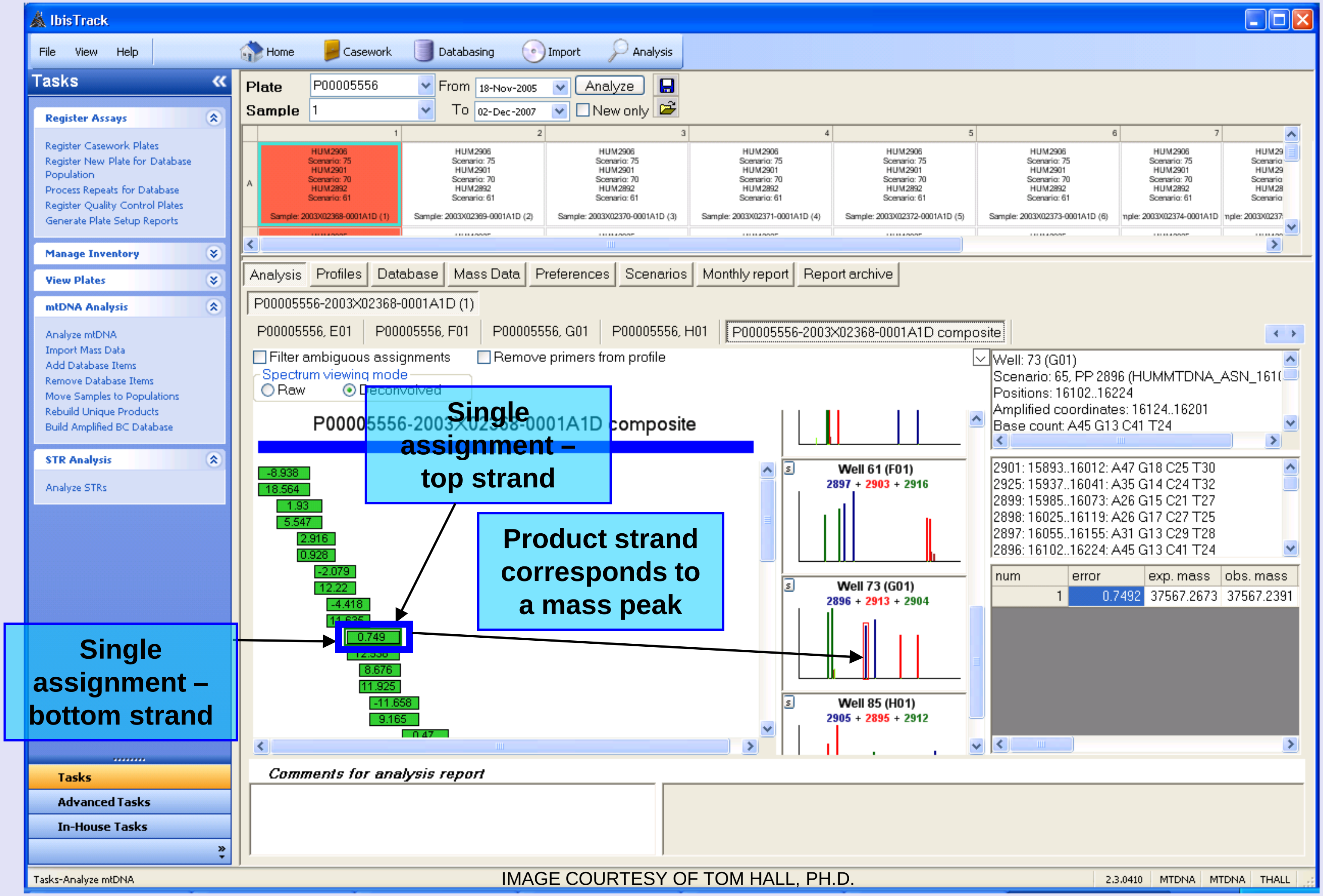

Plate P00005556 From 18-Nov-2005

Sample 1 To 02-Dec-2007 ☐ New only

A1: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02368-0001A1D (1)

A2: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02369-0001A1D (2)

A3: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02370-0001A1D (3)

A4: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02371-0001A1D (4)

A5: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02372-0001A1D (5)

A6: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02373-0001A1D (6)

A7: HUM2906 Scenario: 75 HUM2901 Scenario: 70 HUM2892 Scenario: 61 Sample: 2003X02374-0001A1D

P00005556-2003X02368-0001A1D (1)

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

☐ Filter ambiguous assignments ☐ Remove primers from profile

Spectrum viewing mode: ○ Raw ● Deconvolved

P00005556-2003X02368-0001A1D composite

Well: 73 (G01)
Scenario: 65, PP 2896 (HUMMTDNA_ASN_161
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 T25
2897: 16055..16155: A31 G13 C29 T28
2896: 16102..16224: A45 G13 C41 T24

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

Comments for analysis report

Tasks-Analyze mtDNA | 2.3.0410 | MTDNA | MTDNA | THALL

Single assignment – top strand

Product strand corresponds to a mass peak

Single assignment – bottom strand

IMAGE COURTESY OF TOM HALL, PH.D.

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Single Sample Analysis

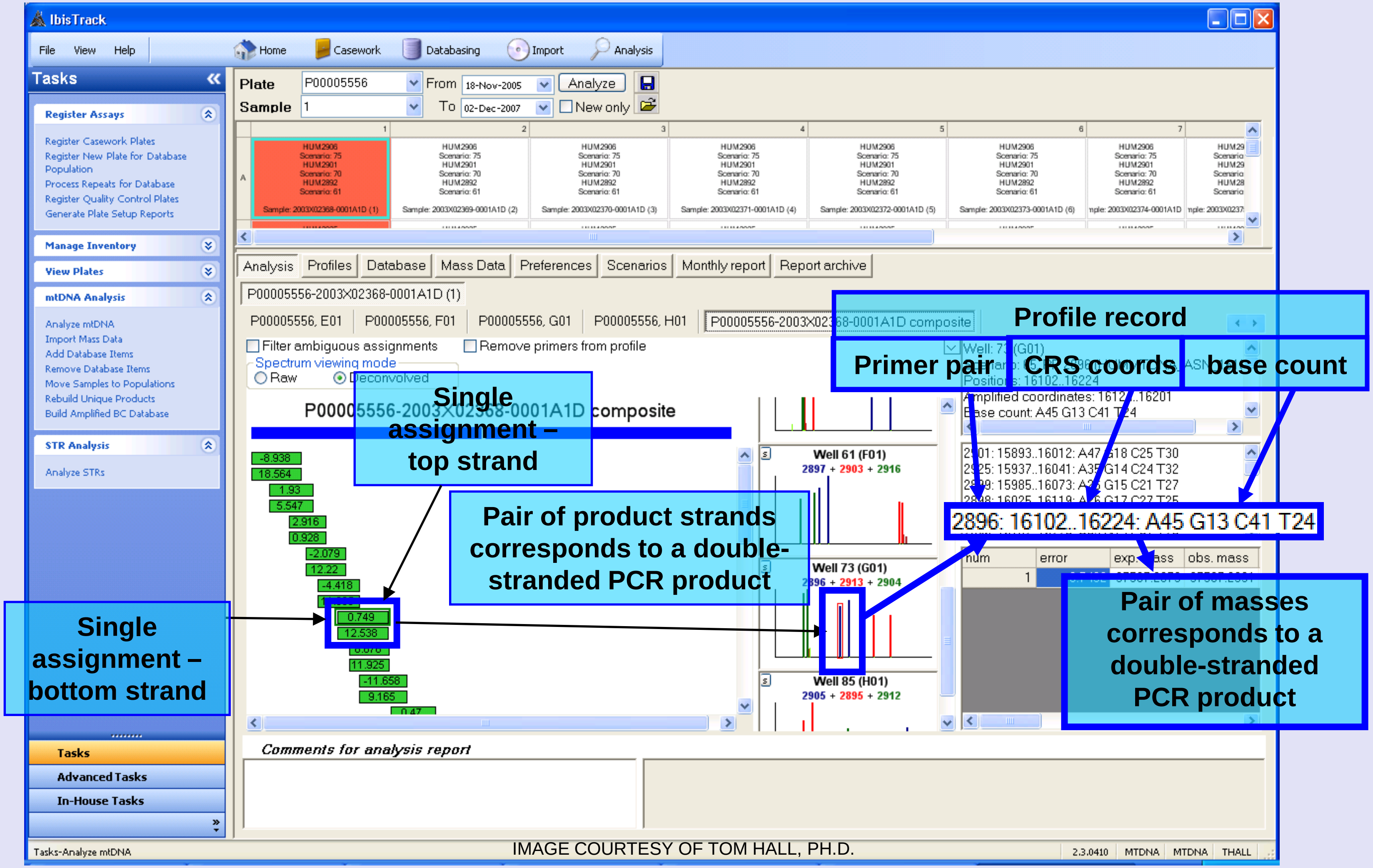

Plate P00005556 From 18-Nov-2005

Sample 1 To 02-Dec-2007 ☐ New only

Sample: 2003X02368-0001A1D (1)

P00005556-2003X02368-0001A1D (1)

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

☐ Filter ambiguous assignments ☐ Remove primers from profile

Spectrum viewing mode ○ Raw ● Deconvolved

P00005556-2003X02368-0001A1D composite

Well: 73 (G01)

Positions: 16102..16224

Amplified coordinates: 16127..16201

Base count: A45 G13 C41 T24

2901: 15893..16012: A47 G18 C25 T30

2925: 15937..16041: A35 G14 C24 T32

2899: 15985..16073: A32 G15 C21 T27

-8.938, 18.564, 1.93, 5.547, 2.916, 0.928, -2.079, 12.22, -4.418, 0.749, 12.538, 11.925, -11.658, 9.165, 0.47

Profile record

Primer pair

CRS coords

base count

2896: 16102..16224: A45 G13 C41 T24

Single assignment – top strand

Pair of product strands corresponds to a double-stranded PCR product

Single assignment – bottom strand

Pair of masses corresponds to a double-stranded PCR product

IMAGE COURTESY OF TOM HALL, PH.D.

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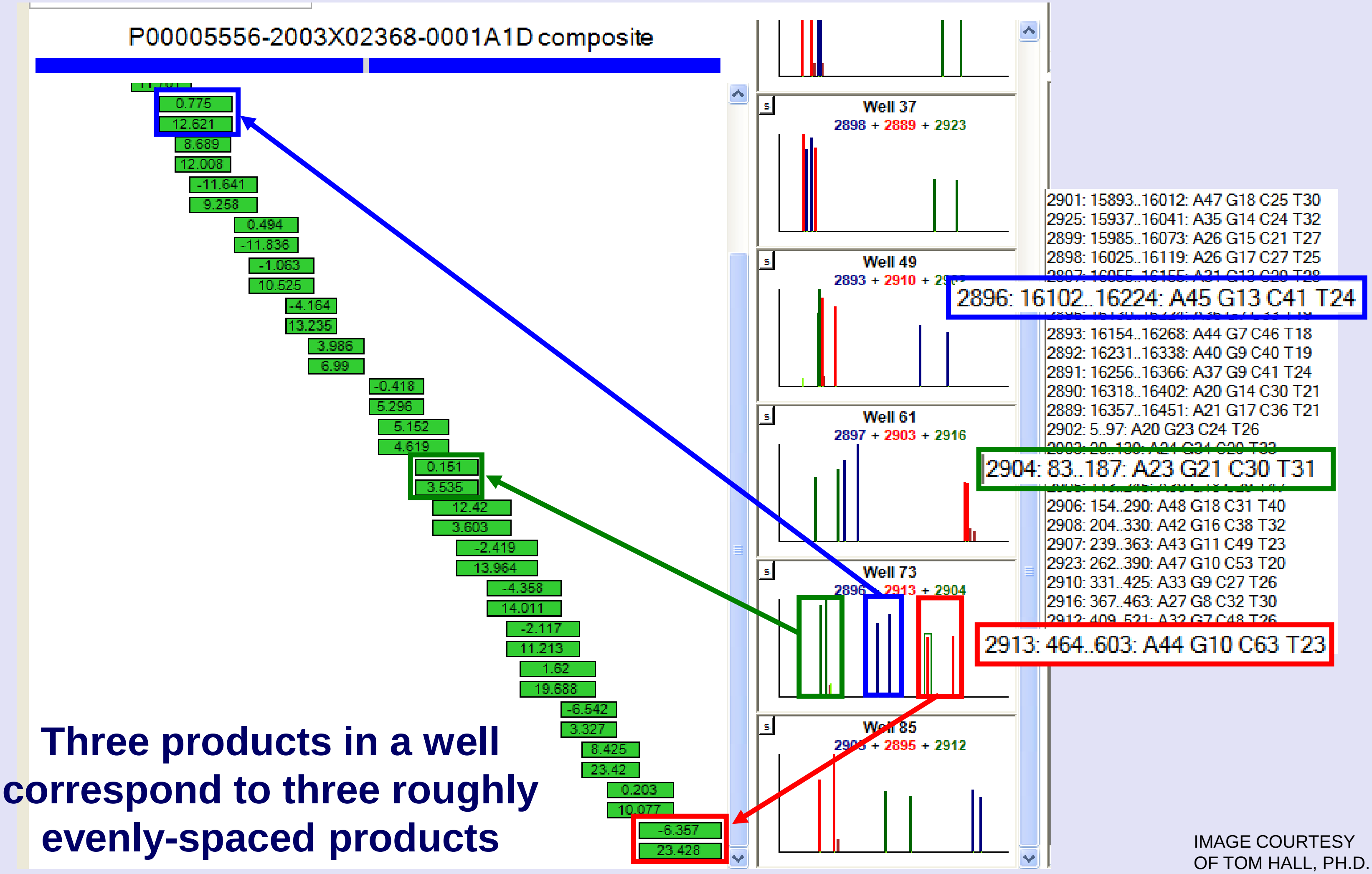
Single Sample Analysis



```
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 T25
2893: 16154..16268: A44 G7 C46 T18
2892: 16231..16338: A40 G9 C40 T19
2891: 16256..16366: A37 G9 C41 T24
2890: 16318..16402: A20 G14 C30 T21
2889: 16357..16451: A21 G17 C36 T21
2902: 5..97: A20 G23 C24 T26
2906: 154..290: A48 G18 C31 T40
2908: 204..330: A42 G16 C38 T32
2907: 239..363: A43 G11 C49 T23
2923: 262..390: A47 G10 C53 T20
2910: 331..425: A33 G9 C27 T26
2916: 367..463: A27 G8 C32 T30
```

2896: 16102..16224: A45 G13 C41 T24

2904: 83..187: A23 G21 C30 T31

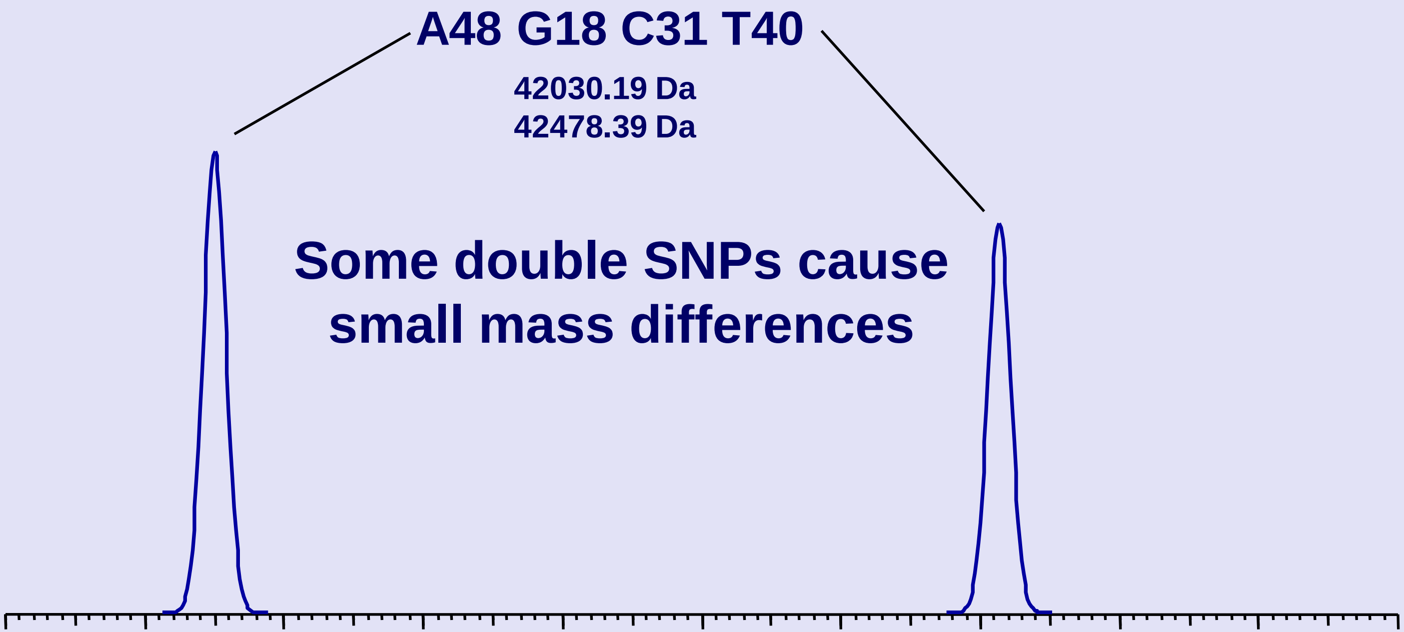
2913: 464..603: A44 G10 C63 T23

Three products in a well correspond to three roughly evenly-spaced products

IMAGE COURTESY
OF TOM HALL, PH.D.

Use of a Mass Tag

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



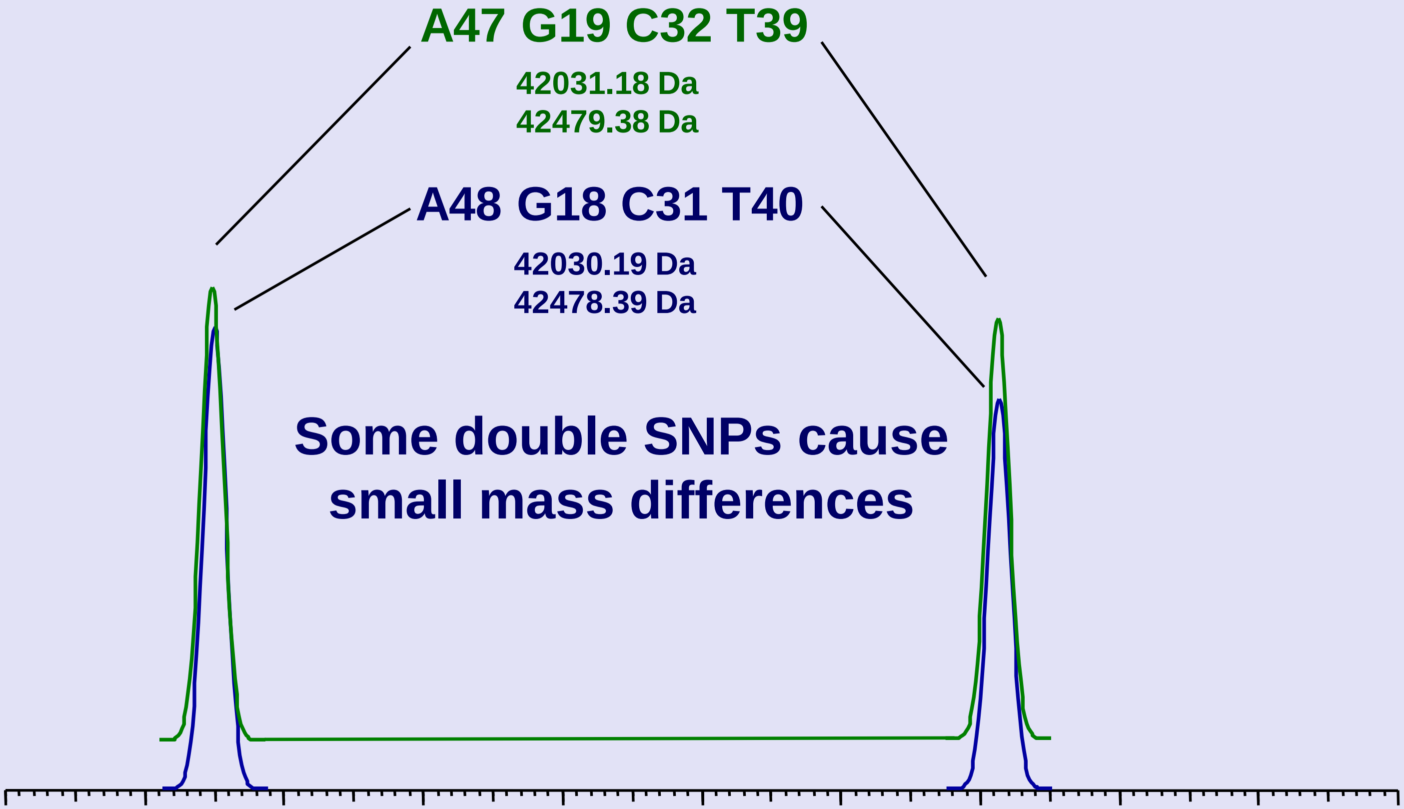
Some double SNPs cause small mass differences

IMAGE COURTESY OF TOM HALL, PH.D.

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.



Some double SNPs cause small mass differences

IMAGE COURTESY OF TOM HALL, PH.D.

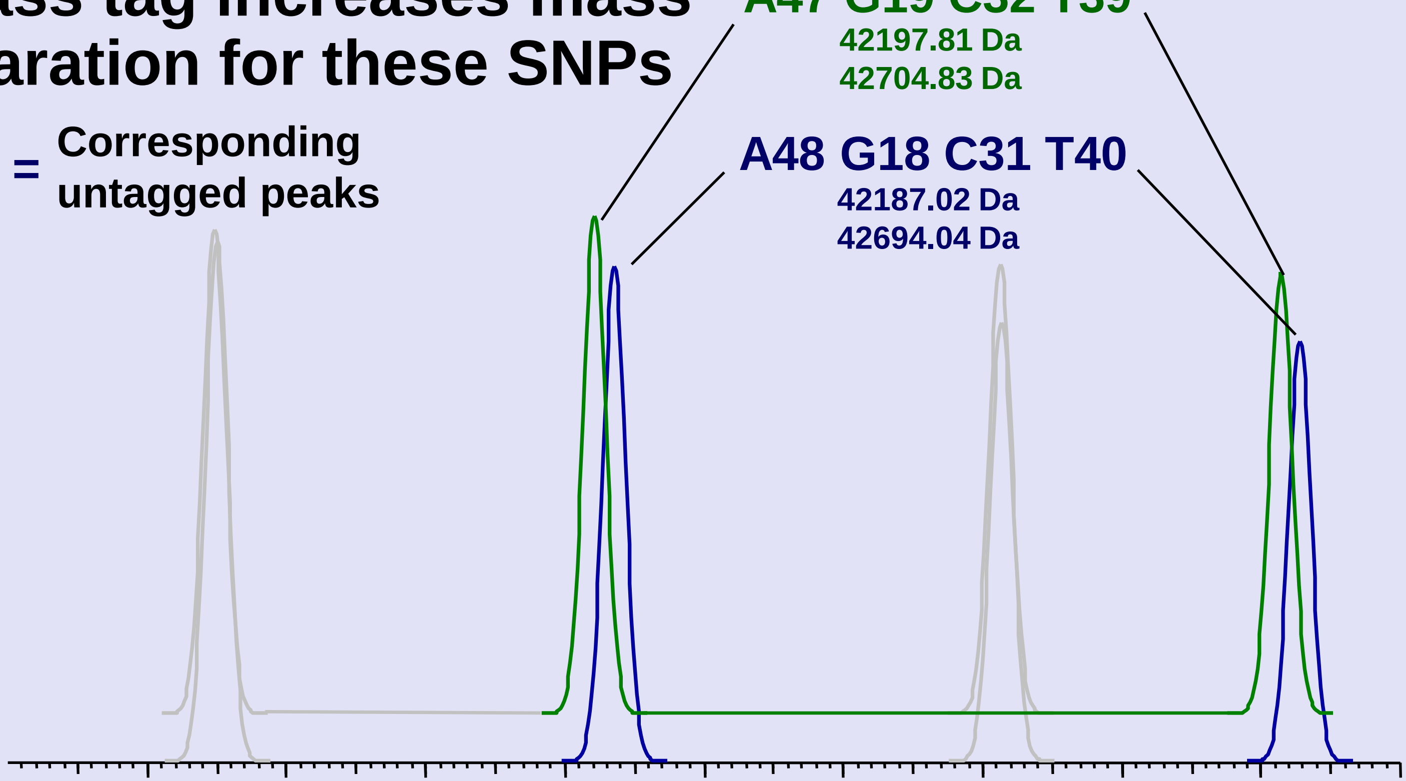
Use of a Mass Tag

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**



A47 G19 C32 T39
42197.81 Da
42704.83 Da

A48 G18 C31 T40
42187.02 Da
42694.04 Da

IMAGE COURTESY OF TOM HALL, PH.D.

Real Data with Mass Tag

Primer pair 2906 product from two representative samples (Data for primer pair 2906 are overlayed).

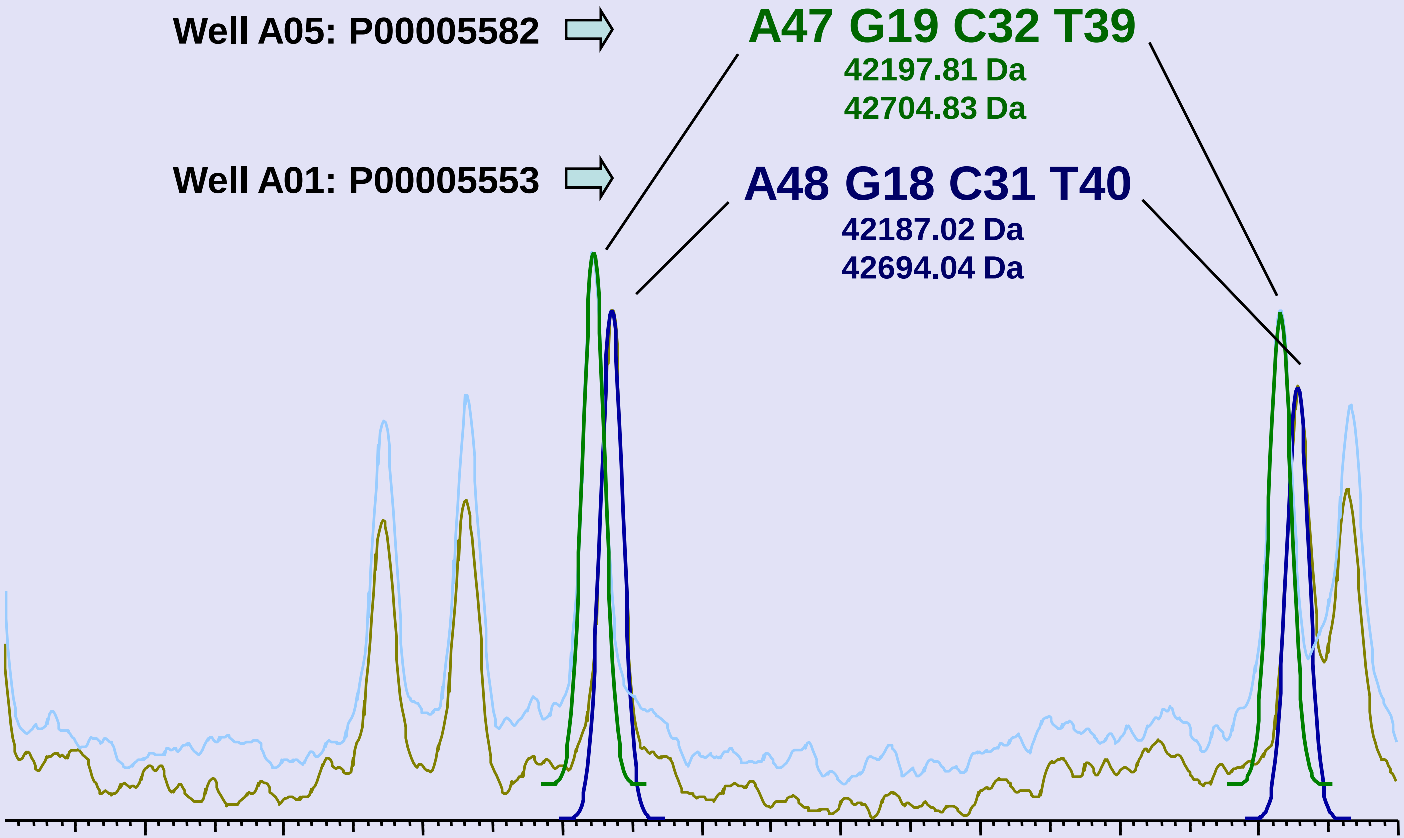
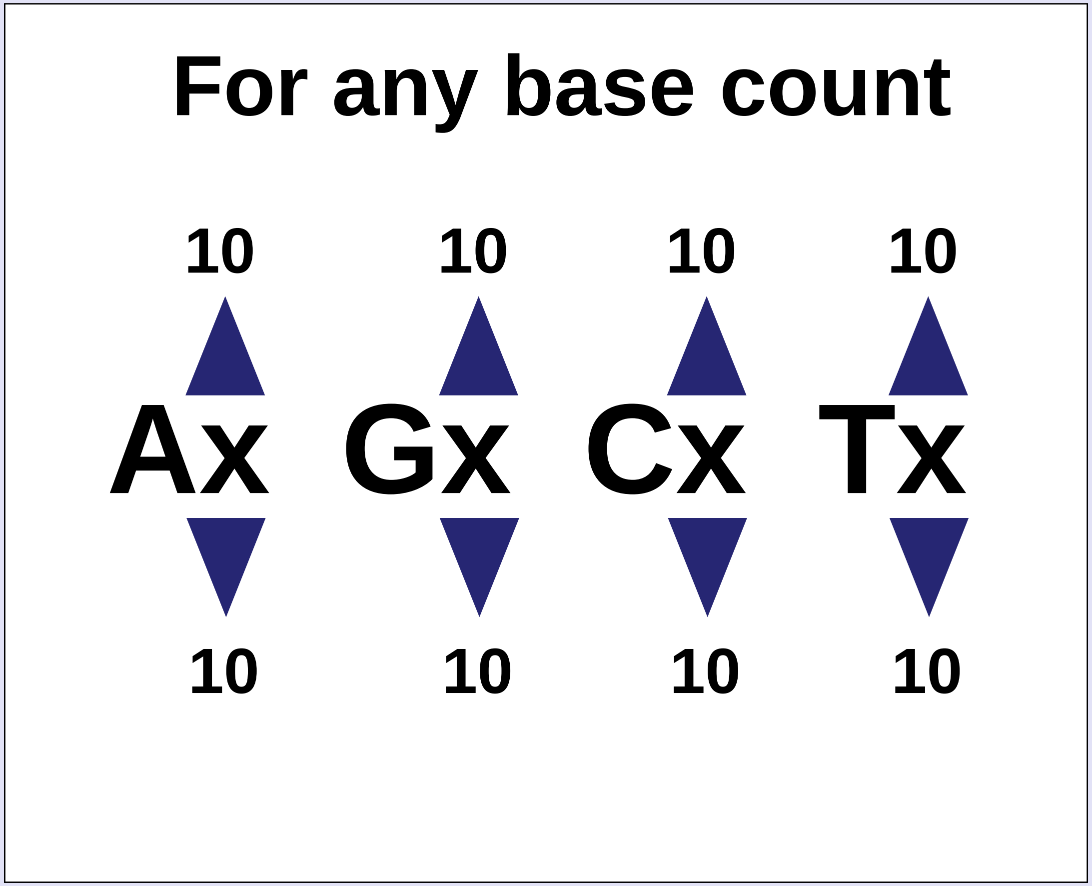


IMAGE COURTESY OF TOM HALL, PH.D.

What Does Mass Tagging Mean?

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



For any base count

IMAGE COURTESY OF TOM HALL, PH.D.

What Does Mass Tagging Mean?

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

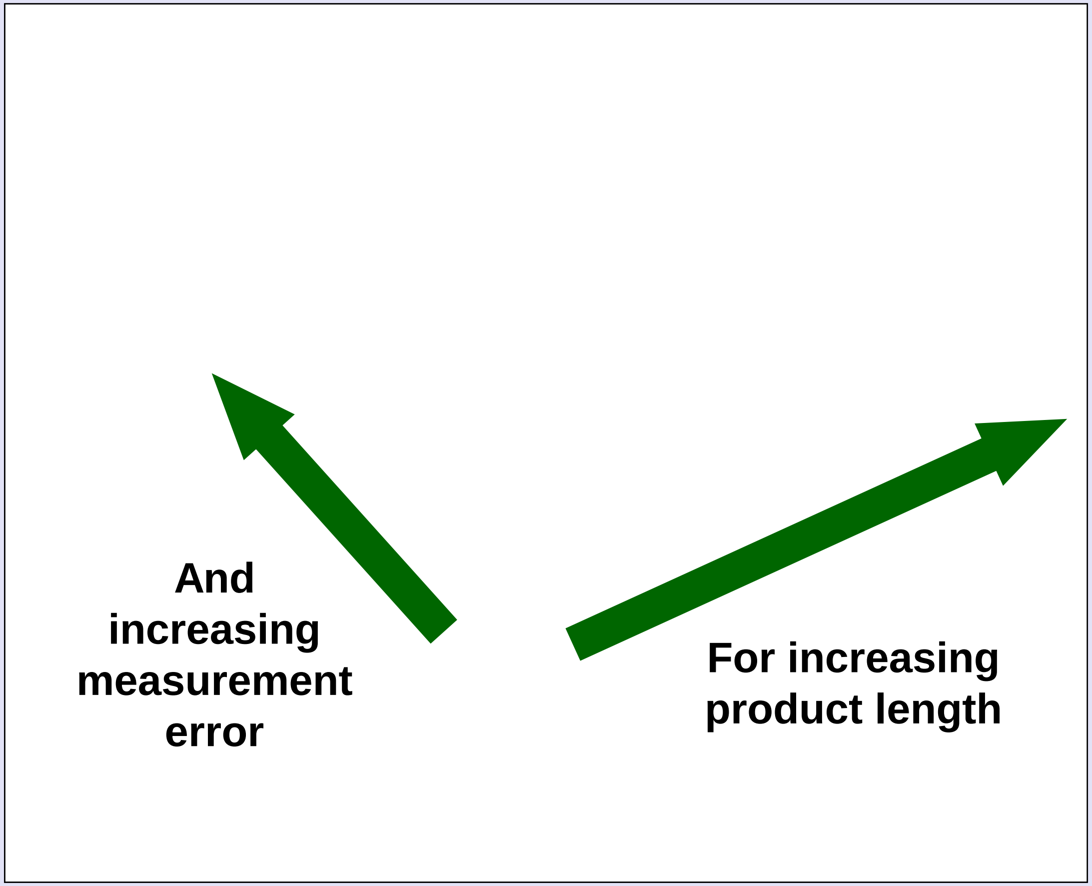


IMAGE COURTESY OF TOM HALL, PH.D.

What Does Mass Tagging Mean?

Potential assignment ambiguities increase dramatically with measurement error and product size.

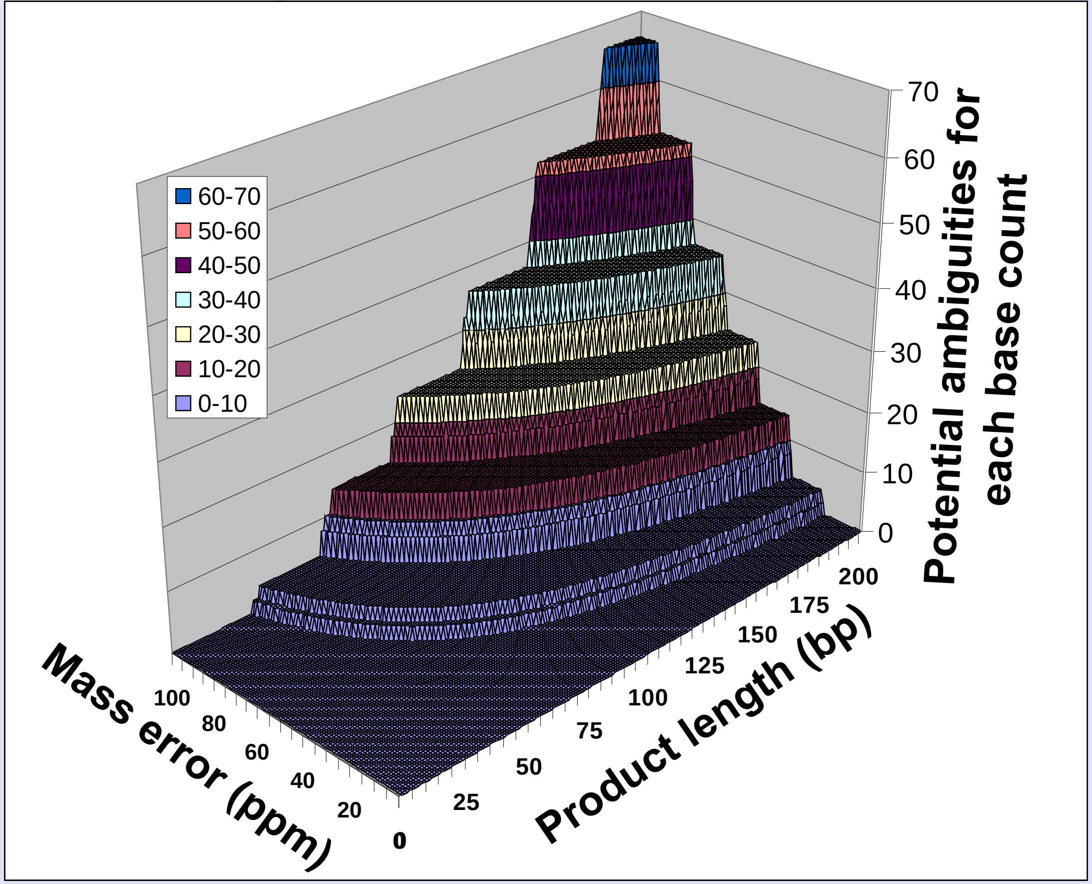


IMAGE COURTESY OF TOM HALL, PH.D.

What Does Mass Tagging Mean?

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

🟨 **Working range for TOF (<20 ppm)**

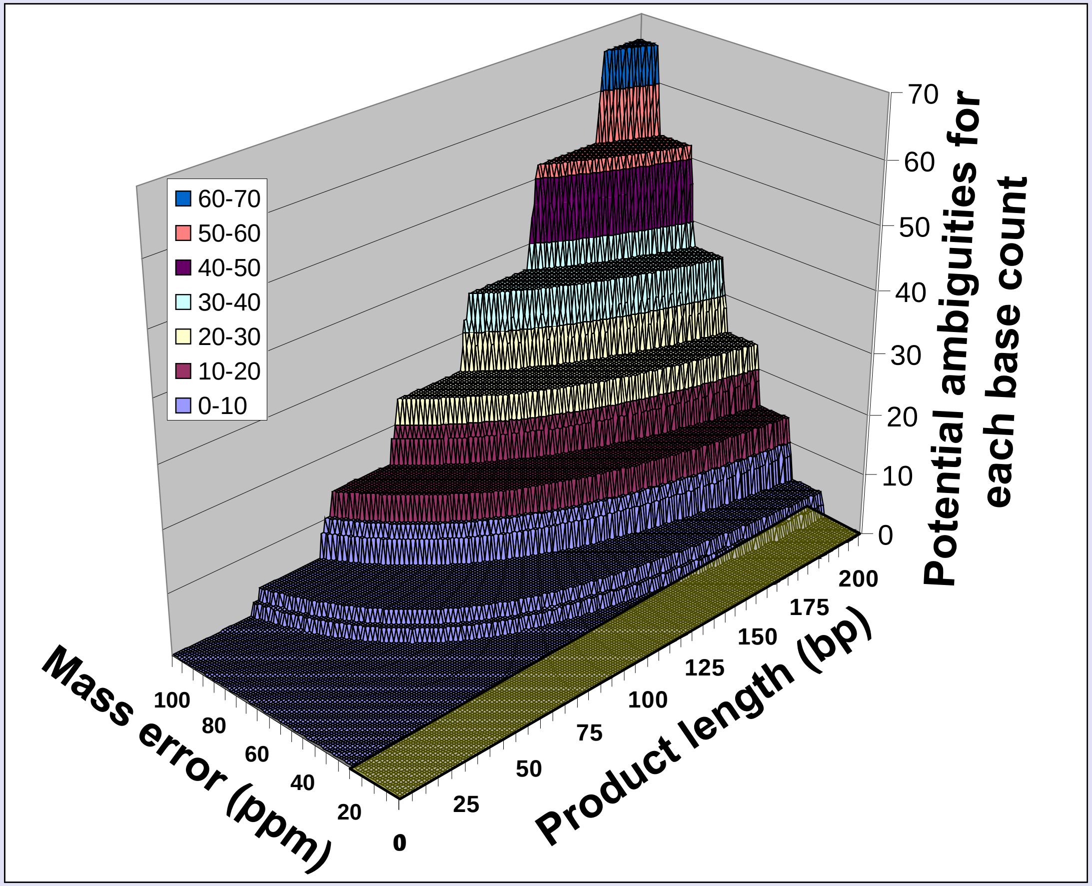


IMAGE COURTESY OF TOM HALL, PH.D.

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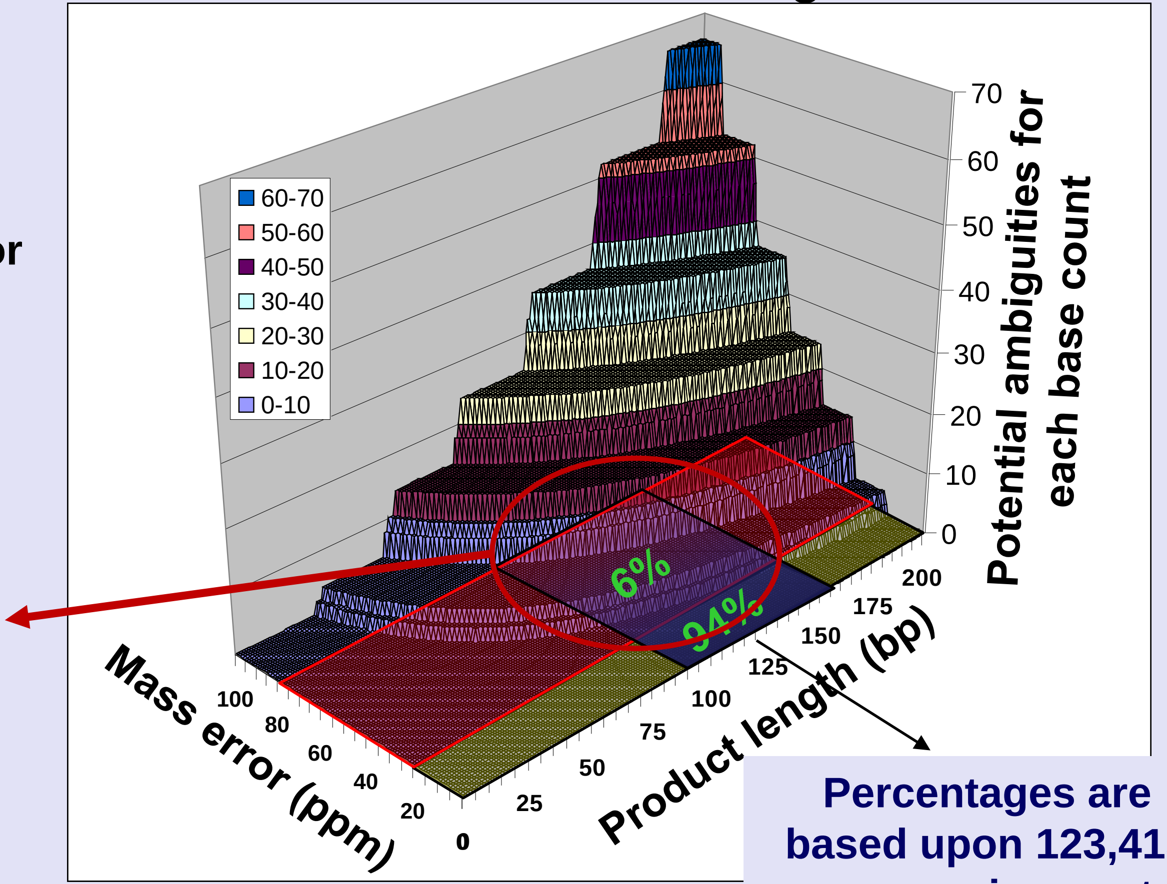
What Does Mass Tagging Mean?

Most **assignments would be fine with natural nucleotides.**

Some **assignments fall outside of “normal” range.**

🟨 **Working range for TOF (<20 ppm)**



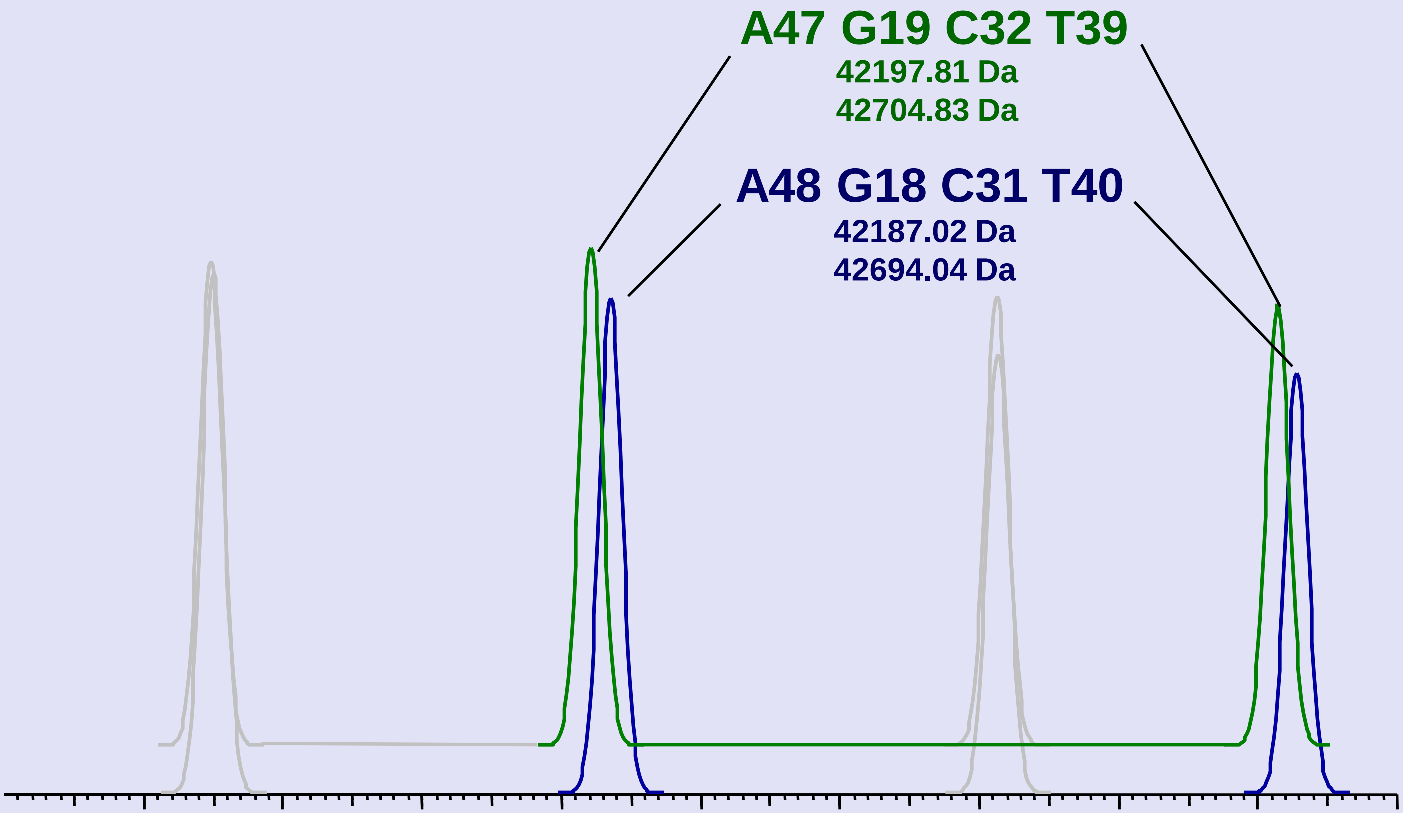
Which 6% of measurements are a problem?

Percentages are based upon 123,415 mass assignments

IMAGE COURTESY OF TOM HALL, PH.D.

Mass Tag Changes Rules

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).



A47 G19 C32 T39
42197.81 Da
42704.83 Da

A48 G18 C31 T40
42187.02 Da
42694.04 Da

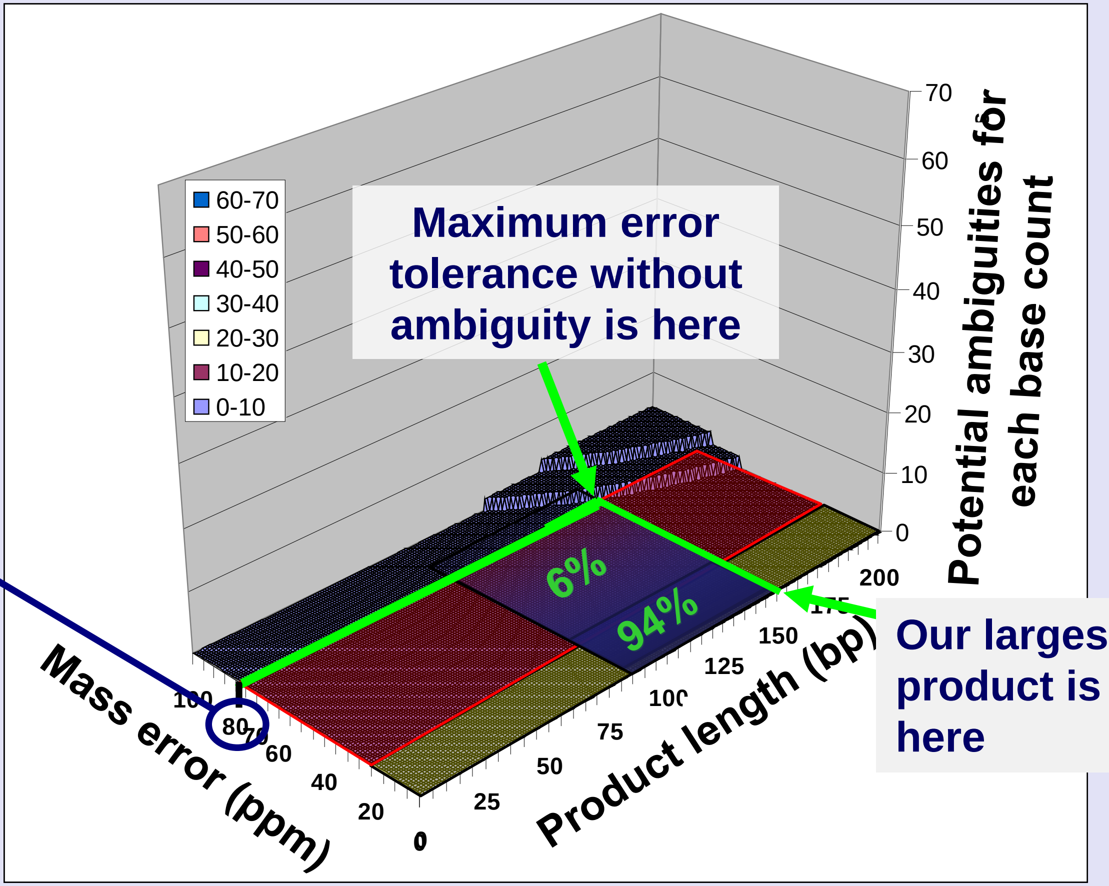
IMAGE COURTESY OF TOM HALL, PH.D.

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**



Maximum error tolerance without ambiguity is here

Our largest product is here

IMAGE COURTESY OF TOM HALL, PH.D.

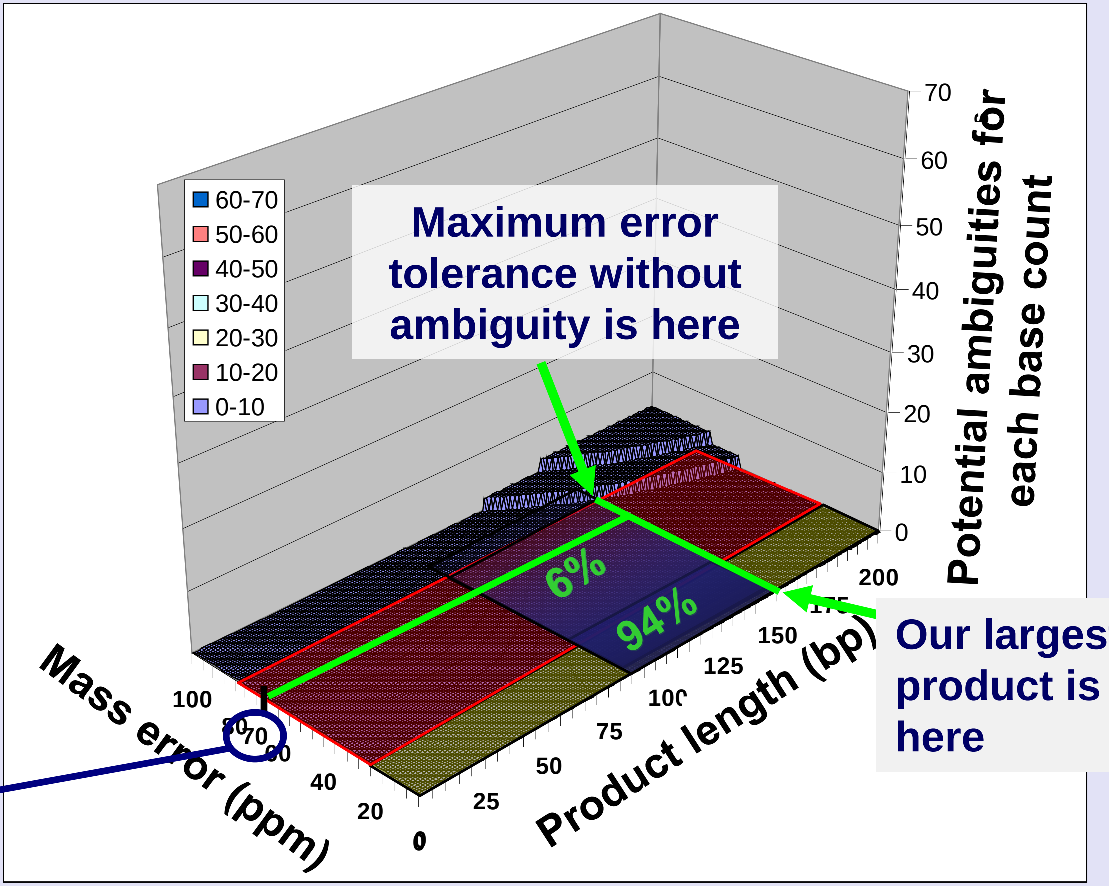
What Does Mass Tagging Mean?

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



Maximum error tolerance without ambiguity is here

Our largest product is here

IMAGE COURTESY OF TOM HALL, PH.D.

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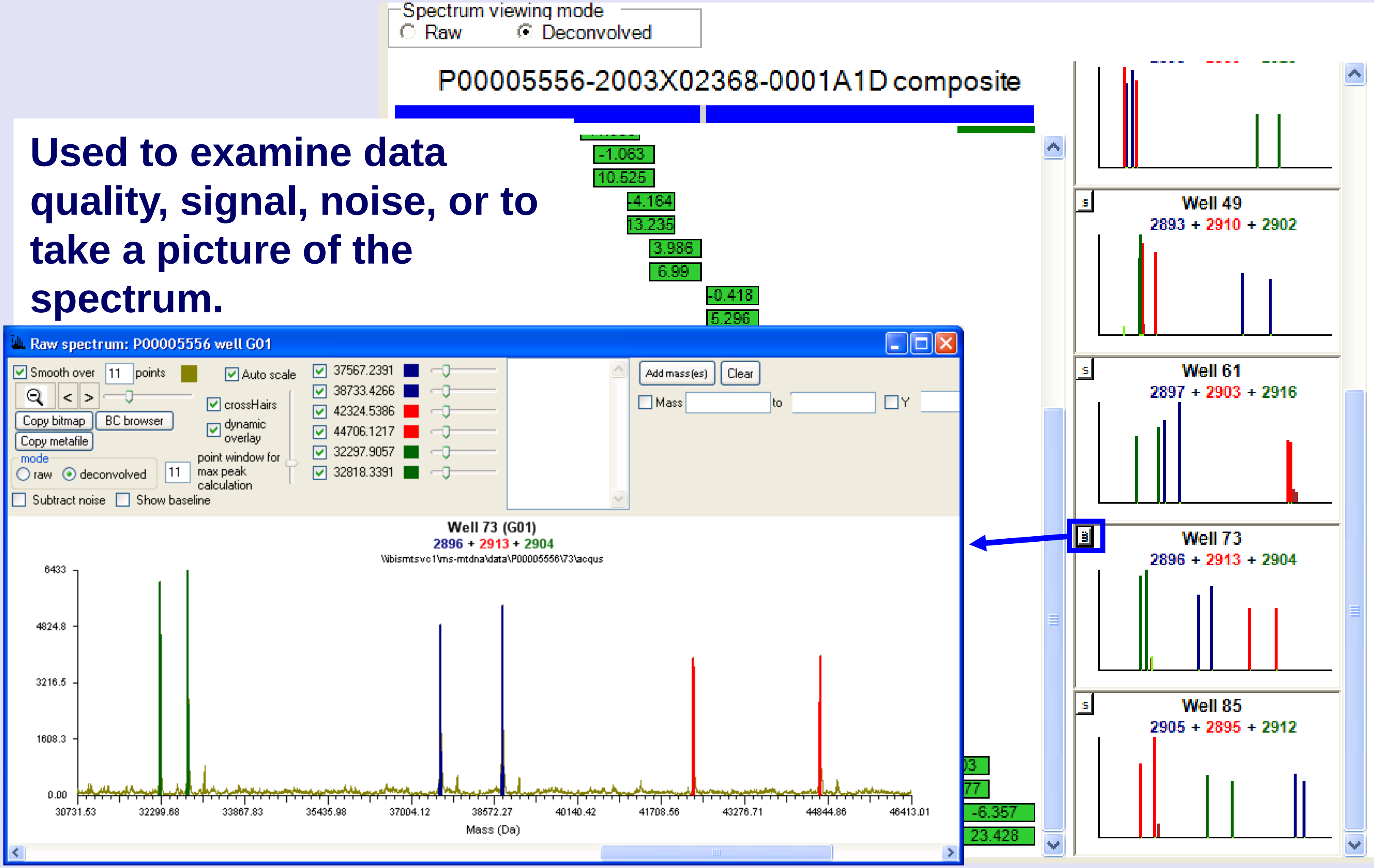
Spectral Viewer

IMAGE COURTESY OF TOM HALL, PH.D.

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



Spectrum viewing mode: ○ Raw ● Deconvolved

P00005556-2003X02368-0001A1D composite

Raw spectrum: P00005556 well G01

☑ Smooth over 11 points

☑ Auto scale

☑ crossHairs

☑ dynamic overlay

mode: ○ raw ● deconvolved

11 point window for max peak calculation

☐ Subtract noise ☐ Show baseline

☑ 37567.2391 🟦

☑ 38733.4266 🟦

☑ 42324.5386 🟥

☑ 44706.1217 🟥

☑ 32297.9057 🟩

☑ 32818.3391 🟩

☐ Mass ___ to ___ ☐ Y

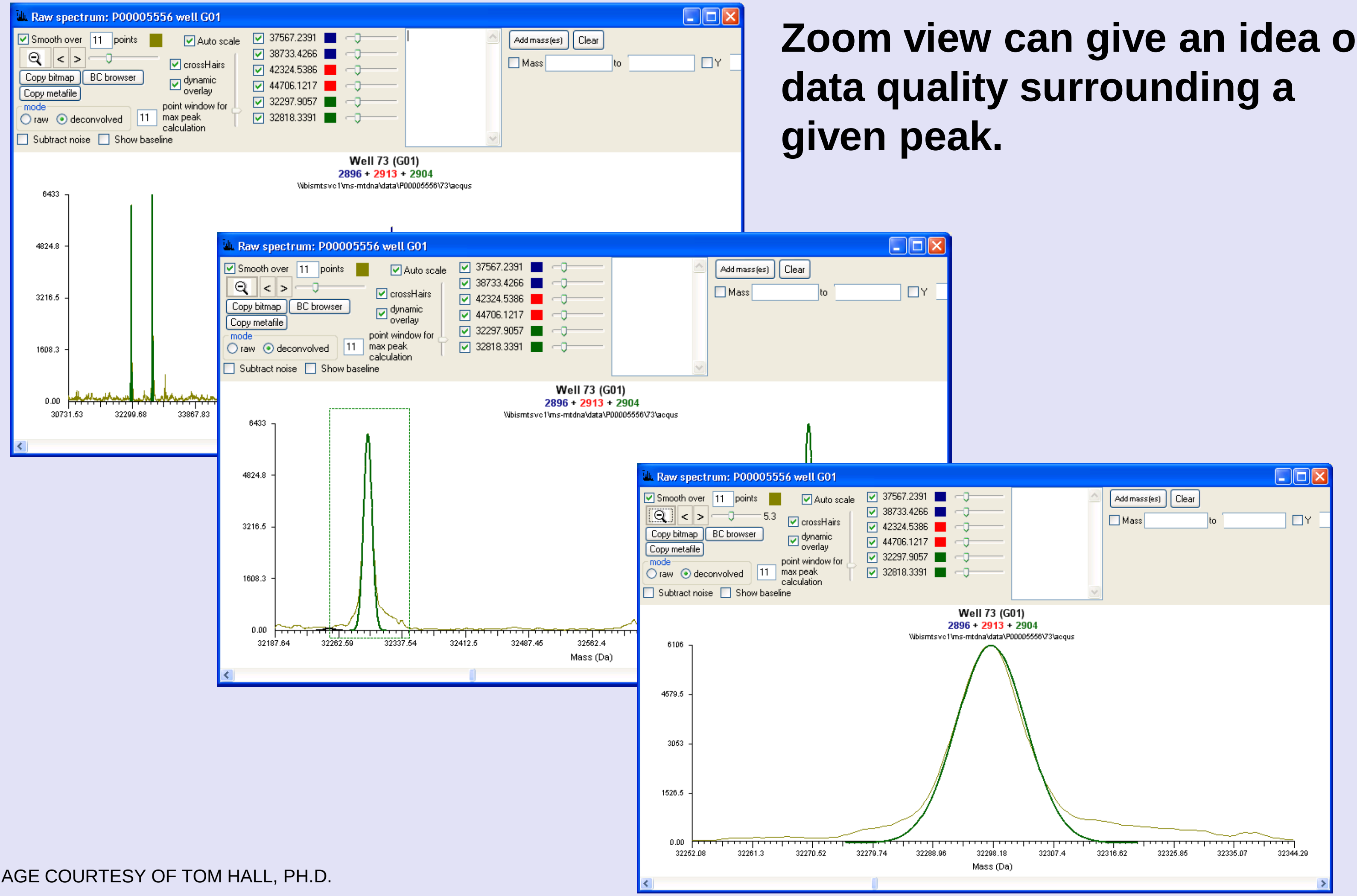
Well 73 (G01)

2896 + 2913 + 2904

\\bismtsvc1\ms-mtdna\data\P00005556\73\acqus

Technology Transition Workshop

Spectral Viewer - Deconvolved



Raw spectrum: P00005556 well G01

☑ Smooth over 11 points

☑ Auto scale

☑ crossHairs

☑ dynamic overlay

mode ○ raw ● deconvolved

11 point window for max peak calculation

☐ Subtract noise ☐ Show baseline

☑	37567.2391	🟦
☑	38733.4266	🟦
☑	42324.5386	🟥
☑	44706.1217	🟥
☑	32297.9057	🟩
☑	32818.3391	🟩

☐ Mass to ☐ Y

Well 73 (G01)

2896 + 2913 + 2904

\\bismtsvc1\ms-mtdna\data\P00005556\73\acqus

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

IMAGE COURTESY OF TOM HALL, PH.D.

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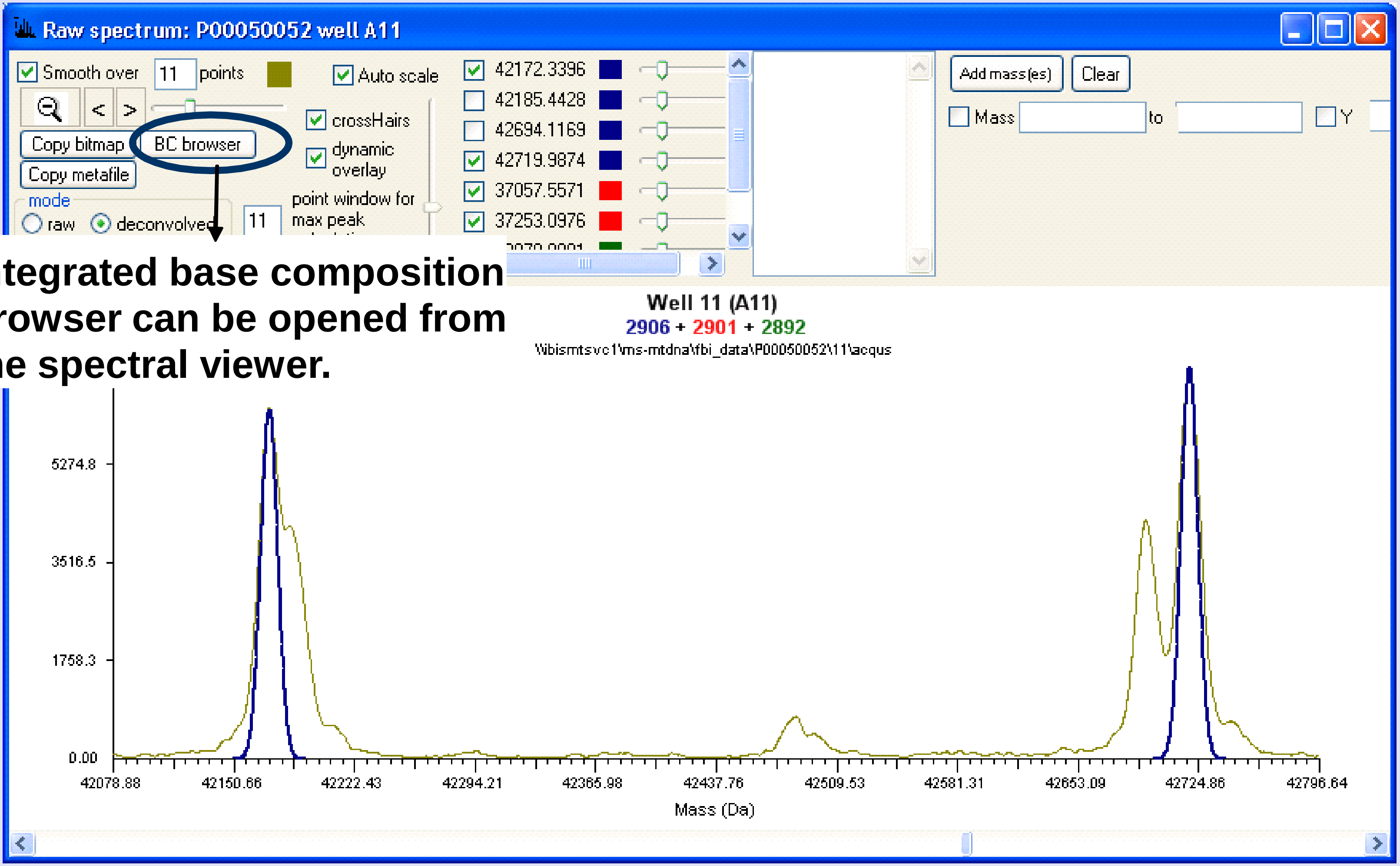
Base Composition Browser

IMAGE COURTESY OF TOM HALL, PH.D.



Raw spectrum: P00050052 well A11

☑ Smooth over 11 points

☑ Auto scale

☑ crossHairs

☑ dynamic overlay

point window for max peak 11

mode ○ raw ● deconvolved

☑ 42172.3396 🟦
☐ 42185.4428 🟦
☐ 42694.1169 🟦
☑ 42719.9874 🟦
☑ 37057.5571 🟥
☑ 37253.0976 🟥

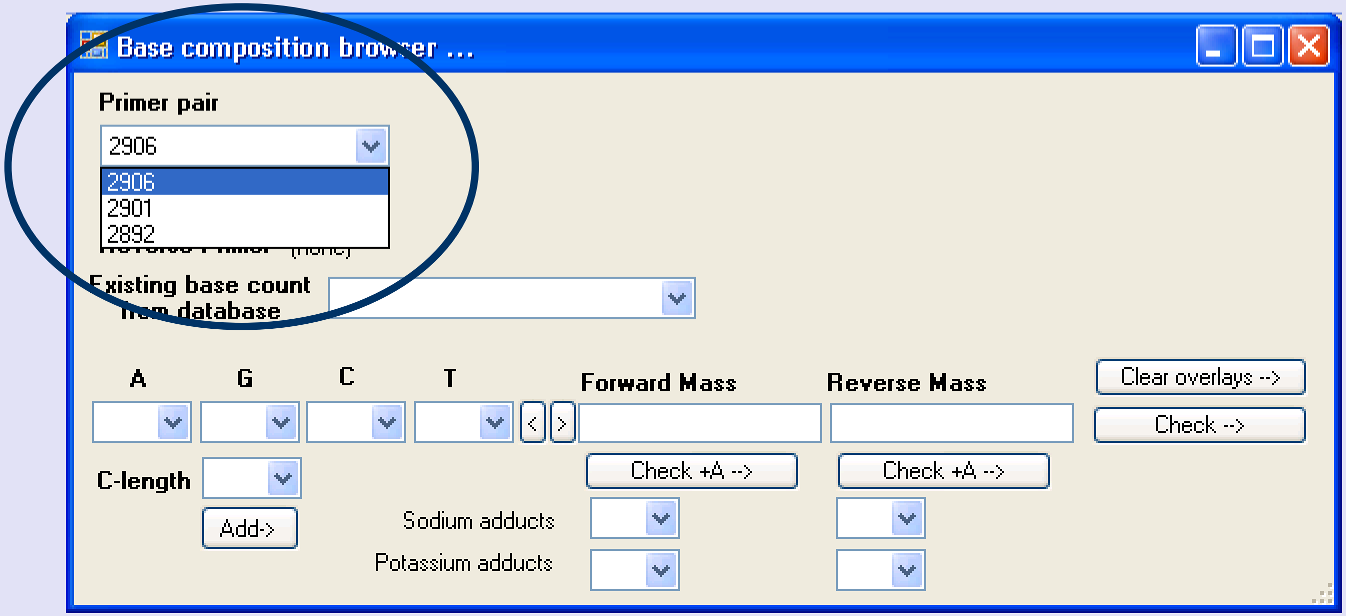
☐ Mass to ☐ Y

Well 11 (A11)
2906 + 2901 + 2892
\\bismtsvc1\ms-mtdna\fbi_data\P00050052\11\acqus

Integrated base composition browser can be opened from the spectral viewer.

Base Composition Browser

Primer pairs in current well are integrated to this view.



Primer pair: 2906

2906
2901
2892

Reverse Primer (none)

IMAGE COURTESY OF TOM HALL, PH.D.

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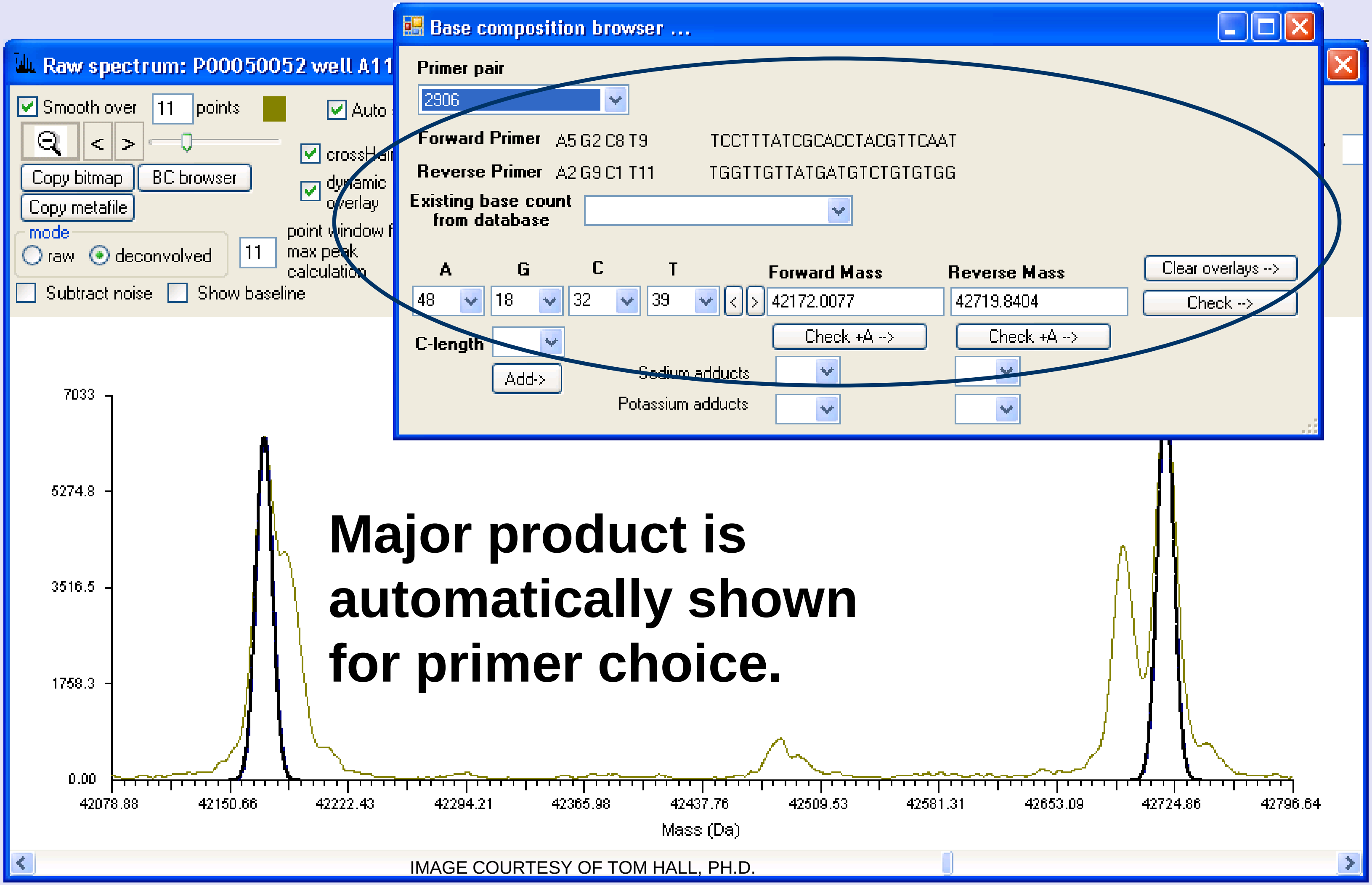
Base Composition Browser



Raw spectrum: P00050052 well A11

☑ Smooth over 11 points

☑ Auto

☑ crossHair

☑ dynamic overlay

mode ○ raw ● deconvolved

11 point window for max peak calculation

☐ Subtract noise ☐ Show baseline

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	32	39	42172.0077	42719.8404

C-length

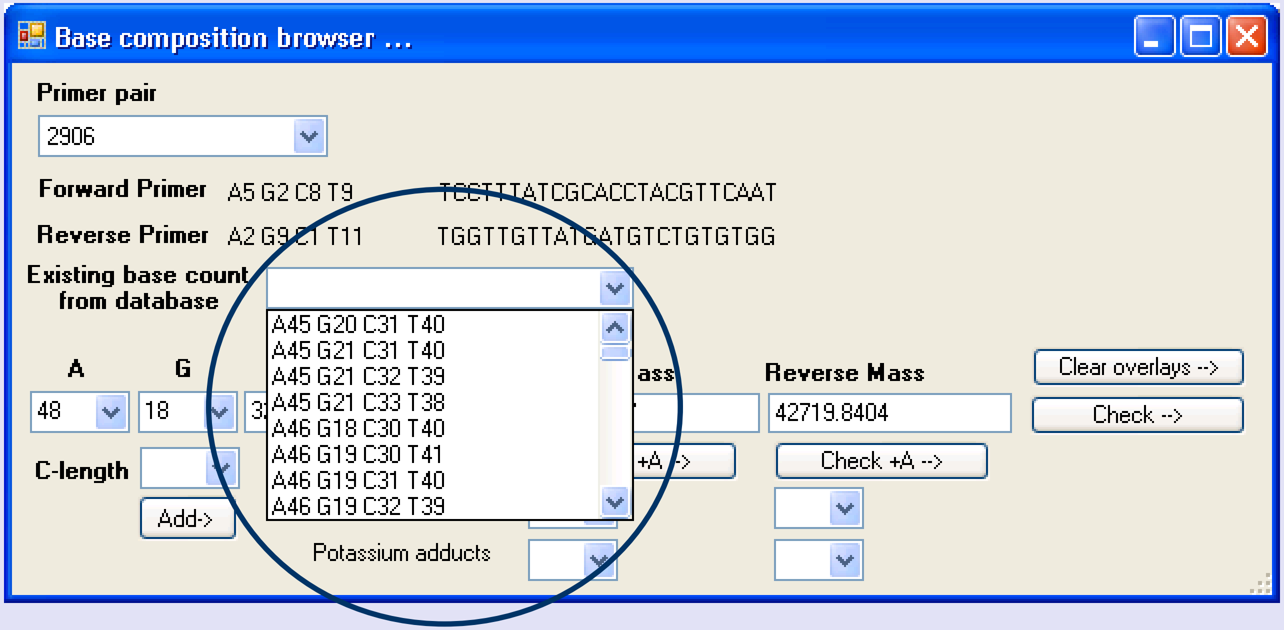
Sodium adducts

Potassium adducts

Major product is automatically shown for primer choice.

IMAGE COURTESY OF TOM HALL, PH.D.

Technology Transition Workshop
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

A45 G20 C31 T40
A45 G21 C31 T40
A45 G21 C32 T39
A45 G21 C33 T38
A46 G18 C30 T40
A46 G19 C30 T41
A46 G19 C31 T40
A46 G19 C32 T39

A: 48

G: 18

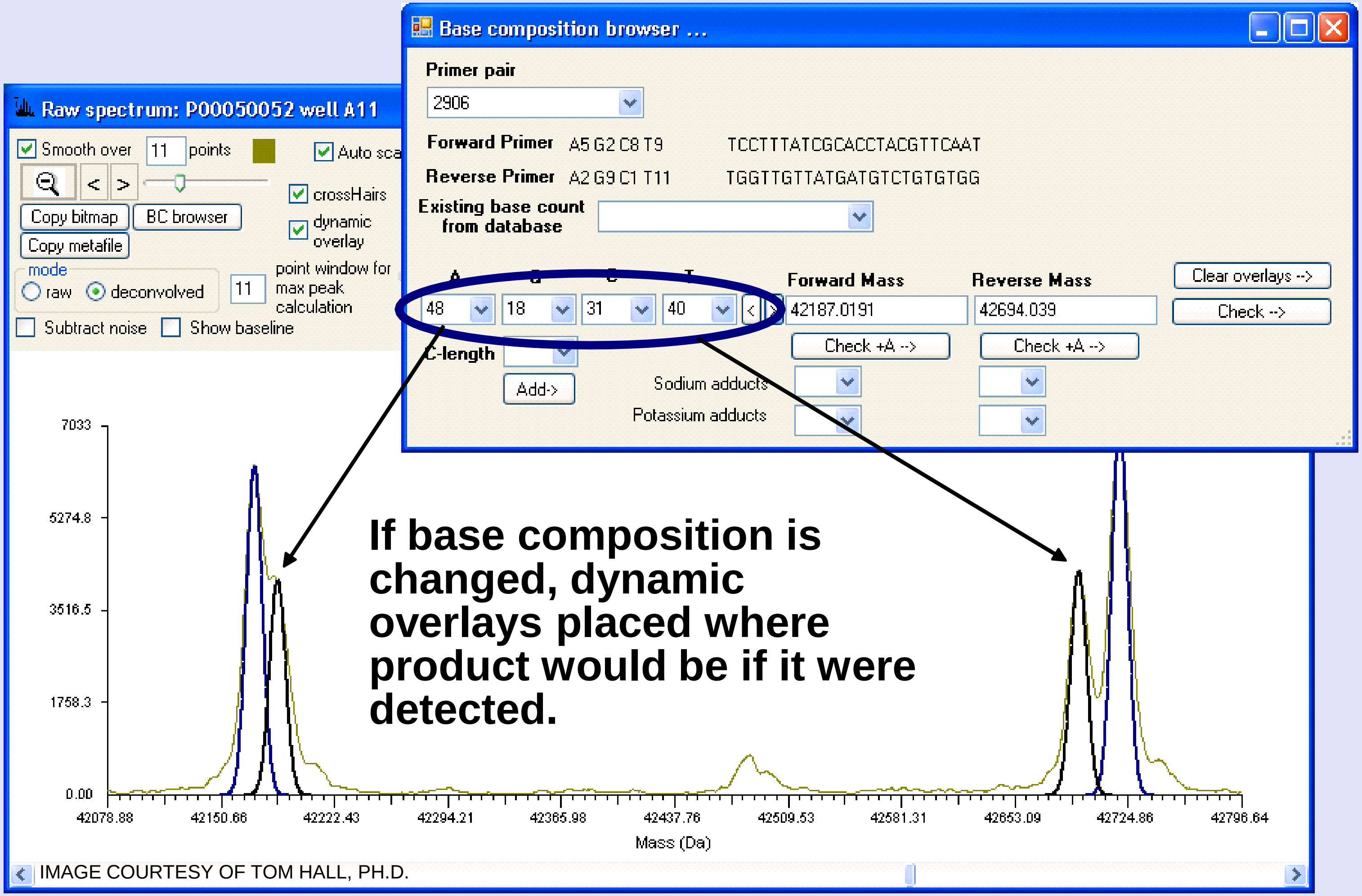
Reverse Mass: 42719.8404

Potassium adducts

All known products for selected primer pair are in this list.

IMAGE COURTESY OF TOM HALL, PH.D.

Base Composition Browser



Raw spectrum: P00050052 well A11

☑ Smooth over 11 points

☑ Auto sca

☑ crossHairs

☑ dynamic overlay

mode ○ raw ● deconvolved

11 point window for max peak calculation

☐ Subtract noise ☐ Show baseline

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	42187.0191	42694.039

If base composition is changed, dynamic overlays placed where product would be if it were detected.

IMAGE COURTESY OF TOM HALL, PH.D.

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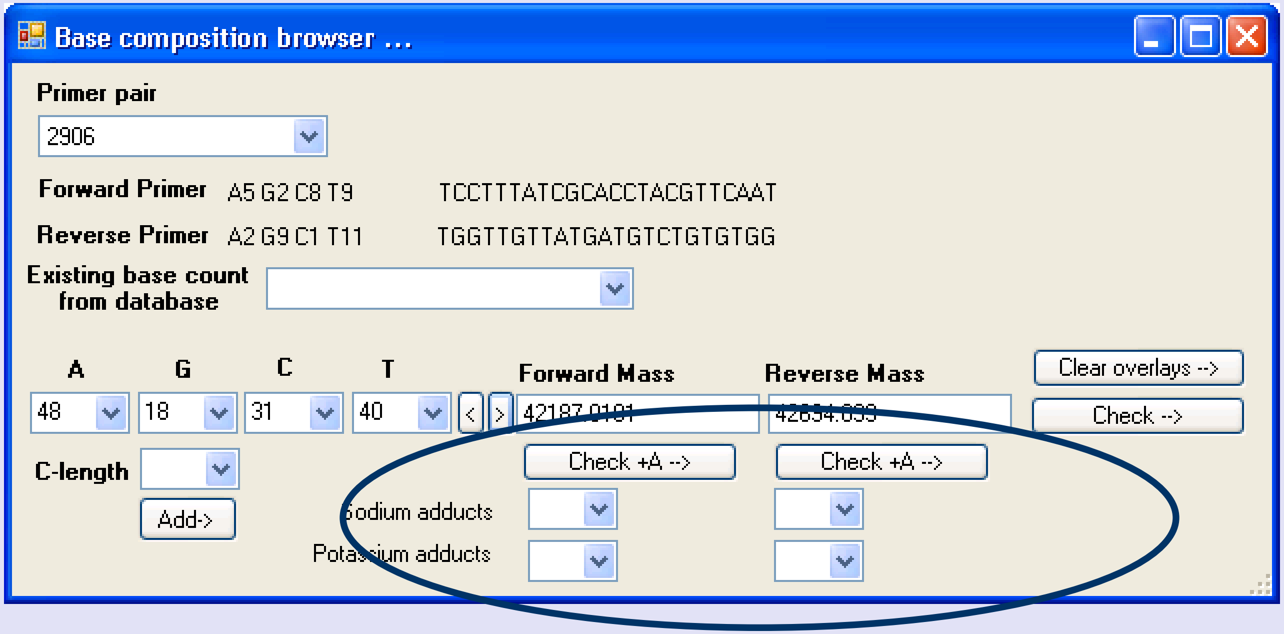
Base Composition Browser



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	42187.0101	42654.039

C-length

Sodium adducts

Potassium adducts

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

IMAGE COURTESY OF TOM HALL, PH.D.

Compare Sample to Database

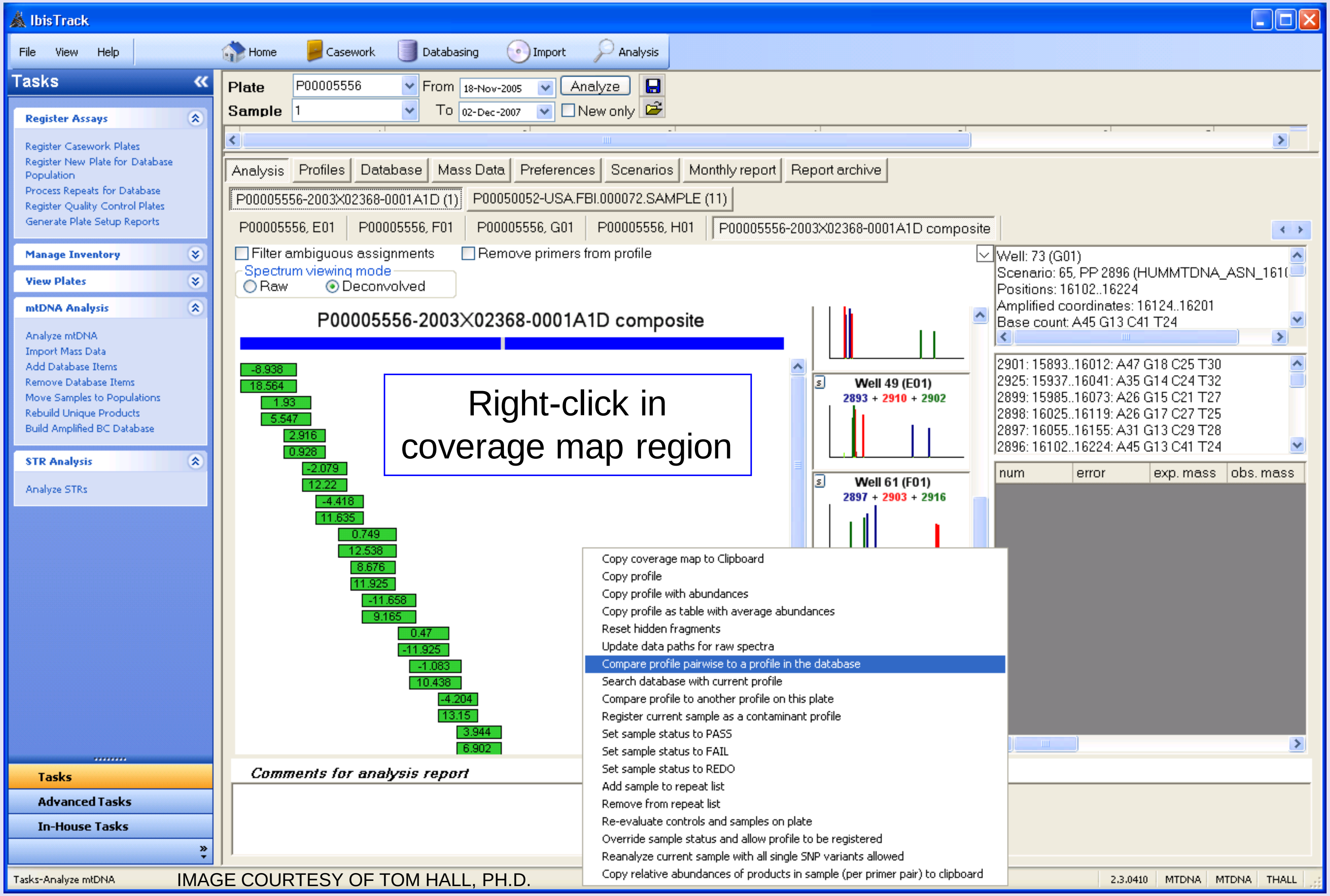


Plate P00005556 From 18-Nov-2005

Sample 1 To 02-Dec-2007 ☐ New only

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

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

☐ Filter ambiguous assignments ☐ Remove primers from profile

Spectrum viewing mode: ○ Raw ● Deconvolved

P00005556-2003X02368-0001A1D composite

Well 49 (E01) 2893 + 2910 + 2902

Well 61 (F01) 2897 + 2903 + 2916

Well: 73 (G01)
Scenario: 65, PP 2896 (HUMMTDNA_ASN_161
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 T25
2897: 16055..16155: A31 G13 C29 T28
2896: 16102..16224: A45 G13 C41 T24

Tasks-Analyze mtDNA 2.3.0410 MTDNA MTDNA THALL

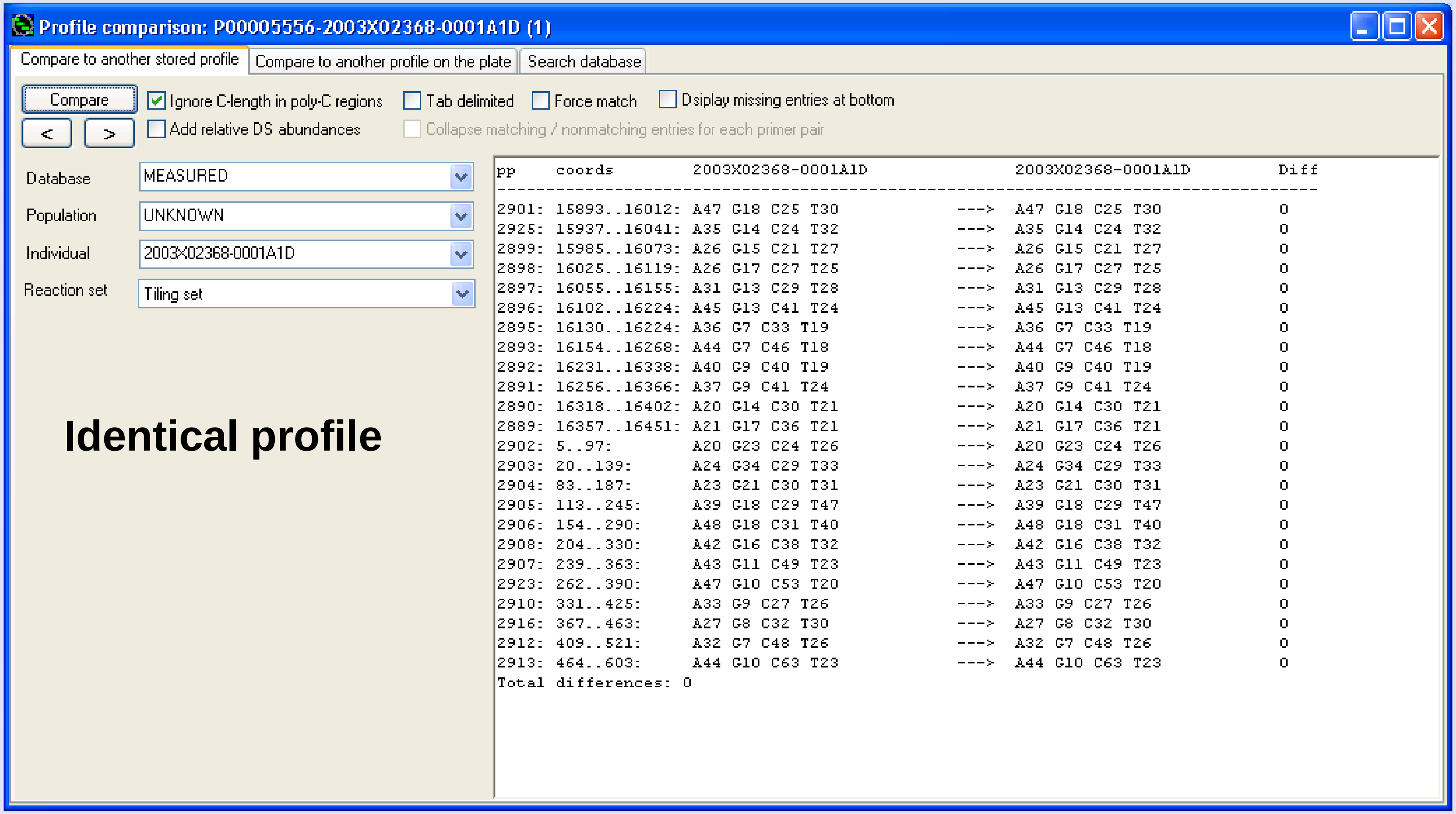
Right-click in coverage map region

IMAGE COURTESY OF TOM HALL, PH.D.

Technology Transition Workshop

Compare Sample to Database

Side-by-side profile comparison shown product-by-product differences between two profiles.



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

☑ Ignore C-length in poly-C regions
☐ Tab delimited
☐ Force match
☐ Dsiplay missing entries at bottom
☐ Add relative DS abundances
☐ Collapse matching / nonmatching entries for each primer pair

Database: MEASURED
Population: UNKNOWN
Individual: 2003X02368-0001A1D
Reaction set: Tiling set

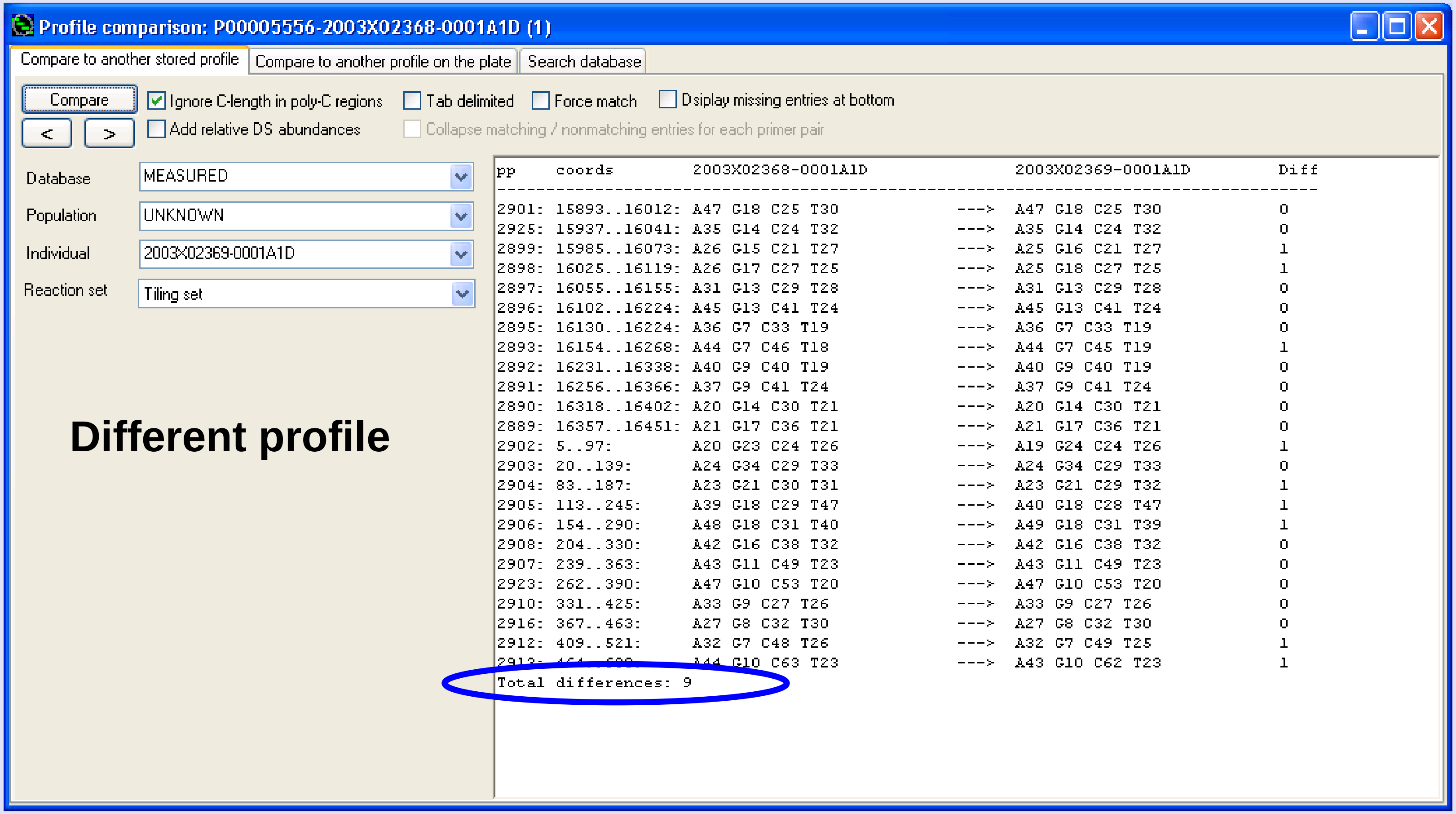
```
pp    coords        2003X02368-0001A1D               2003X02368-0001A1D         Diff
------------------------------------------------------------------------------------
2901: 15893..16012: A47 G18 C25 T30            --->  A47 G18 C25 T30            0
2925: 15937..16041: A35 G14 C24 T32            --->  A35 G14 C24 T32            0
2899: 15985..16073: A26 G15 C21 T27            --->  A26 G15 C21 T27            0
2898: 16025..16119: A26 G17 C27 T25            --->  A26 G17 C27 T25            0
2897: 16055..16155: A31 G13 C29 T28            --->  A31 G13 C29 T28            0
2896: 16102..16224: A45 G13 C41 T24            --->  A45 G13 C41 T24            0
2895: 16130..16224: A36 G7 C33 T19             --->  A36 G7 C33 T19             0
2893: 16154..16268: A44 G7 C46 T18             --->  A44 G7 C46 T18             0
2892: 16231..16338: A40 G9 C40 T19             --->  A40 G9 C40 T19             0
2891: 16256..16366: A37 G9 C41 T24             --->  A37 G9 C41 T24             0
2890: 16318..16402: A20 G14 C30 T21            --->  A20 G14 C30 T21            0
2889: 16357..16451: A21 G17 C36 T21            --->  A21 G17 C36 T21            0
2902: 5..97:        A20 G23 C24 T26            --->  A20 G23 C24 T26            0
2903: 20..139:      A24 G34 C29 T33            --->  A24 G34 C29 T33            0
2904: 83..187:      A23 G21 C30 T31            --->  A23 G21 C30 T31            0
2905: 113..245:     A39 G18 C29 T47            --->  A39 G18 C29 T47            0
2906: 154..290:     A48 G18 C31 T40            --->  A48 G18 C31 T40            0
2908: 204..330:     A42 G16 C38 T32            --->  A42 G16 C38 T32            0
2907: 239..363:     A43 G11 C49 T23            --->  A43 G11 C49 T23            0
2923: 262..390:     A47 G10 C53 T20            --->  A47 G10 C53 T20            0
2910: 331..425:     A33 G9 C27 T26             --->  A33 G9 C27 T26             0
2916: 367..463:     A27 G8 C32 T30             --->  A27 G8 C32 T30             0
2912: 409..521:     A32 G7 C48 T26             --->  A32 G7 C48 T26             0
2913: 464..603:     A44 G10 C63 T23            --->  A44 G10 C63 T23            0
Total differences: 0
```

Identical profile

IMAGE COURTESY OF TOM HALL, PH.D.

Compare Sample to Database

Side-by-side profile comparison shown product-by-product differences between two profiles.



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

☑ Ignore C-length in poly-C regions
☐ Tab delimited
☐ Force match
☐ Dsiplay missing entries at bottom
☐ Add relative DS abundances
☐ Collapse matching / nonmatching entries for each primer pair

Database: MEASURED
Population: UNKNOWN
Individual: 2003X02369-0001A1D
Reaction set: Tiling set

Different profile

```
pp    coords         2003X02368-0001A1D                2003X02369-0001A1D          Diff
-----------------------------------------------------------------------------------------
2901: 15893..16012: A47 G18 C25 T30           --->  A47 G18 C25 T30             0
2925: 15937..16041: A35 G14 C24 T32           --->  A35 G14 C24 T32             0
2899: 15985..16073: A26 G15 C21 T27           --->  A25 G16 C21 T27             1
2898: 16025..16119: A26 G17 C27 T25           --->  A25 G18 C27 T25             1
2897: 16055..16155: A31 G13 C29 T28           --->  A31 G13 C29 T28             0
2896: 16102..16224: A45 G13 C41 T24           --->  A45 G13 C41 T24             0
2895: 16130..16224: A36 G7 C33 T19            --->  A36 G7 C33 T19              0
2893: 16154..16268: A44 G7 C46 T18            --->  A44 G7 C45 T19              1
2892: 16231..16338: A40 G9 C40 T19            --->  A40 G9 C40 T19              0
2891: 16256..16366: A37 G9 C41 T24            --->  A37 G9 C41 T24              0
2890: 16318..16402: A20 G14 C30 T21           --->  A20 G14 C30 T21             0
2889: 16357..16451: A21 G17 C36 T21           --->  A21 G17 C36 T21             0
2902: 5..97:        A20 G23 C24 T26           --->  A19 G24 C24 T26             1
2903: 20..139:      A24 G34 C29 T33           --->  A24 G34 C29 T33             0
2904: 83..187:      A23 G21 C30 T31           --->  A23 G21 C29 T32             1
2905: 113..245:     A39 G18 C29 T47           --->  A40 G18 C28 T47             1
2906: 154..290:     A48 G18 C31 T40           --->  A49 G18 C31 T39             1
2908: 204..330:     A42 G16 C38 T32           --->  A42 G16 C38 T32             0
2907: 239..363:     A43 G11 C49 T23           --->  A43 G11 C49 T23             0
2923: 262..390:     A47 G10 C53 T20           --->  A47 G10 C53 T20             0
2910: 331..425:     A33 G9 C27 T26            --->  A33 G9 C27 T26              0
2916: 367..463:     A27 G8 C32 T30            --->  A27 G8 C32 T30              0
2912: 409..521:     A32 G7 C48 T26            --->  A32 G7 C49 T25              1
2913: 464..60[illegible]: A44 G10 C63 T23     --->  A43 G10 C62 T23             1
Total differences: 9
```

IMAGE COURTESY OF TOM HALL, PH.D.

NIJ National Institute of Justice

Technology Transition Workshop

Search Database

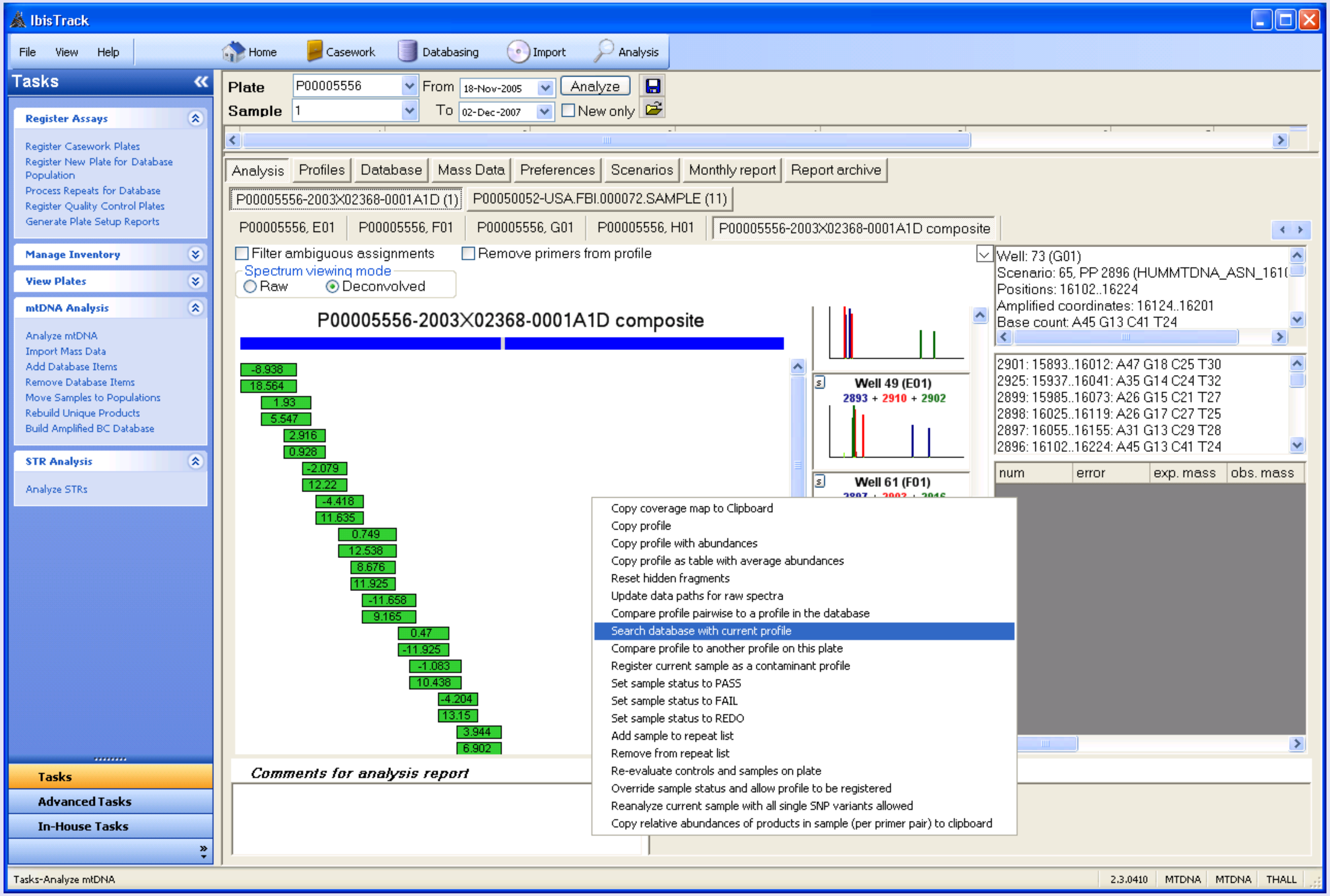


Plate P00005556
Sample 1
From 18-Nov-2005
To 02-Dec-2007
☐ New only

☐ Filter ambiguous assignments
☐ Remove primers from profile

Spectrum viewing mode: ○ Raw ● Deconvolved

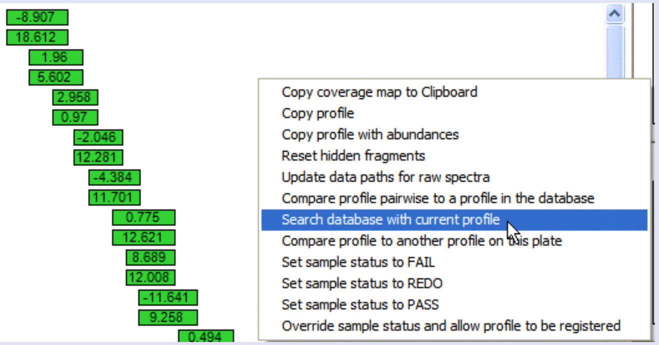
Well: 73 (G01)
Scenario: 65, PP 2896 (HUMMTDNA_ASN_161
Positions: 16102..16224
Amplified coordinates: 16124..16201
Base count: A45 G13 C41 T24

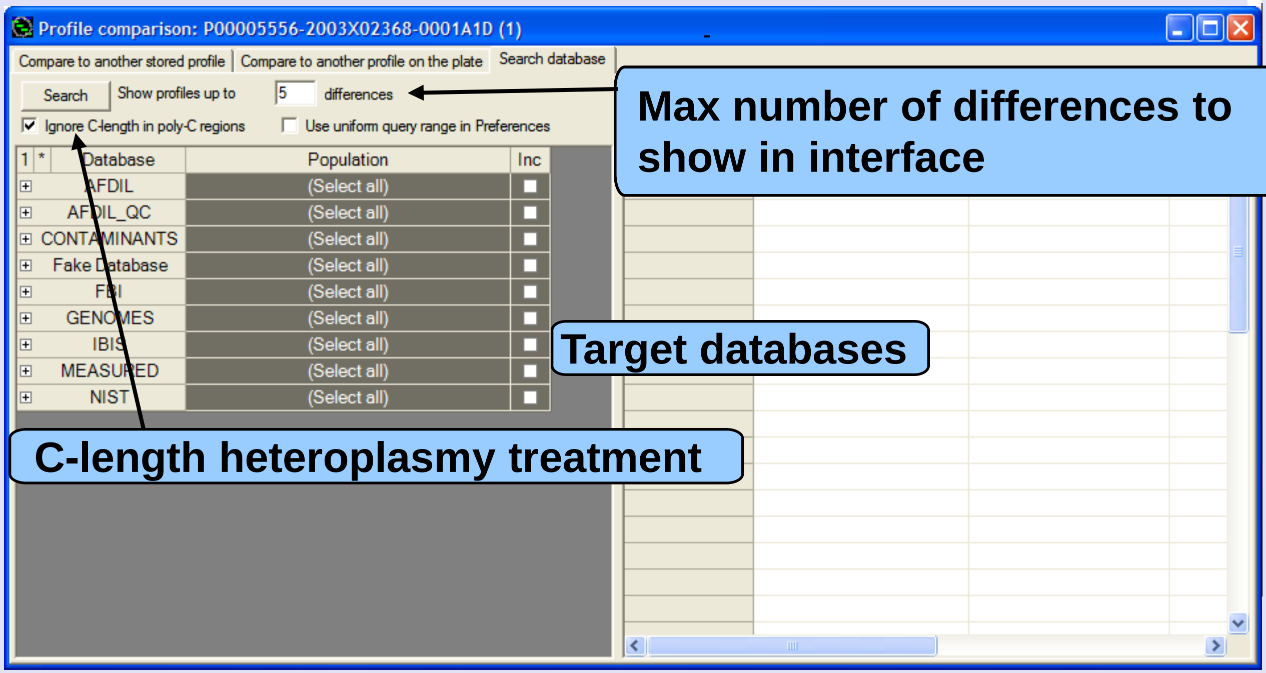
2901: 15893..16012: A47 G18 C25 T30
2925: 15937..16041: A35 G14 C24 T32
2899: 15985..16073: A26 G15 C21 T27
2898: 16025..16119: A26 G17 C27 T25
2897: 16055..16155: A31 G13 C29 T28
2896: 16102..16224: A45 G13 C41 T24

Tasks-Analyze mtDNA | 2.3.0410 | MTDNA | MTDNA | THALL

IMAGE COURTESY OF TOM HALL, PH.D.

Search Database





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)	☐
AFDIL_QC	(Select all)	☐
CONTAMINANTS	(Select all)	☐
Fake Database	(Select all)	☐
FBI	(Select all)	☐
GENOMES	(Select all)	☐
IBIS	(Select all)	☐
MEASURED	(Select all)	☐
NIST	(Select all)	☐

Max number of differences to show in interface

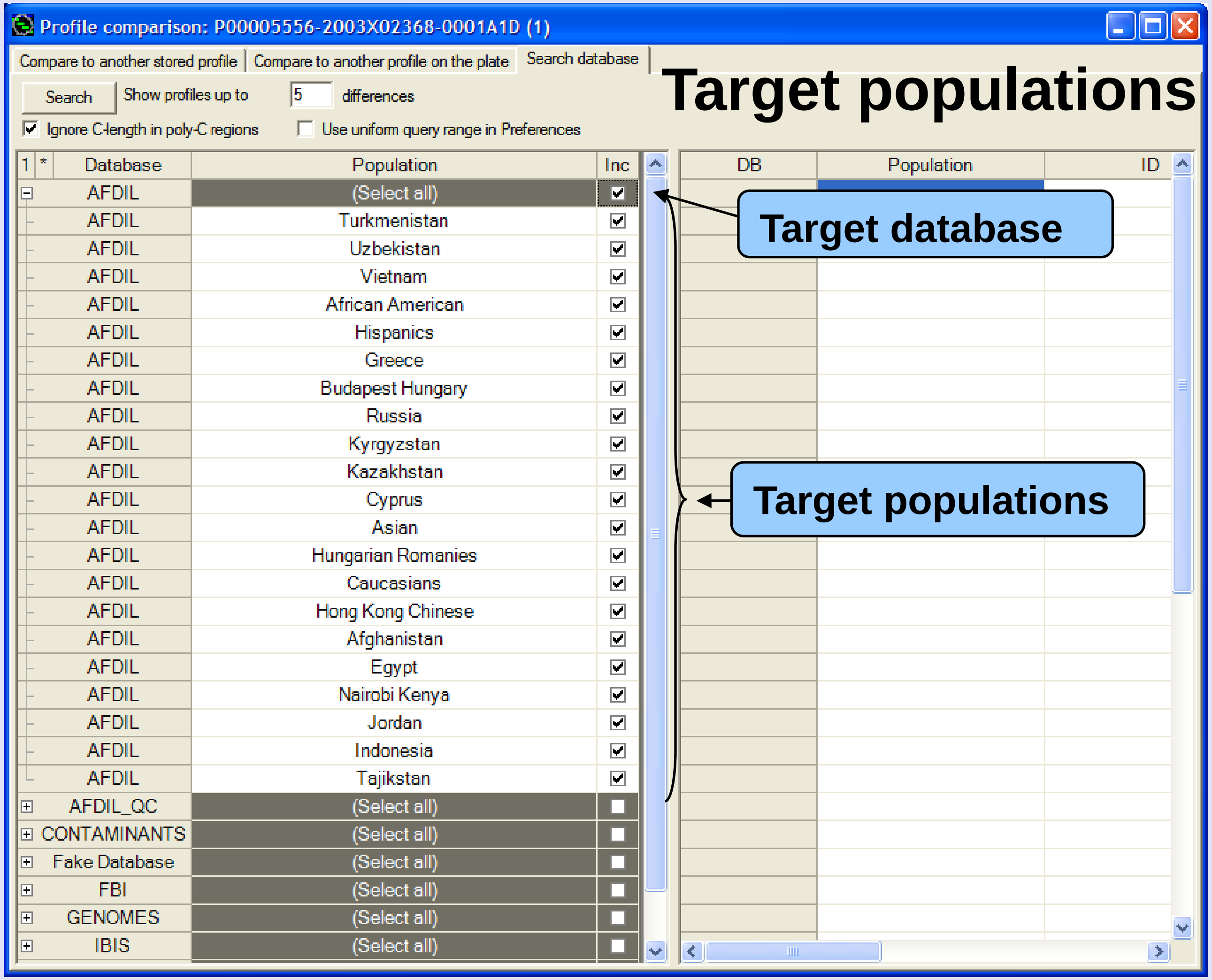
Target databases

C-length heteroplasmy treatment

IMAGE COURTESY
OF TOM HALL, PH.D.

Search Database

Target populations choice



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

Show profiles up to 5 differences

☑ Ignore C-length in poly-C regions

☐ Use uniform query range in Preferences

1	*	Database	Population	Inc
⊟		AFDIL	(Select all)	☑
		AFDIL	Turkmenistan	☑
		AFDIL	Uzbekistan	☑
		AFDIL	Vietnam	☑
		AFDIL	African American	☑
		AFDIL	Hispanics	☑
		AFDIL	Greece	☑
		AFDIL	Budapest Hungary	☑
		AFDIL	Russia	☑
		AFDIL	Kyrgyzstan	☑
		AFDIL	Kazakhstan	☑
		AFDIL	Cyprus	☑
		AFDIL	Asian	☑
		AFDIL	Hungarian Romanies	☑
		AFDIL	Caucasians	☑
		AFDIL	Hong Kong Chinese	☑
		AFDIL	Afghanistan	☑
		AFDIL	Egypt	☑
		AFDIL	Nairobi Kenya	☑
		AFDIL	Jordan	☑
		AFDIL	Indonesia	☑
		AFDIL	Tajikstan	☑
⊞		AFDIL_QC	(Select all)	☐
⊞		CONTAMINANTS	(Select all)	☐
⊞		Fake Database	(Select all)	☐
⊞		FBI	(Select all)	☐
⊞		GENOMES	(Select all)	☐
⊞		IBIS	(Select all)	☐

DB	Population	ID

Target database

Target populations

IMAGE COURTESY
OF TOM HALL, PH.D.

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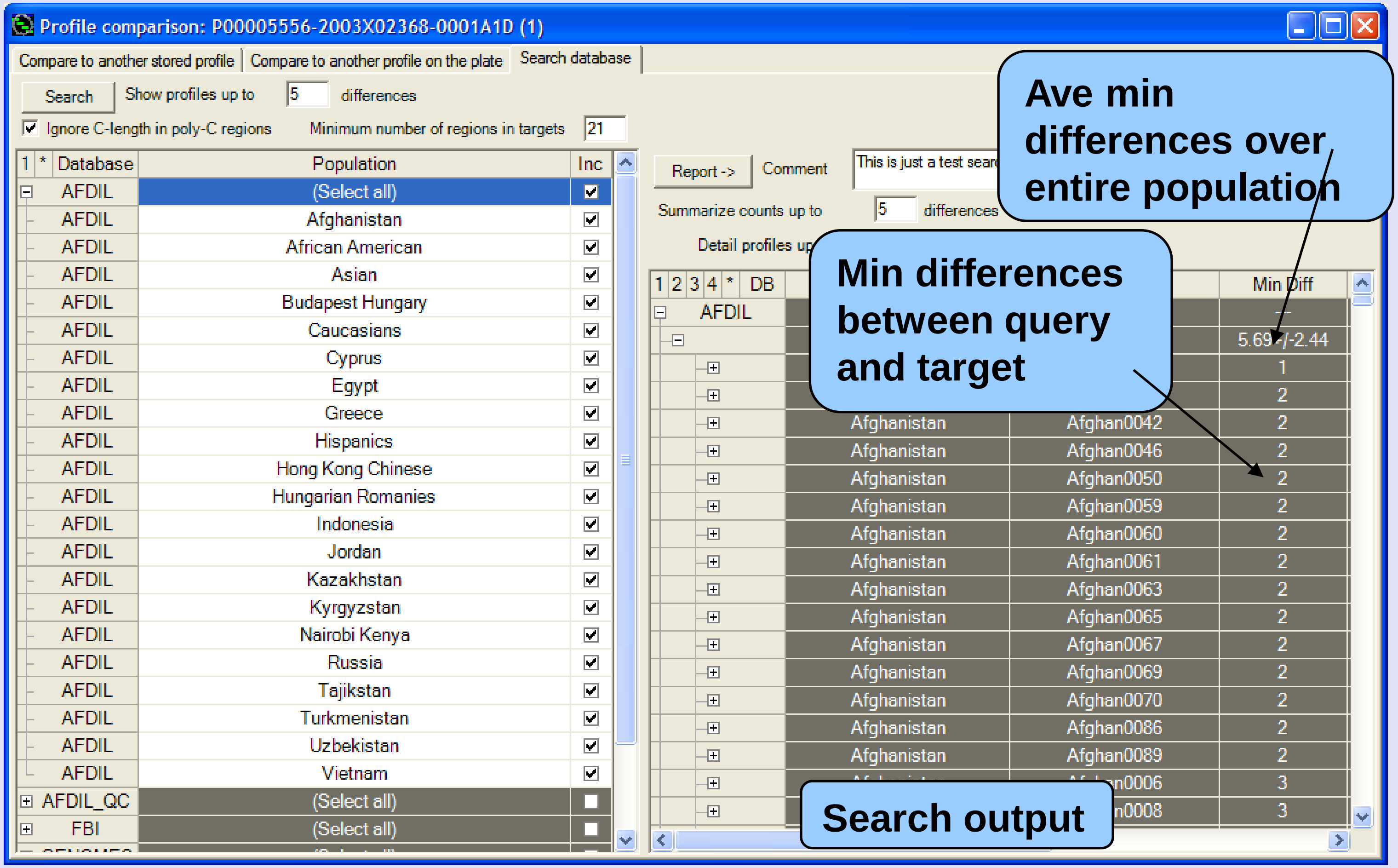
Search Database



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

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)	☑
		AFDIL	Afghanistan	☑
		AFDIL	African American	☑
		AFDIL	Asian	☑
		AFDIL	Budapest Hungary	☑
		AFDIL	Caucasians	☑
		AFDIL	Cyprus	☑
		AFDIL	Egypt	☑
		AFDIL	Greece	☑
		AFDIL	Hispanics	☑
		AFDIL	Hong Kong Chinese	☑
		AFDIL	Hungarian Romanies	☑
		AFDIL	Indonesia	☑
		AFDIL	Jordan	☑
		AFDIL	Kazakhstan	☑
		AFDIL	Kyrgyzstan	☑
		AFDIL	Nairobi Kenya	☑
		AFDIL	Russia	☑
		AFDIL	Tajikstan	☑
		AFDIL	Turkmenistan	☑
		AFDIL	Uzbekistan	☑
		AFDIL	Vietnam	☑
⊞		AFDIL_QC	(Select all)	☐
⊞		FBI	(Select all)	☐

Comment: This is just a test sear

Summarize counts up to 5 differences

Detail profiles up

1 2 3 4 * DB			Min Diff
⊟ AFDIL			--
⊟			5.69+/-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
⊞		n0006	3
⊞		n0008	3

Ave min differences over entire population

Min differences between query and target

Search output

IMAGE COURTESY OF TOM HALL, PH.D.

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Comparing Profiles

Accounting for overlaps

AF-2		USA.FBI.000070	diff	
2901: 15893..16012: no data		2901: 15893..16012: no data		
2925: 15937..16041: no data		2925: 15937..16041: no data		
2899: 15985..16073: no data		2899: 16015..16051: A7 G10 C5 T15		
2898: 16048..16098: A15 G7 C17 T12	✗	2898: 16048..16098: A15 G7 C16 T13	1	1
2897: 16078..16129: A15 G8 C14 T15	→	2897: 16078..16129: A15 G8 C14 T15		
2896: 16124..16201: A27 G7 C27 T17	✗	2896: 16124..16201: A26 G7 C29 T16	2	2
2895: 16157..16201: A17 G1 C19 T8	✗	2895: 16157..16201: A16 G1 C21 T7	2	
2893: 16182..16250: A24 G5 C28 T12	✗	2893: 16182..16250: A23 G5 C29 T12	1	
2892: 16254..16305: A17 G4 C22 T8 N	→	2892: 16254..16305: A18 G4 C22 T8		
2891: 16283..16344: A23 G5 C18 T15 N	→	2891: 16283..16344: A24 G5 C19 T14		
2890: 16318..16402: no data		2890: 16342..16381: A8 G5 C17 T10		
2889: 16357..16451: no data		2889: 16377..16428: A12 G9 C20 T11		
2902: 5..97: no data		2902: 31..76: A5 G15 C12 T15		
2903: 20..139: no data		2903: 41..114: A12 G24 C21 T18		
2904: 103..162: A10 G10 C20 T20	✗	2904: 103..162: A9 G11 C18 T22	3	3
2905: 138..217: A23 G9 C21 T27	✗	2905: 138..217: A22 G10 C19 T29	3	
2906: 178..267: A32 G15 C15 T28	→	2906: 178..267: A32 G15 C15 T28		
2908: 234..313: A30 G6 C30 T16	→	2908: 234..313: A30 G6 C31 T16		
2907: 263..340: A25 G6 C35 T14	→	2907: 263..340: A25 G6 C36 T14		
2923: 262..390: no data		2923: 289..367: A27 G6 C37 T12		
2910: 331..425: no data		2910: 355..401: A21 G3 C14 T9		
2916: 367..463: no data		2916: 389..437: A11 G7 C12 T19		
2912: 409..521: no data		2912: 431..501: A20 G1 C34 T16		
2913: 464..603: no data		2913: 493..576: A27 G6 C46 T5		

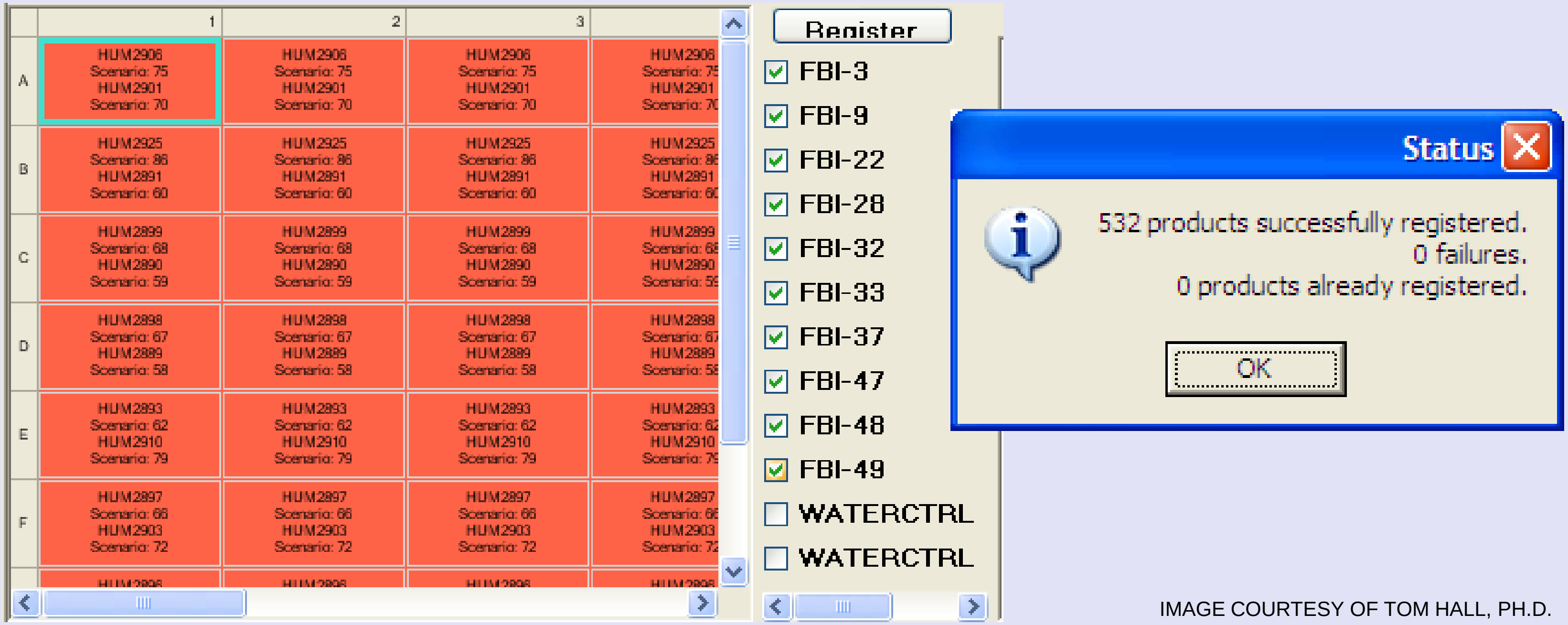
Total minimum differences **6**

Technology Transition Workshop

Profile Registration

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**



	1	2	3	
A	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 70	HUM2906 Scenario: 75 HUM2901 Scenario: 7
B	HUM2925 Scenario: 86 HUM2891 Scenario: 60	HUM2925 Scenario: 86 HUM2891 Scenario: 60	HUM2925 Scenario: 86 HUM2891 Scenario: 60	HUM2925 Scenario: 8 HUM2891 Scenario: 6
C	HUM2899 Scenario: 68 HUM2890 Scenario: 59	HUM2899 Scenario: 68 HUM2890 Scenario: 59	HUM2899 Scenario: 68 HUM2890 Scenario: 59	HUM2899 Scenario: 6 HUM2890 Scenario: 5
D	HUM2898 Scenario: 67 HUM2889 Scenario: 58	HUM2898 Scenario: 67 HUM2889 Scenario: 58	HUM2898 Scenario: 67 HUM2889 Scenario: 58	HUM2898 Scenario: 6 HUM2889 Scenario: 5
E	HUM2893 Scenario: 62 HUM2910 Scenario: 79	HUM2893 Scenario: 62 HUM2910 Scenario: 79	HUM2893 Scenario: 62 HUM2910 Scenario: 79	HUM2893 Scenario: 6 HUM2910 Scenario: 7
F	HUM2897 Scenario: 66 HUM2903 Scenario: 72	HUM2897 Scenario: 66 HUM2903 Scenario: 72	HUM2897 Scenario: 66 HUM2903 Scenario: 72	HUM2897 Scenario: 6 HUM2903 Scenario: 7

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

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

IMAGE COURTESY OF TOM HALL, PH.D.

Technology Transition Workshop

Report Generation

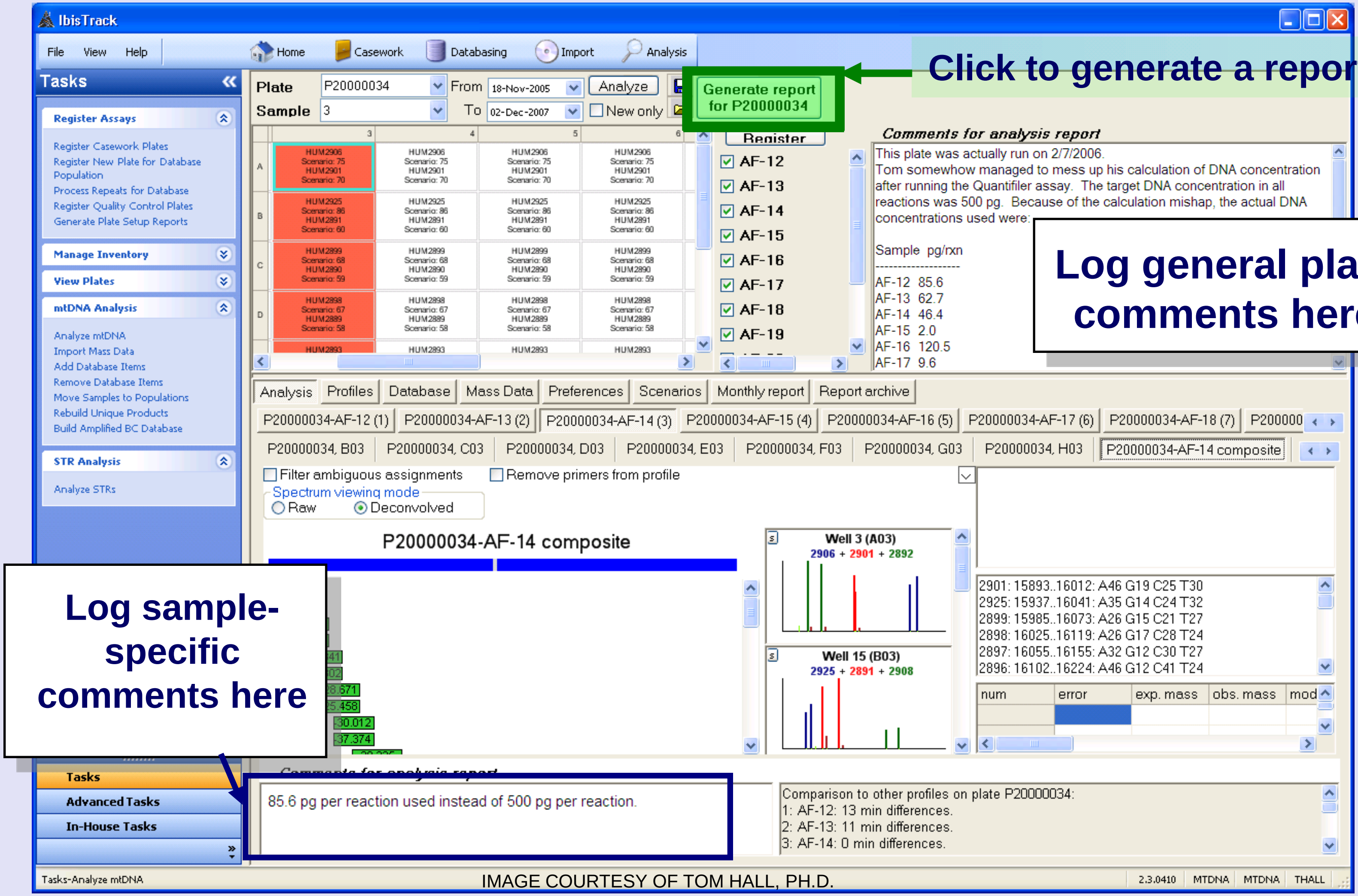


Plate P20000034
Sample 3
From 18-Nov-2005
To 02-Dec-2007
☐ New only

☑ AF-12
☑ AF-13
☑ AF-14
☑ AF-15
☑ AF-16
☑ AF-17
☑ AF-18
☑ AF-19

Click to generate a report

Comments for analysis report

This plate was actually run on 2/7/2006.
Tom somewhow managed to mess up his calculation of DNA concentration after running the Quantifiler 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

Log general plate comments here

P20000034-AF-12 (1) | P20000034-AF-13 (2) | P20000034-AF-14 (3) | P20000034-AF-15 (4) | P20000034-AF-16 (5) | P20000034-AF-17 (6) | P20000034-AF-18 (7)

P20000034, B03 | P20000034, C03 | P20000034, D03 | P20000034, E03 | P20000034, F03 | P20000034, G03 | P20000034, H03 | P20000034-AF-14 composite

☐ Filter ambiguous assignments
☐ Remove primers from profile

Spectrum viewing mode: ○ Raw ● Deconvolved

P20000034-AF-14 composite

Well 3 (A03): 2906 + 2901 + 2892

Well 15 (B03): 2925 + 2891 + 2908

2901: 15893..16012: A46 G19 C25 T30
2925: 15937..16041: A35 G14 C24 T32
2899: 15985..16073: A26 G15 C21 T27
2898: 16025..16119: A26 G17 C28 T24
2897: 16055..16155: A32 G12 C30 T27
2896: 16102..16224: A46 G12 C41 T24

num	error	exp. mass	obs. mass	mod

Log sample-specific comments here

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.

IMAGE COURTESY OF TOM HALL, PH.D.

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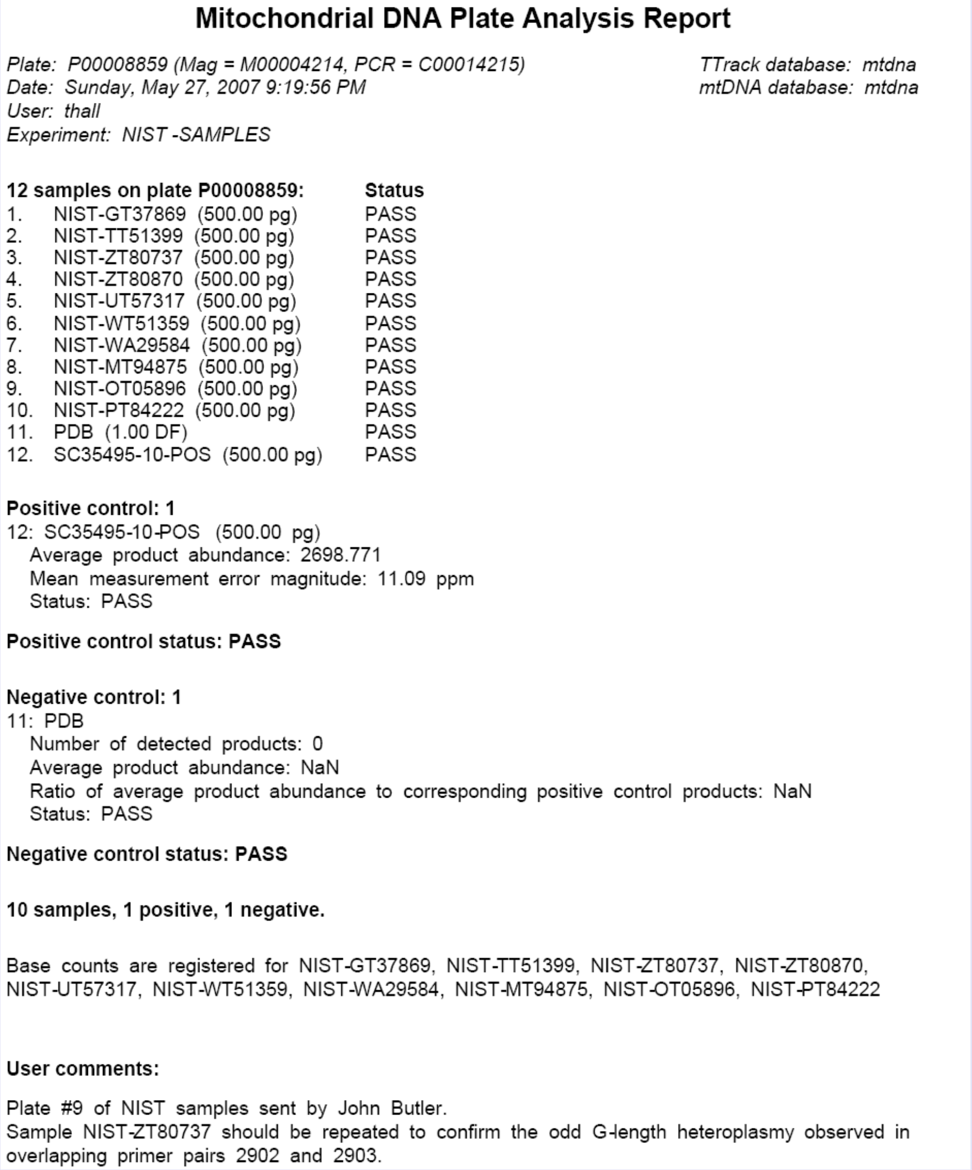
First page of report summarizes samples and controls on a plate.

- **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)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST -SAMPLES

TTrack database: mtdna
mtDNA database: mtdna

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.

IMAGE COURTESY OF TOM HALL, PH.D.

Second page of report summarizes analysis parameters used.

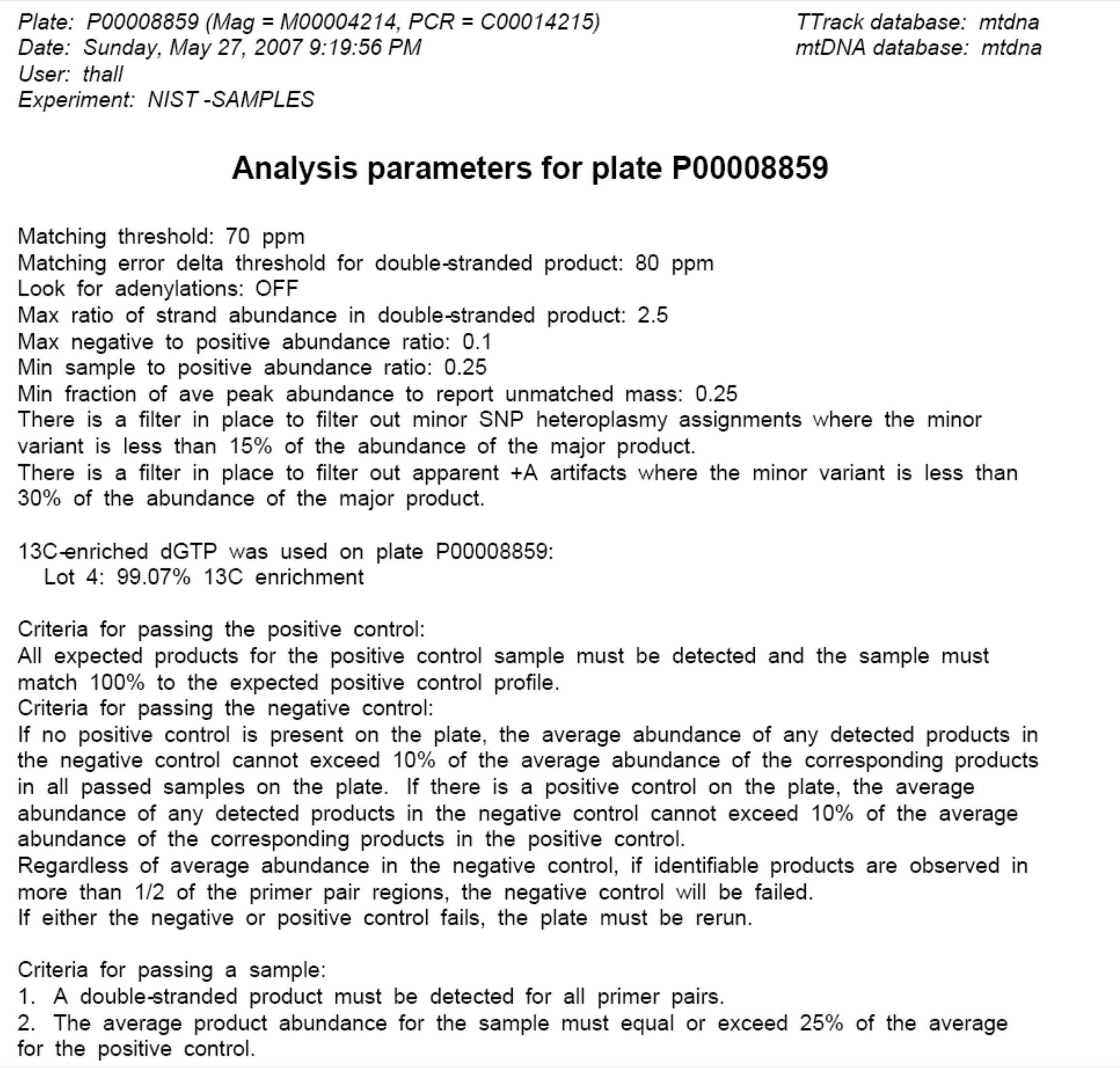


Plate: P00008859 (Mag = M00004214, PCR = C00014215)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST -SAMPLES

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.

IMAGE COURTESY OF TOM HALL, PH.D.

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

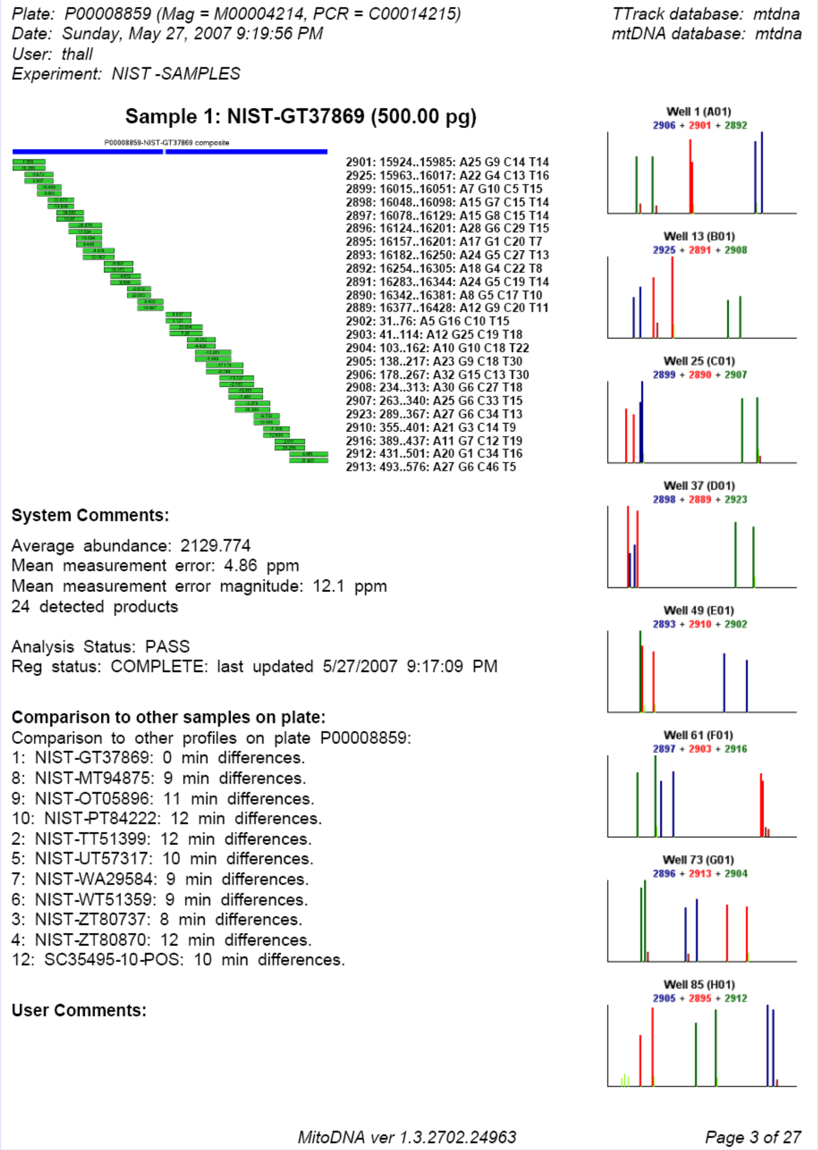


Plate: P00008859 (Mag = M00004214, PCR = C00014215)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST -SAMPLES

TTrack database: mtdna
mtDNA database: mtdna

Sample 1: NIST-GT37869 (500.00 pg)

2901: 15924..15985: A25 G9 C14 T14
2925: 15963..16017: A22 G4 C13 T16
2899: 16015..16051: A7 G10 C5 T15
2898: 16048..16098: A15 G7 C15 T14
2897: 16078..16129: A15 G8 C15 T14
2896: 16124..16201: A28 G6 C29 T15
2895: 16157..16201: A17 G1 C20 T7
2893: 16182..16250: A24 G5 C27 T13
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 G16 C10 T15
2903: 41..114: A12 G25 C19 T18
2904: 103..162: A10 G10 C18 T22
2905: 138..217: A23 G9 C18 T30
2906: 178..267: A32 G15 C13 T30
2908: 234..313: A30 G6 C27 T18
2907: 263..340: A25 G6 C33 T15
2923: 289..367: A27 G6 C34 T13
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

System Comments:

Average abundance: 2129.774
Mean measurement error: 4.86 ppm
Mean measurement error magnitude: 12.1 ppm
24 detected products

Analysis Status: PASS
Reg status: COMPLETE: last updated 5/27/2007 9:17:09 PM

Comparison to other samples on plate:
Comparison to other profiles on plate P00008859:
1: NIST-GT37869: 0 min differences.
8: NIST-MT94875: 9 min differences.
9: NIST-OT05896: 11 min differences.
10: NIST-PT84222: 12 min differences.
2: NIST-TT51399: 12 min differences.
5: NIST-UT57317: 10 min differences.
7: NIST-WA29584: 9 min differences.
6: NIST-WT51359: 9 min differences.
3: NIST-ZT80737: 8 min differences.
4: NIST-ZT80870: 12 min differences.
12: SC35495-10-POS: 10 min differences.

User Comments:

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Summary of raw data signal corresponding to primers in each well of negative control(s).

If there are any products in the negative control, a comparison to each sample (one sample per page) will follow.

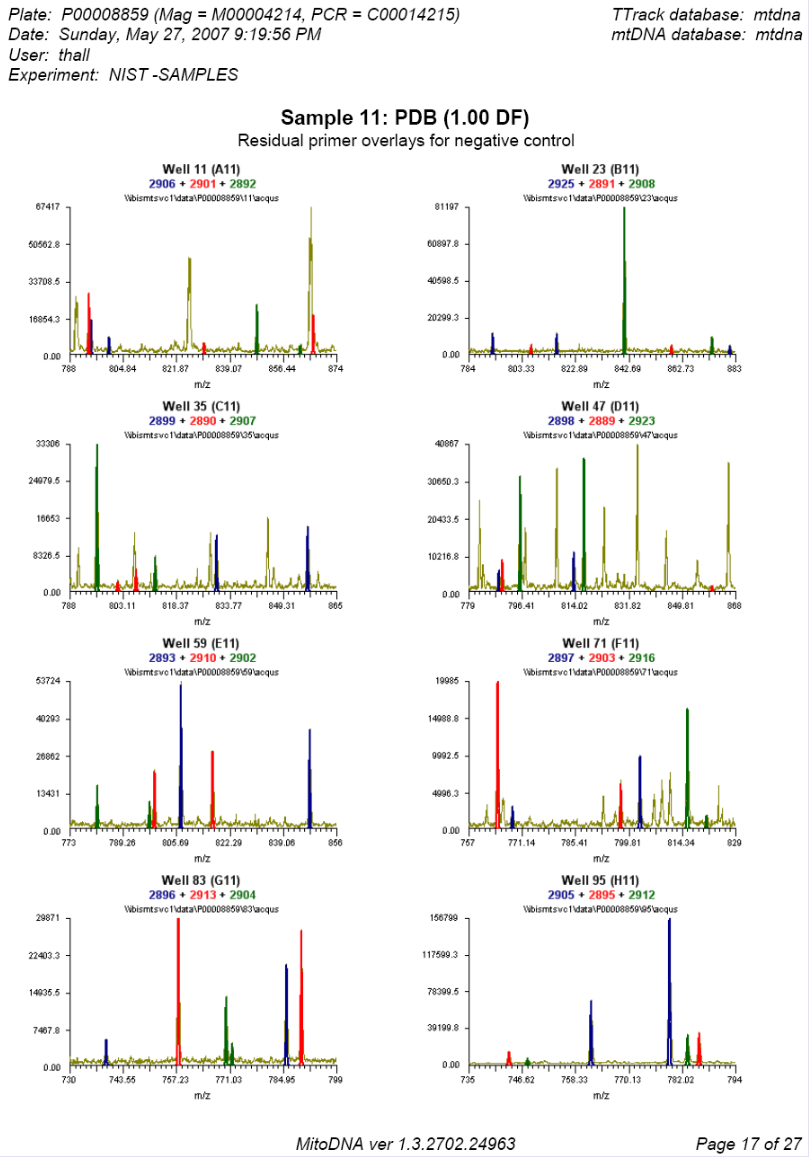

Plate: P00008859 (Mag = M00004214, PCR = C00014215)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST -SAMPLES

TTrack database: mtdna
mtDNA database: mtdna

Sample 11: PDB (1.00 DF)

Residual primer overlays for negative control

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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.

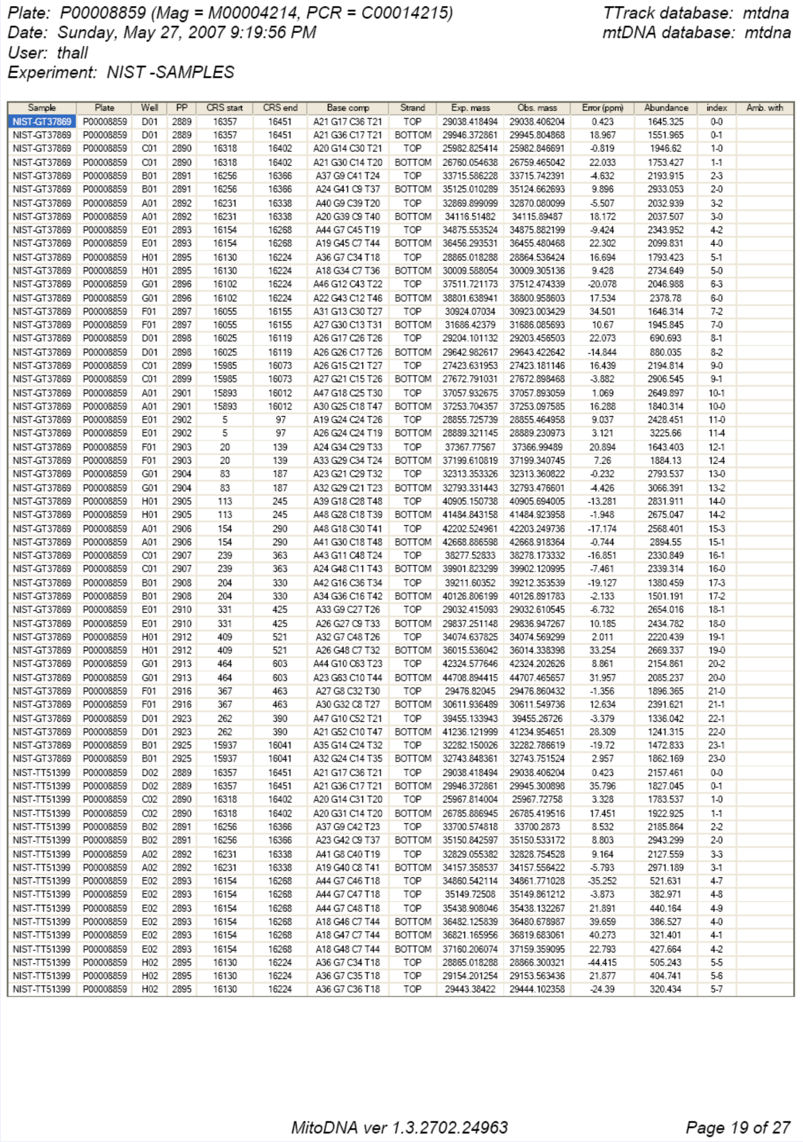

Plate: P00008859 (Mag = M00004214, PCR = C00014215)
Date: Sunday, May 27, 2007 9:19:56 PM
User: thall
Experiment: NIST -SAMPLES

TTrack database: mtdna
mtDNA database: mtdna

Sample	Plate	Well	PP	CRS start	CRS end	Base comp	Strand	Exp. mass	Obs. mass	Error (ppm)	Abundance	index	Amb. with
NIST-GT37869	P00008859	D01	2889	16357	16451	A21 G17 C36 T21	TOP	29038.418494	29038.406204	0.423	1645.325	0-0	
NIST-GT37869	P00008859	D01	2889	16357	16451	A21 G36 C17 T21	BOTTOM	29946.372861	29945.804868	18.967	1551.965	0-1	
NIST-GT37869	P00008859	C01	2890	16318	16402	A20 G14 C30 T21	TOP	25982.825414	25982.846691	-0.819	1946.62	1-0	
NIST-GT37869	P00008859	C01	2890	16318	16402	A21 G30 C14 T20	BOTTOM	26760.054638	26759.465042	22.033	1753.427	1-1	
NIST-GT37869	P00008859	B01	2891	16256	16366	A37 G9 C41 T24	TOP	33715.586228	33715.742391	-4.632	2193.915	2-3	
NIST-GT37869	P00008859	B01	2891	16256	16366	A24 G41 C9 T37	BOTTOM	35125.010289	35124.662693	9.896	2933.053	2-0	
NIST-GT37869	P00008859	A01	2892	16231	16338	A40 G9 C39 T20	TOP	32869.899099	32870.080099	-5.507	2032.939	3-2	
NIST-GT37869	P00008859	A01	2892	16231	16338	A20 G39 C9 T40	BOTTOM	34116.51482	34115.89487	18.172	2037.507	3-0	
NIST-GT37869	P00008859	E01	2893	16154	16268	A44 G7 C45 T19	TOP	34875.553524	34875.882199	-9.424	2343.952	4-2	
NIST-GT37869	P00008859	E01	2893	16154	16268	A19 G45 C7 T44	BOTTOM	36456.293531	36455.480468	22.302	2099.831	4-0	
NIST-GT37869	P00008859	H01	2895	16130	16224	A36 G7 C34 T18	TOP	28865.018288	28864.536424	16.694	1793.423	5-1	
NIST-GT37869	P00008859	H01	2895	16130	16224	A18 G34 C7 T36	BOTTOM	30009.588054	30009.305136	9.428	2734.649	5-0	
NIST-GT37869	P00008859	G01	2896	16102	16224	A46 G12 C43 T22	TOP	37511.721173	37512.474339	-20.078	2046.988	6-3	
NIST-GT37869	P00008859	G01	2896	16102	16224	A22 G43 C12 T46	BOTTOM	38801.638941	38800.958603	17.534	2378.78	6-0	
NIST-GT37869	P00008859	F01	2897	16055	16155	A31 G13 C30 T27	TOP	30924.07034	30923.003429	34.501	1646.314	7-2	
NIST-GT37869	P00008859	F01	2897	16055	16155	A27 G30 C13 T31	BOTTOM	31686.42379	31686.085693	10.67	1945.845	7-0	
NIST-GT37869	P00008859	D01	2898	16025	16119	A26 G17 C26 T26	TOP	29204.101132	29203.456503	22.073	690.693	8-1	
NIST-GT37869	P00008859	D01	2898	16025	16119	A26 G26 C17 T26	BOTTOM	29642.982617	29643.422642	-14.844	880.035	8-2	
NIST-GT37869	P00008859	C01	2899	15985	16073	A26 G15 C21 T27	TOP	27423.631953	27423.181146	16.439	2194.814	9-0	
NIST-GT37869	P00008859	C01	2899	15985	16073	A27 G21 C15 T26	BOTTOM	27672.791031	27672.898468	-3.882	2906.545	9-1	
NIST-GT37869	P00008859	A01	2901	15893	16012	A47 G18 C25 T30	TOP	37057.932675	37057.893059	1.069	2649.897	10-1	
NIST-GT37869	P00008859	A01	2901	15893	16012	A30 G25 C18 T47	BOTTOM	37253.704357	37253.097585	16.288	1840.314	10-0	
NIST-GT37869	P00008859	E01	2902	5	97	A19 G24 C24 T26	TOP	28855.725739	28855.464958	9.037	2428.451	11-0	
NIST-GT37869	P00008859	E01	2902	5	97	A26 G24 C24 T19	BOTTOM	28889.321145	28889.230973	3.121	3225.66	11-4	
NIST-GT37869	P00008859	F01	2903	20	139	A24 G34 C29 T33	TOP	37367.77567	37366.99489	20.894	1643.403	12-1	
NIST-GT37869	P00008859	F01	2903	20	139	A33 G29 C34 T24	BOTTOM	37199.610819	37199.340745	7.26	1884.13	12-4	
NIST-GT37869	P00008859	G01	2904	83	187	A23 G21 C29 T32	TOP	32313.353326	32313.360822	-0.232	2793.537	13-0	
NIST-GT37869	P00008859	G01	2904	83	187	A32 G29 C21 T23	BOTTOM	32793.331443	32793.476601	-4.426	3066.391	13-2	
NIST-GT37869	P00008859	H01	2905	113	245	A39 G18 C28 T48	TOP	40905.150738	40905.694005	-13.281	2831.911	14-0	
NIST-GT37869	P00008859	H01	2905	113	245	A48 G28 C18 T39	BOTTOM	41484.843158	41484.923958	-1.948	2675.047	14-2	
NIST-GT37869	P00008859	A01	2906	154	290	A48 G18 C30 T41	TOP	42202.524961	42203.249736	-17.174	2568.401	15-3	
NIST-GT37869	P00008859	A01	2906	154	290	A41 G30 C18 T48	BOTTOM	42668.886598	42668.918364	-0.744	2894.55	15-1	
NIST-GT37869	P00008859	C01	2907	239	363	A43 G11 C48 T24	TOP	38277.52833	38278.173332	-16.851	2330.849	16-1	
NIST-GT37869	P00008859	C01	2907	239	363	A24 G48 C11 T43	BOTTOM	39901.823299	39902.120995	-7.461	2339.314	16-0	
NIST-GT37869	P00008859	B01	2908	204	330	A42 G16 C36 T34	TOP	39211.60352	39212.353539	-19.127	1380.459	17-3	
NIST-GT37869	P00008859	B01	2908	204	330	A34 G36 C16 T42	BOTTOM	40126.806199	40126.891783	-2.133	1501.191	17-2	
NIST-GT37869	P00008859	E01	2910	331	425	A33 G9 C27 T26	TOP	29032.415093	29032.610545	-6.732	2654.016	18-1	
NIST-GT37869	P00008859	E01	2910	331	425	A26 G27 C9 T33	BOTTOM	29837.251148	29836.947267	10.185	2434.782	18-0	
NIST-GT37869	P00008859	H01	2912	409	521	A32 G7 C48 T26	TOP	34074.637825	34074.569299	2.011	2220.439	19-1	
NIST-GT37869	P00008859	H01	2912	409	521	A26 G48 C7 T32	BOTTOM	36015.536042	36014.338398	33.254	2669.337	19-0	
NIST-GT37869	P00008859	G01	2913	464	603	A44 G10 C63 T23	TOP	42324.577646	42324.202626	8.861	2154.861	20-2	
NIST-GT37869	P00008859	G01	2913	464	603	A23 G63 C10 T44	BOTTOM	44708.894415	44707.465657	31.957	2085.237	20-0	
NIST-GT37869	P00008859	F01	2916	367	463	A27 G8 C32 T30	TOP	29476.82045	29476.860432	-1.356	1896.365	21-0	
NIST-GT37869	P00008859	F01	2916	367	463	A30 G32 C8 T27	BOTTOM	30611.936489	30611.549736	12.634	2391.621	21-1	
NIST-GT37869	P00008859	D01	2923	262	390	A47 G10 C52 T21	TOP	39455.133943	39455.26726	-3.379	1336.042	22-1	
NIST-GT37869	P00008859	D01	2923	262	390	A21 G52 C10 T47	BOTTOM	41236.121999	41234.954651	28.309	1241.315	22-0	
NIST-GT37869	P00008859	B01	2925	15937	16041	A35 G14 C24 T32	TOP	32282.150026	32282.786619	-19.72	1472.833	23-1	
NIST-GT37869	P00008859	B01	2925	15937	16041	A32 G24 C14 T35	BOTTOM	32743.848361	32743.751524	2.957	1862.169	23-0	
NIST-TT51399	P00008859	D02	2889	16357	16451	A21 G17 C36 T21	TOP	29038.418494	29038.406204	0.423	2157.461	0-0	
NIST-TT51399	P00008859	D02	2889	16357	16451	A21 G36 C17 T21	BOTTOM	29946.372861	29945.300898	35.796	1827.045	0-1	
NIST-TT51399	P00008859	C02	2890	16318	16402	A20 G14 C31 T20	TOP	25967.814004	25967.72758	3.328	1783.537	1-0	
NIST-TT51399	P00008859	C02	2890	16318	16402	A20 G31 C14 T20	BOTTOM	26785.886945	26785.419516	17.451	1922.925	1-1	
NIST-TT51399	P00008859	B02	2891	16256	16366	A37 G9 C42 T23	TOP	33700.574818	33700.2873	8.532	2185.864	2-2	
NIST-TT51399	P00008859	B02	2891	16256	16366	A23 G42 C9 T37	BOTTOM	35150.842597	35150.533172	8.803	2943.299	2-0	
NIST-TT51399	P00008859	A02	2892	16231	16338	A41 G8 C40 T19	TOP	32829.055382	32828.754528	9.164	2127.559	3-3	
NIST-TT51399	P00008859	A02	2892	16231	16338	A19 G40 C8 T41	BOTTOM	34157.358537	34157.556422	-5.793	2971.189	3-1	
NIST-TT51399	P00008859	E02	2893	16154	16268	A44 G7 C46 T18	TOP	34860.542114	34861.771028	-35.252	521.631	4-7	
NIST-TT51399	P00008859	E02	2893	16154	16268	A44 G7 C47 T18	TOP	35149.72508	35149.861212	-3.873	382.971	4-8	
NIST-TT51399	P00008859	E02	2893	16154	16268	A44 G7 C48 T18	TOP	35438.908046	35438.132267	21.891	440.164	4-9	
NIST-TT51399	P00008859	E02	2893	16154	16268	A18 G46 C7 T44	BOTTOM	36482.125839	36480.678987	39.659	386.527	4-0	
NIST-TT51399	P00008859	E02	2893	16154	16268	A18 G47 C7 T44	BOTTOM	36821.165956	36819.683061	40.273	321.401	4-1	
NIST-TT51399	P00008859	E02	2893	16154	16268	A18 G48 C7 T44	BOTTOM	37160.206074	37159.359095	22.793	427.664	4-2	
NIST-TT51399	P00008859	H02	2895	16130	16224	A36 G7 C34 T18	TOP	28865.018288	28866.300321	-44.415	505.243	5-5	
NIST-TT51399	P00008859	H02	2895	16130	16224	A36 G7 C35 T18	TOP	29154.201254	29153.563436	21.877	404.741	5-6	
NIST-TT51399	P00008859	H02	2895	16130	16224	A36 G7 C36 T18	TOP	29443.38422	29444.102358	-24.39	320.434	5-7	

MitoDNA ver 1.3.2702.24963

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IMAGE COURTESY OF TOM HALL, PH.D.

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
- Automated comparison of profiles to database entries
- Search database
- Add sequences and convert to base compositions in the database

Contact Information:

Tom Hall, Ph.D.
Ibis Biosciences, Inc.
thall@ibisbio.com