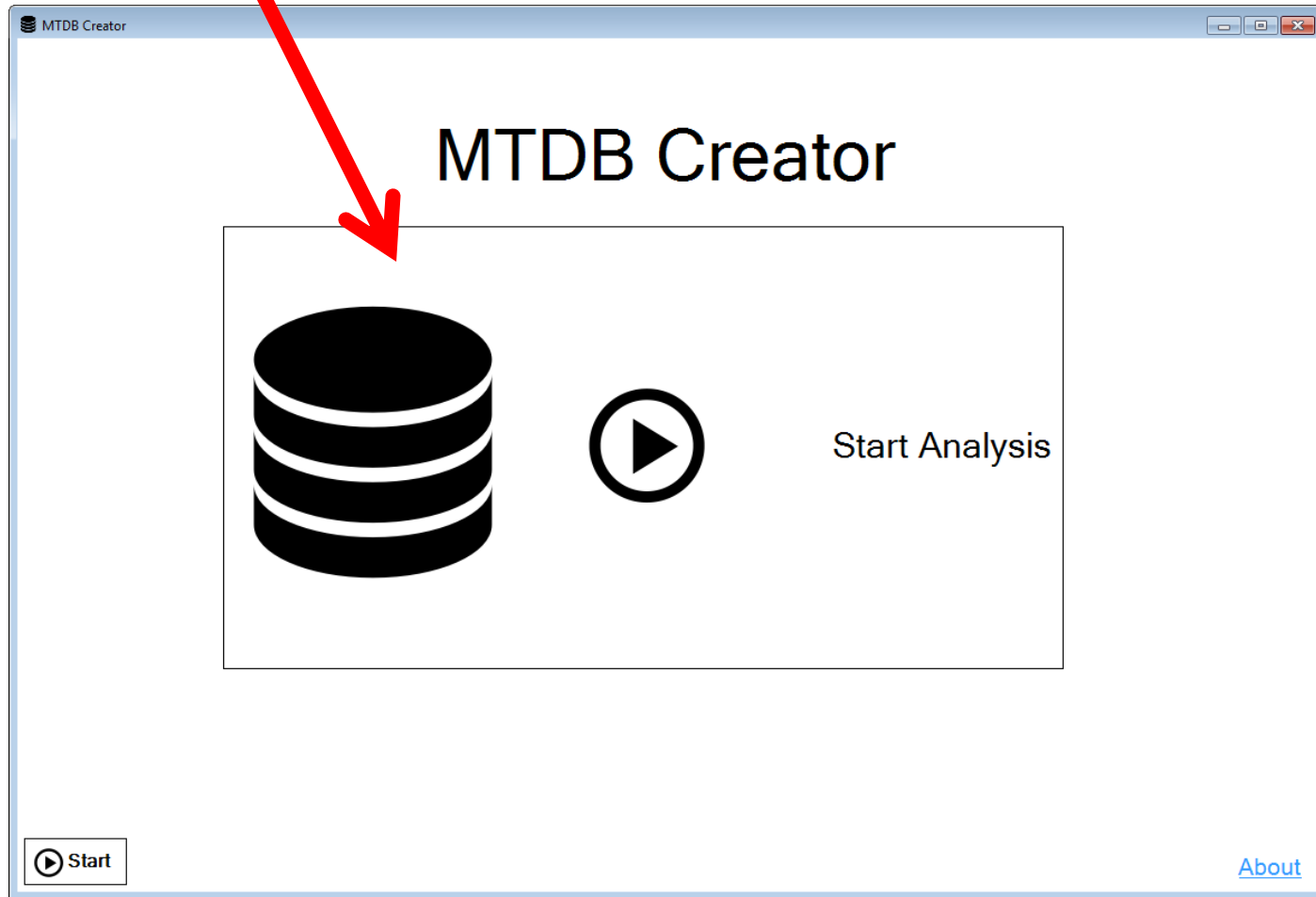



Click Here

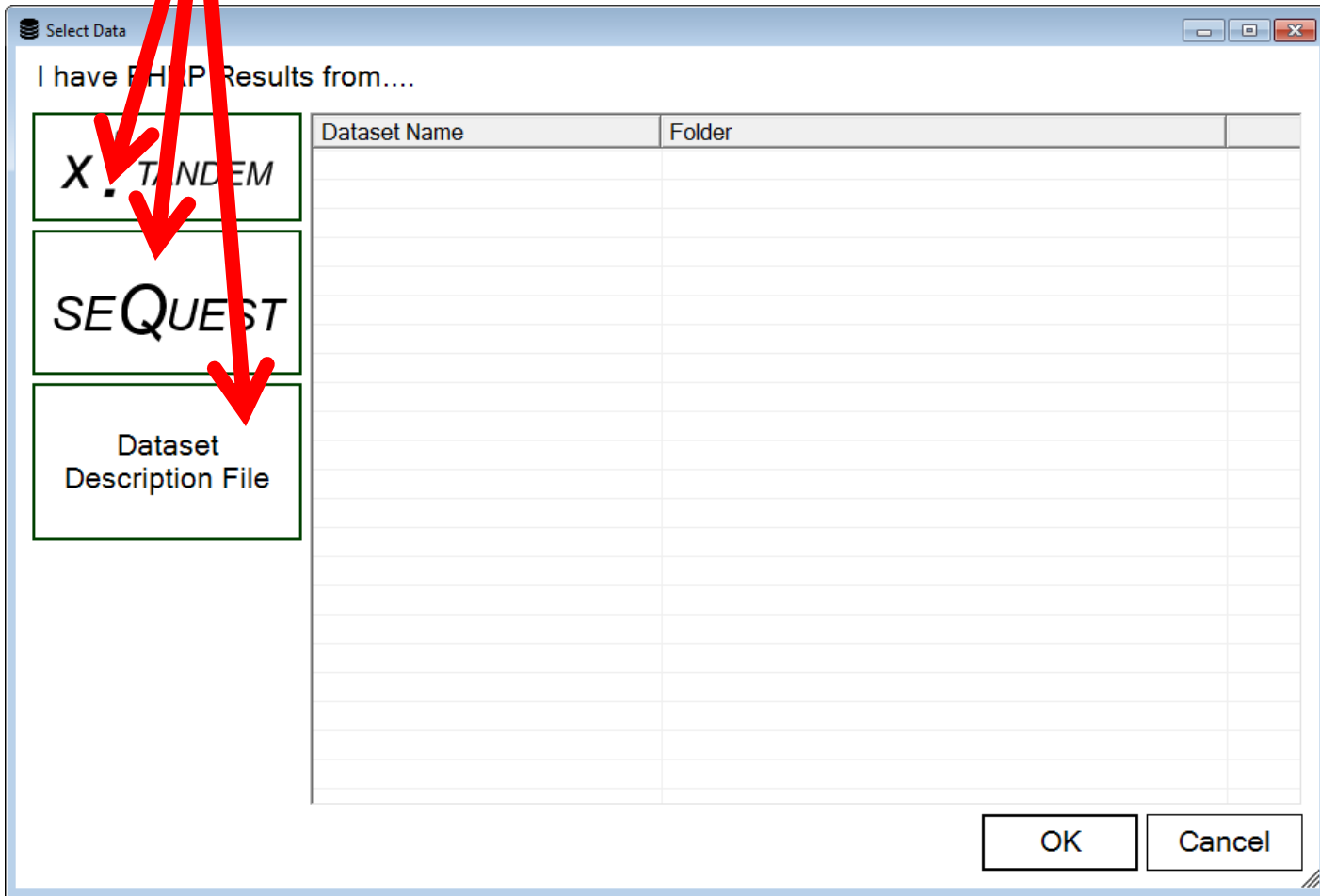
# Startup



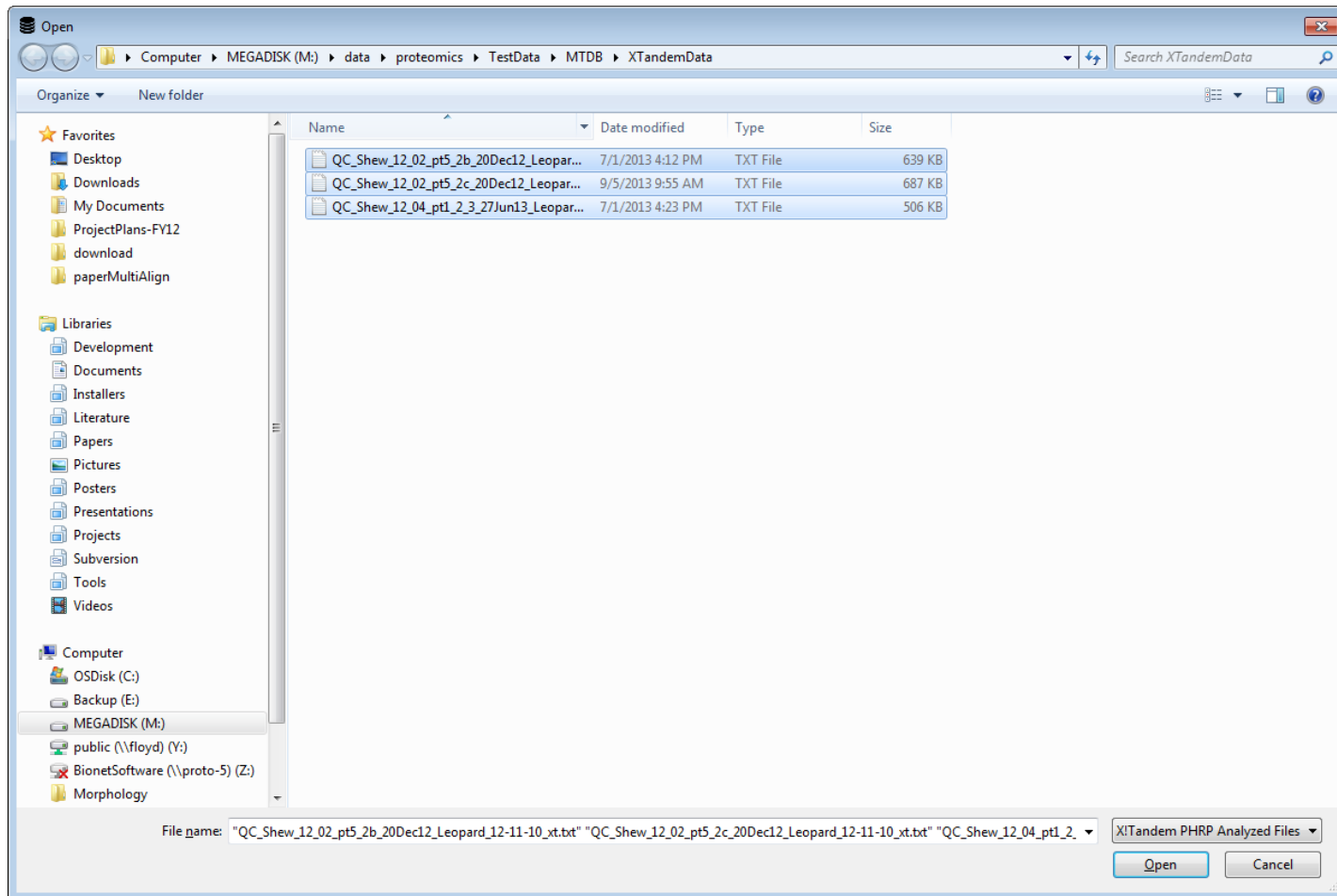


The screenshot shows a database selection window titled "Select Data". It contains a list of database entries. Two red arrows point to the entries "X.TANDEM" and "SEQUENCE".

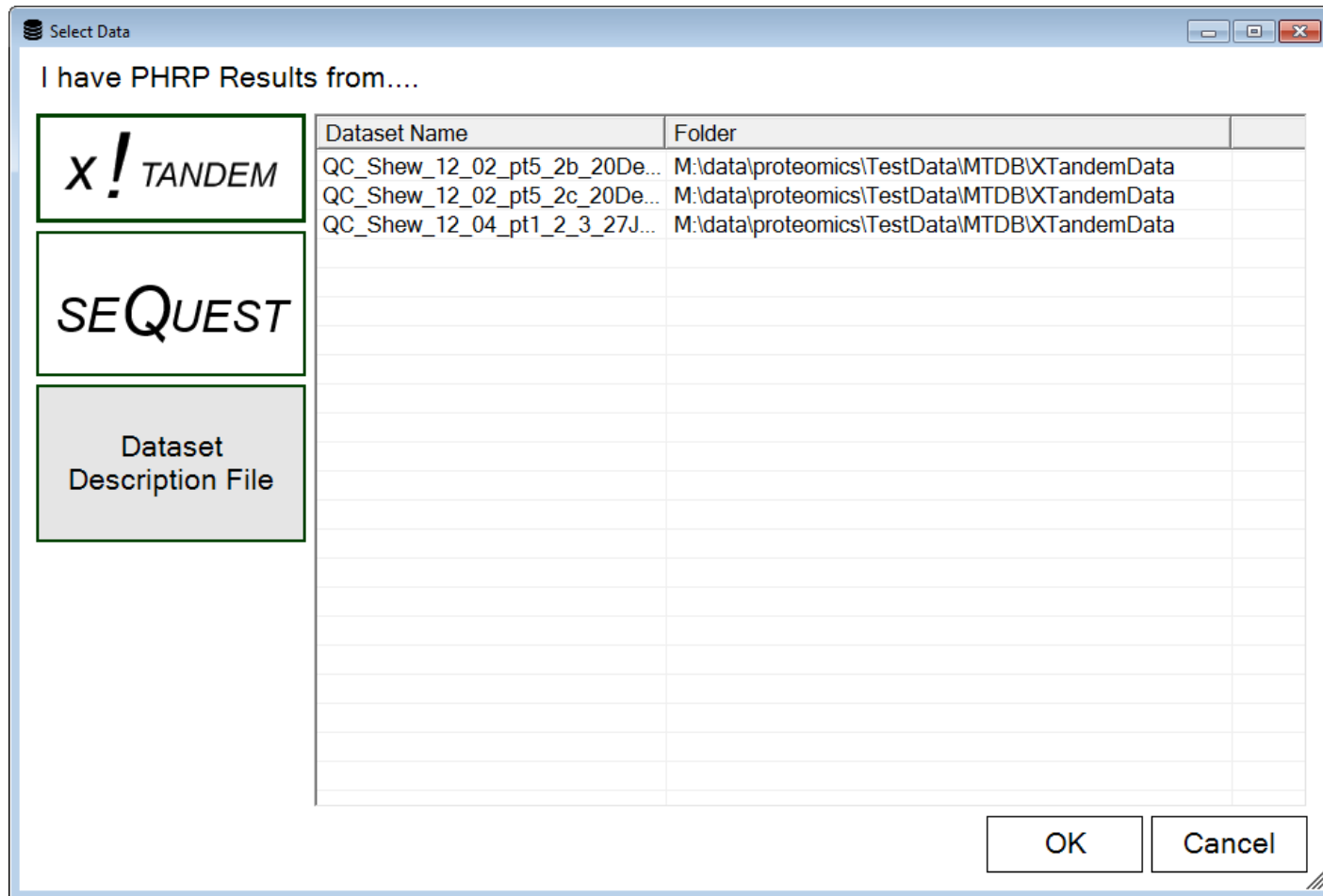
# Select Your Data



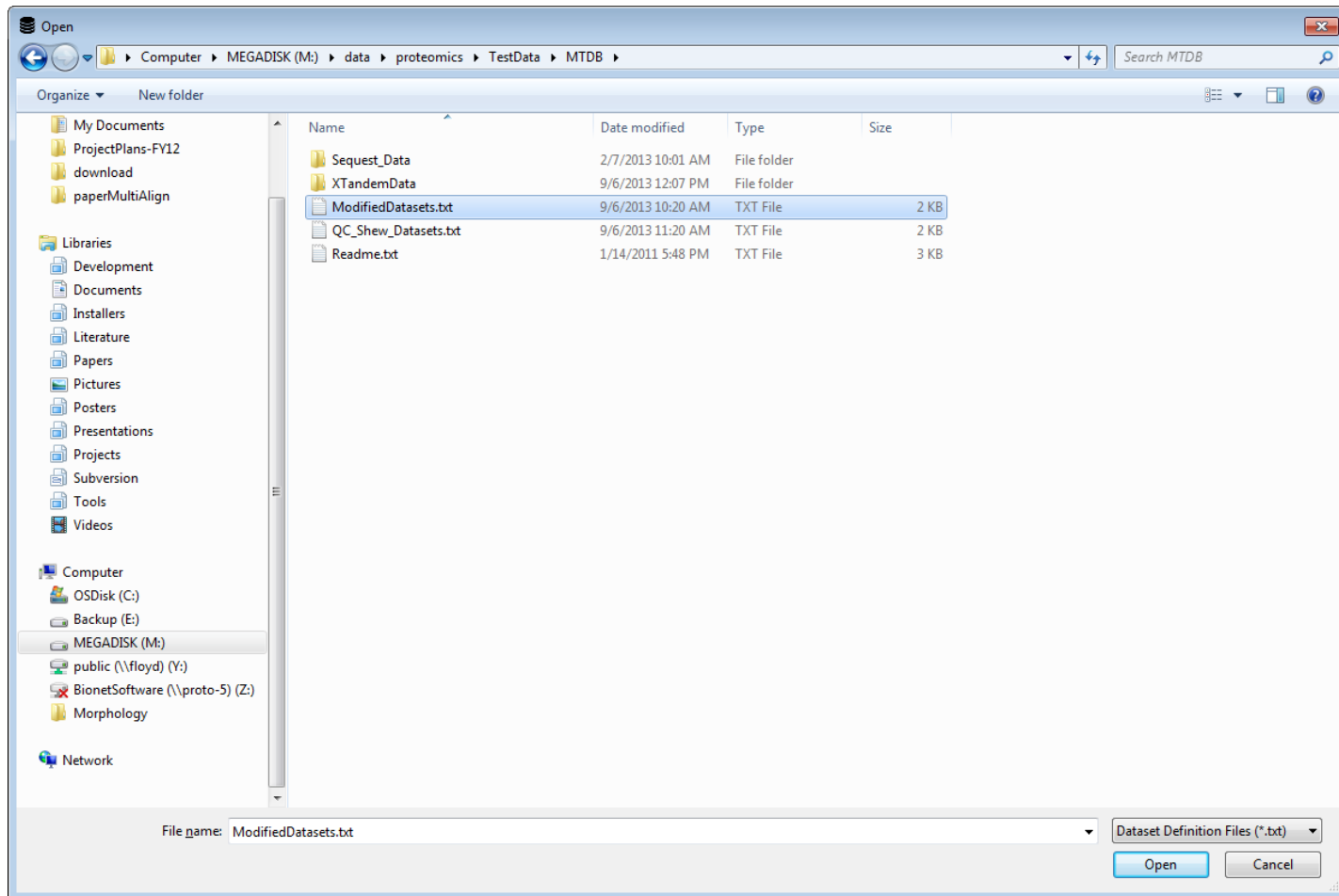
# Multi-Select – MTDB figures out where rest of data is based on the search results files



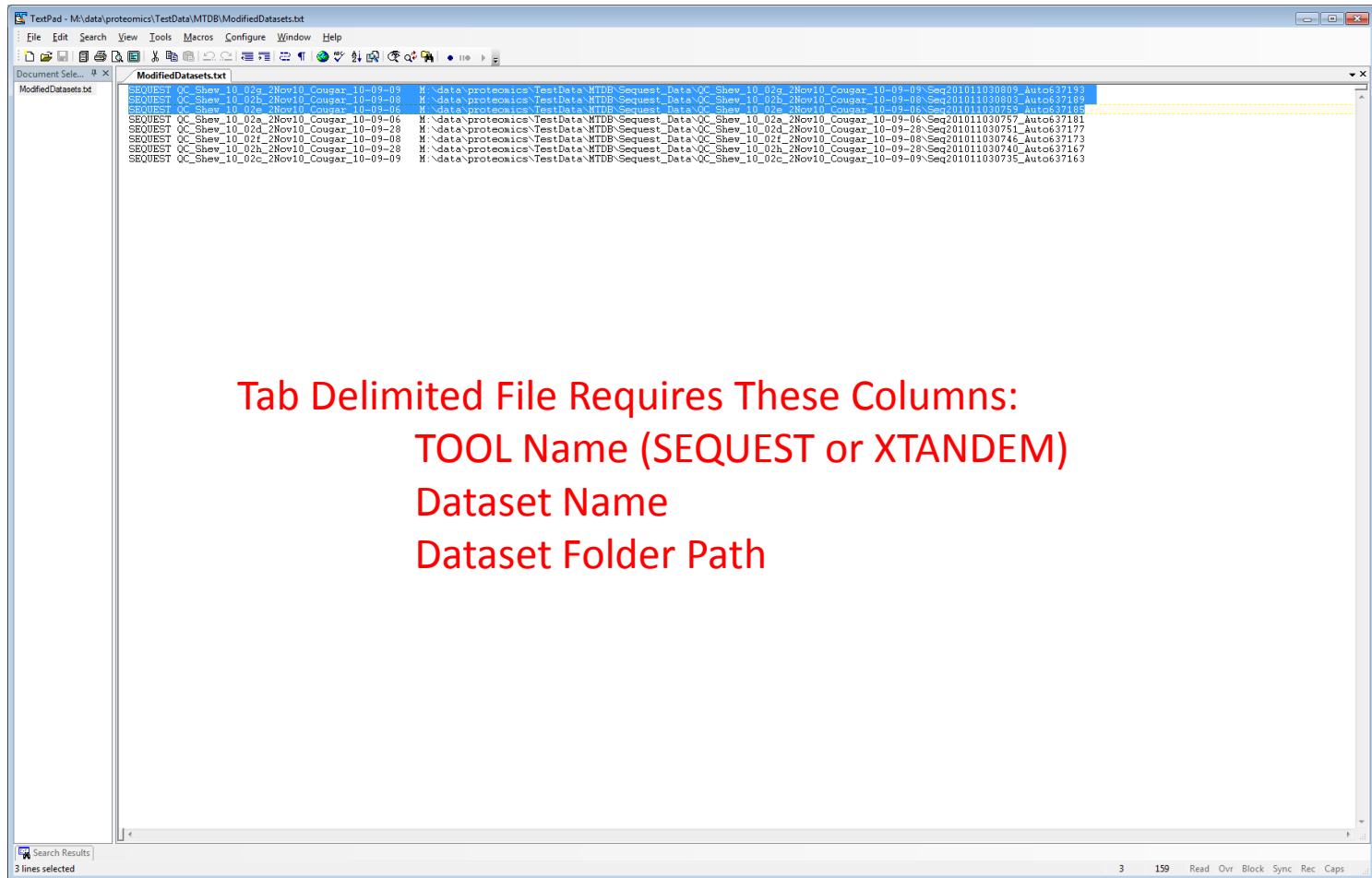
# Datasets are listed in window



# Or you could just do it the old way with a data definition file.



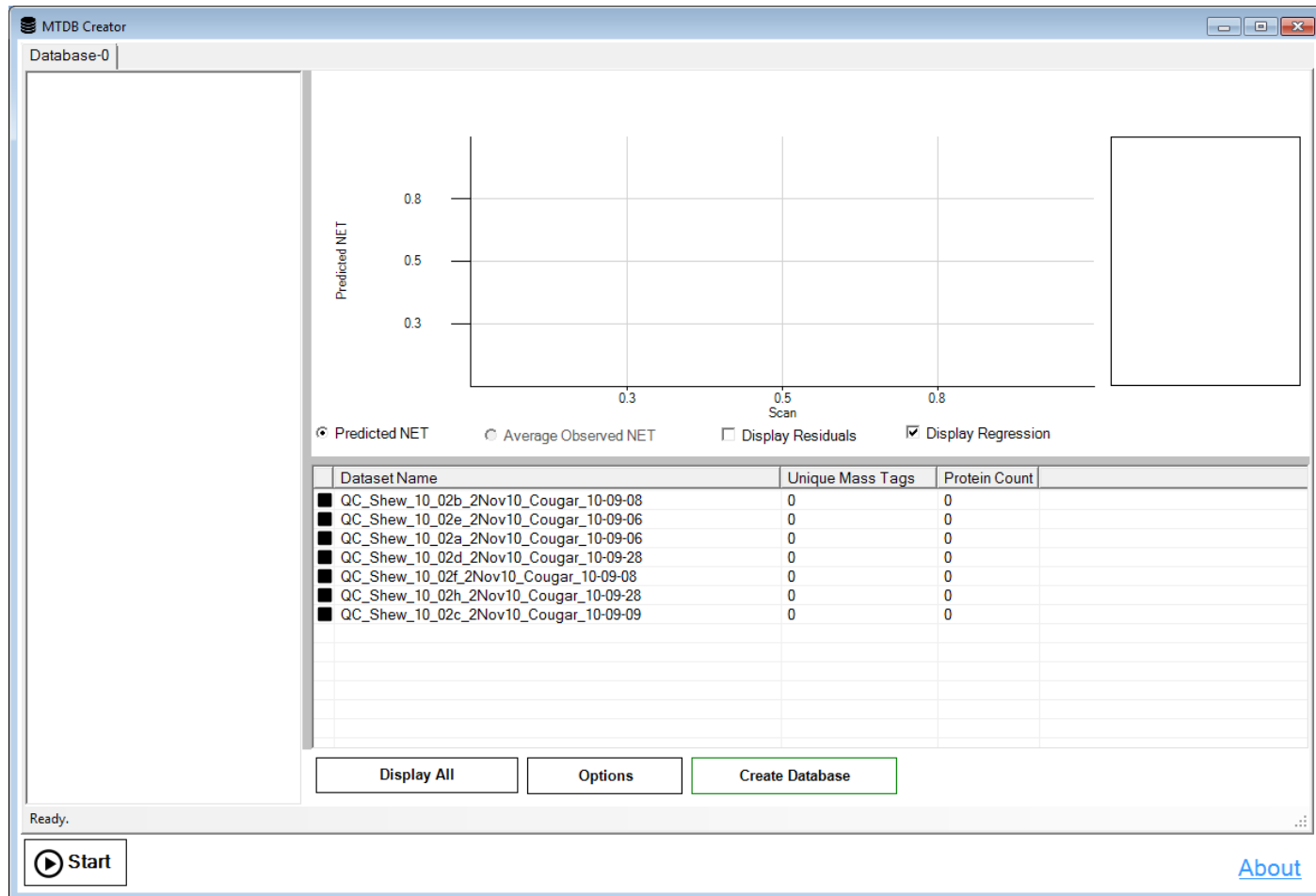
# Dataset Definition File



Tab Delimited File Requires These Columns:

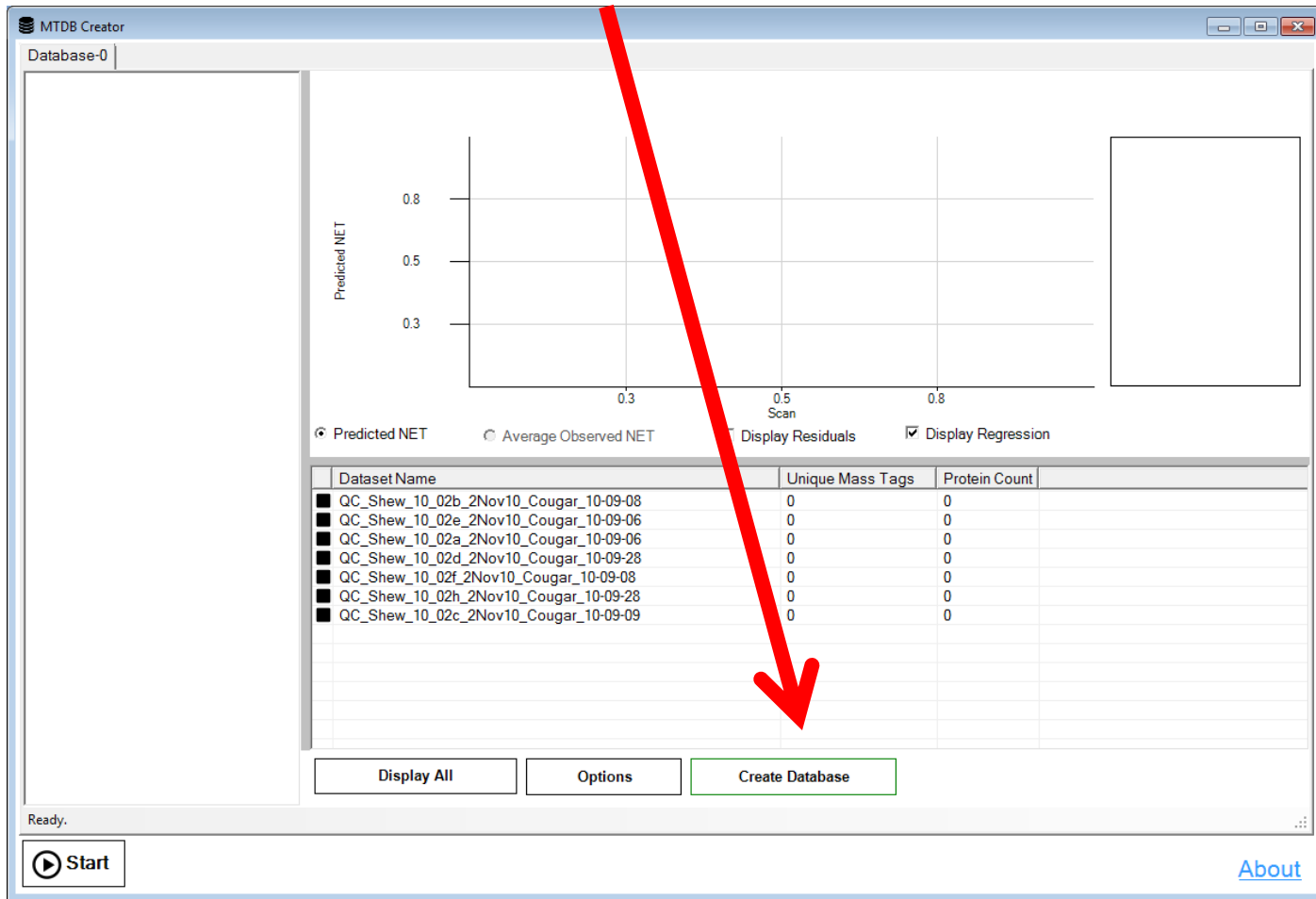
- TOOL Name (SEQUEST or XTANDEM)
- Dataset Name
- Dataset Folder Path

# After you select your data



# Start Processing

Click Here To Start Processing



The screenshot shows the MTDB Creator application window. The title bar reads 'MTDB Creator'. The main area is divided into a left sidebar labeled 'Database-0', a central plot area, and a bottom section with a table and buttons.

The central plot area has a y-axis labeled 'Predicted NET' with values 0.3, 0.5, and 0.8, and an x-axis labeled 'Scan' with values 0.3, 0.5, and 0.8. Below the plot are three radio buttons: 'Predicted NET' (selected), 'Average Observed NET', and 'Display Residuals'. To the right of these is a checked checkbox for 'Display Regression'.

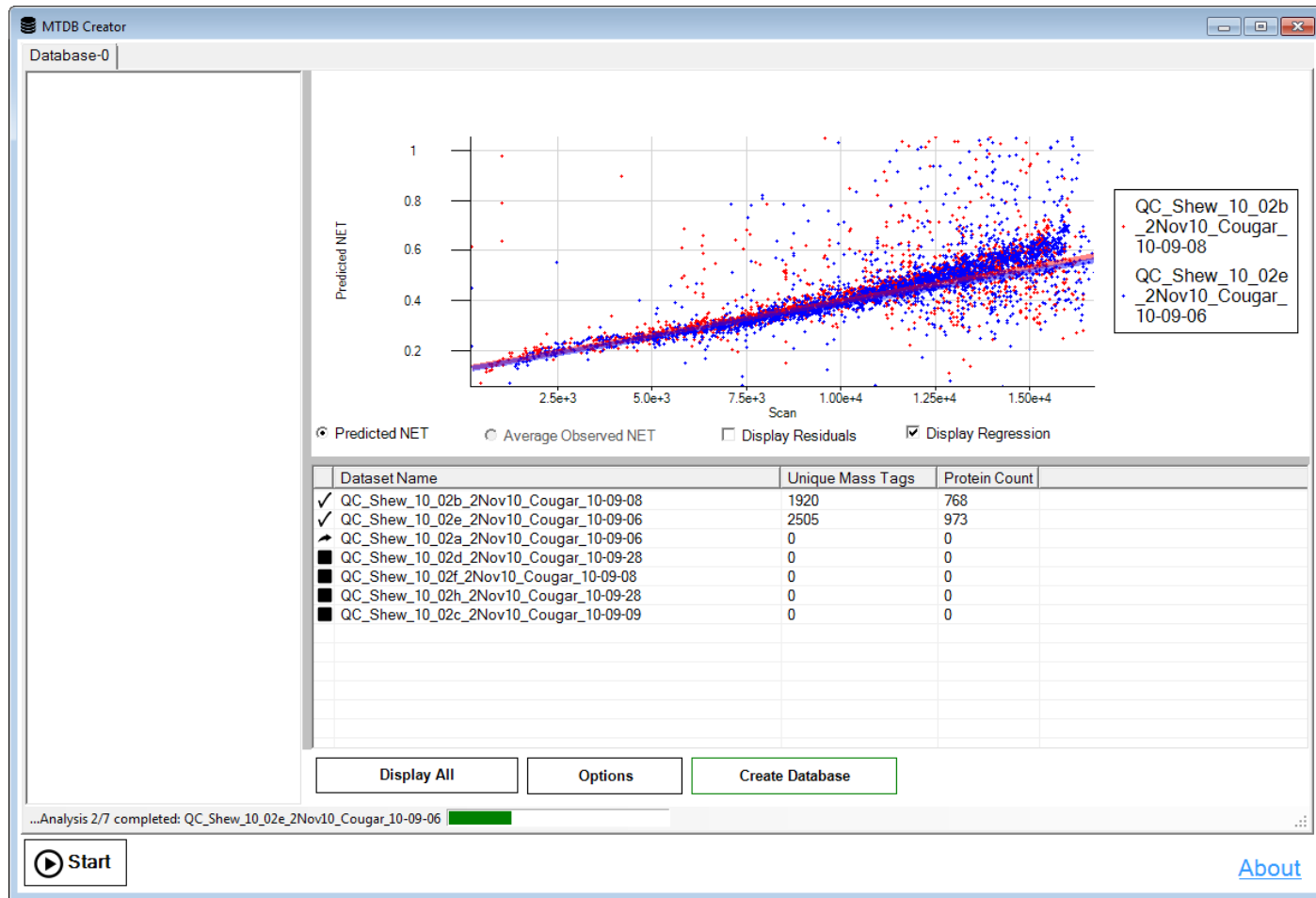
Below the plot is a table with the following data:

Dataset Name	Unique Mass Tags	Protein Count
■ QC_Shew_10_02b_2Nov10_Cougar_10-09-08	0	0
■ QC_Shew_10_02e_2Nov10_Cougar_10-09-06	0	0
■ QC_Shew_10_02a_2Nov10_Cougar_10-09-06	0	0
■ QC_Shew_10_02d_2Nov10_Cougar_10-09-28	0	0
■ QC_Shew_10_02f_2Nov10_Cougar_10-09-08	0	0
■ QC_Shew_10_02h_2Nov10_Cougar_10-09-28	0	0
■ QC_Shew_10_02c_2Nov10_Cougar_10-09-09	0	0

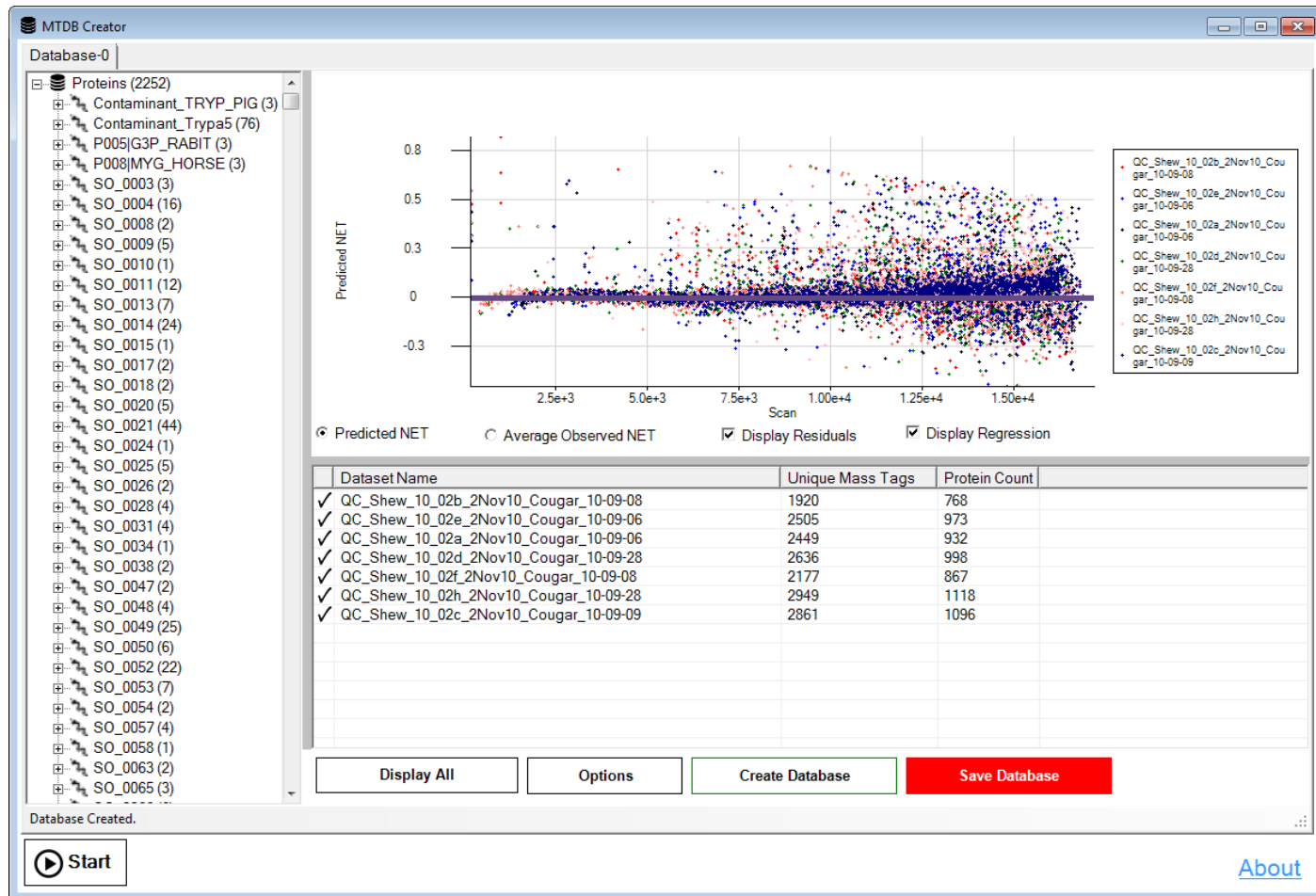
At the bottom of the window, there are three buttons: 'Display All', 'Options', and 'Create Database' (which is highlighted with a green border). Below these buttons is a status bar that says 'Ready.' and a 'Start' button with a play icon. An 'About' link is visible in the bottom right corner.



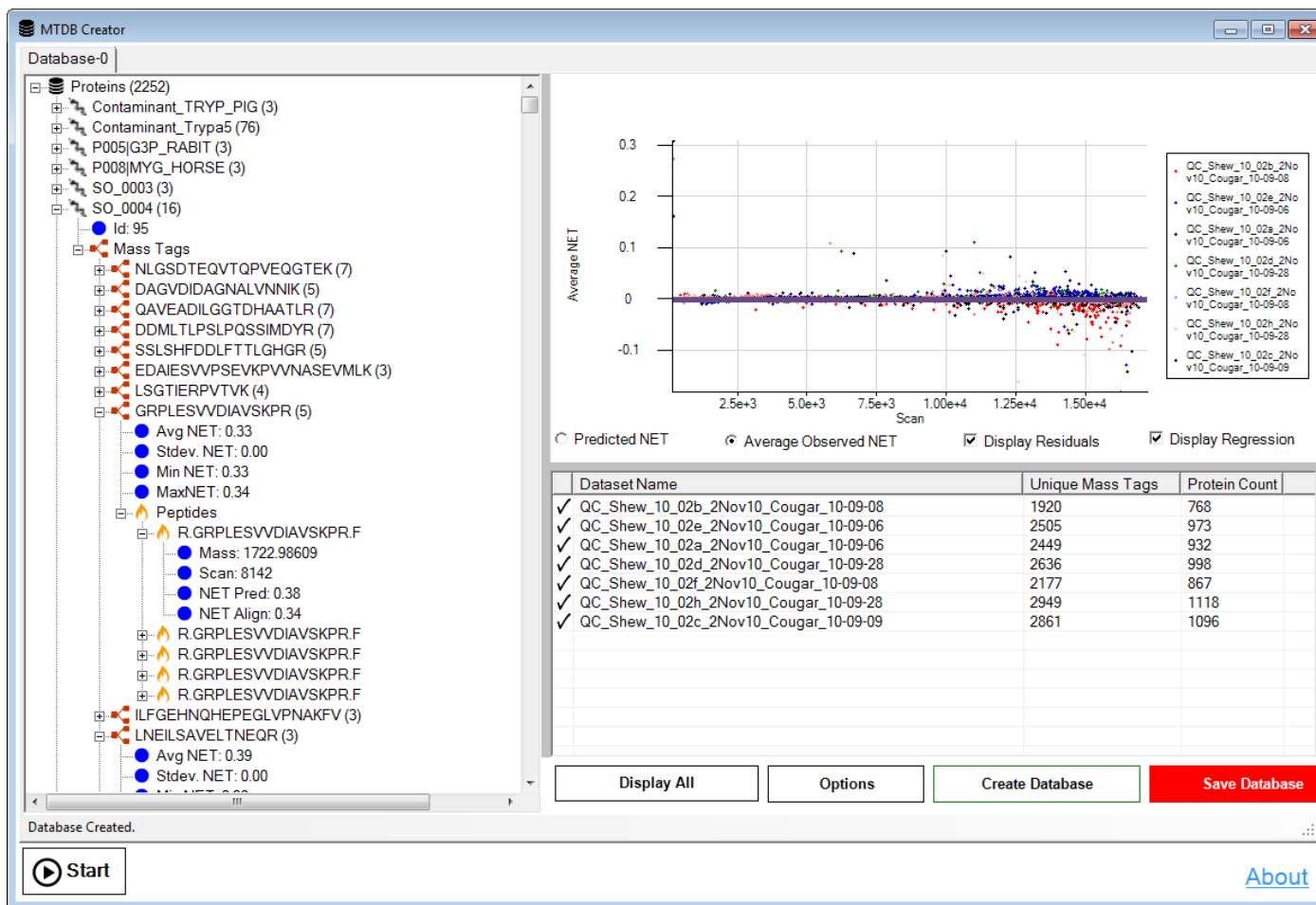
# Processing Screen...



# Processing Complete



# Processing Complete – Protein Collection



# Save Your Database

Click Here To Save Your Database

The screenshot shows the MTDB Creator application window. On the left is a tree view of the database contents, including Proteins (2252), Contaminants, and Mass Tags. The central area displays a scatter plot of Average NET vs. Predicted NET. Below the plot is a table of datasets with their unique mass tags and protein counts. At the bottom, there are buttons for 'Display All', 'Options', 'Create Database', and 'Save Database'. A red arrow points from the text above to the 'Save Database' button.

Database-0

Proteins (2252)

- Contaminant\_TRYP\_PIG (3)
- Contaminant\_Trypa5 (76)
- P005[G3P\_RABIT (3)
- P008[MYG\_HORSE (3)
- SO\_0003 (3)
- SO\_0004 (16)
- Id: 95
- Mass Tags
  - NLGSDTEQVTQPVEQGTEK (7)
  - DAGVIDDAGNALVNNIK (5)
  - QAVEADILGGTDHAATLR (7)
  - DDMLTLPSPQSSIMDYR (7)
  - SSLSHFDDLFTTLGHGR (5)
  - EDAIESVVPSEVKPVVNASEVMLK (3)
  - LSGTIERPVTVK (4)
  - GRPLESVVDIAVSKPR (5)
- Peptides
  - R.GRPLESVVDIAVSKPR.F
    - Mass: 1722.98609
    - Scan: 8142
    - NET Pred: 0.38
    - NET Align: 0.34
  - R.GRPLESVVDIAVSKPR.F
  - R.GRPLESVVDIAVSKPR.F
  - R.GRPLESVVDIAVSKPR.F
  - R.GRPLESVVDIAVSKPR.F
  - ILFGEHNQHEPEGLVPNAKFV (3)
  - LNEILSAVELTNEQR (3)

Avg NET: 0.33  
Stdev. NET: 0.00  
Min NET: 0.33  
MaxNET: 0.34

Average NET

Predicted NET

Average Observed NET

Display Residuals

Display Regression

Dataset Name	Unique Mass Tags	Protein Count
✓ QC_Shew_10_02b_2Nov10_Cougar_10-09-08	1920	768
✓ QC_Shew_10_02e_2Nov10_Cougar_10-09-06	2505	973
✓ QC_Shew_10_02a_2Nov10_Cougar_10-09-06	2449	932
✓ QC_Shew_10_02d_2Nov10_Cougar_10-09-28	2636	998
✓ QC_Shew_10_02f_2Nov10_Cougar_10-09-08	2777	867
✓ QC_Shew_10_02h_2Nov10_Cougar_10-09-28	2911	1118
✓ QC_Shew_10_02c_2Nov10_Cougar_10-09-09	2861	1096

Display All

Options

Create Database

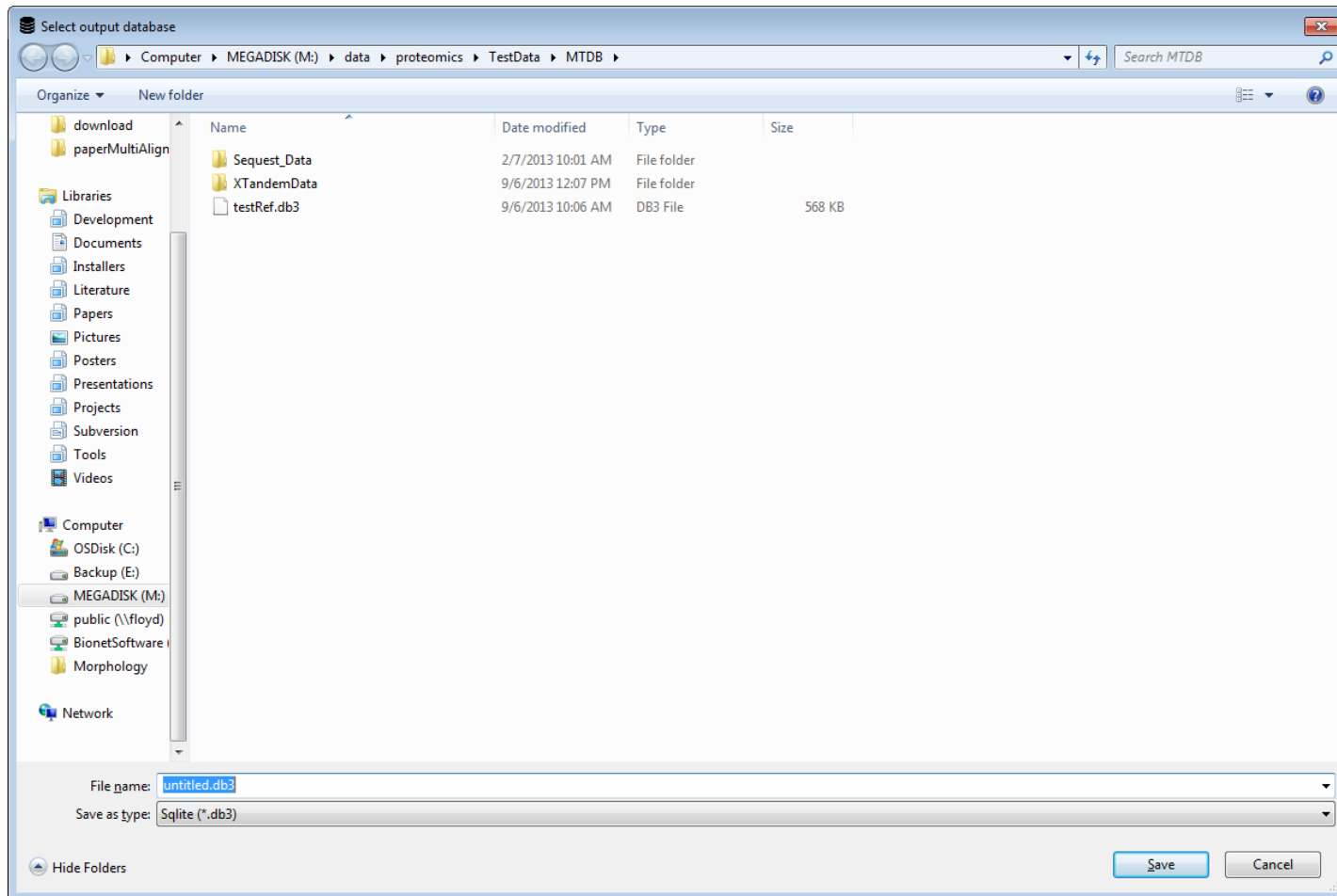
Save Database

Database Created.

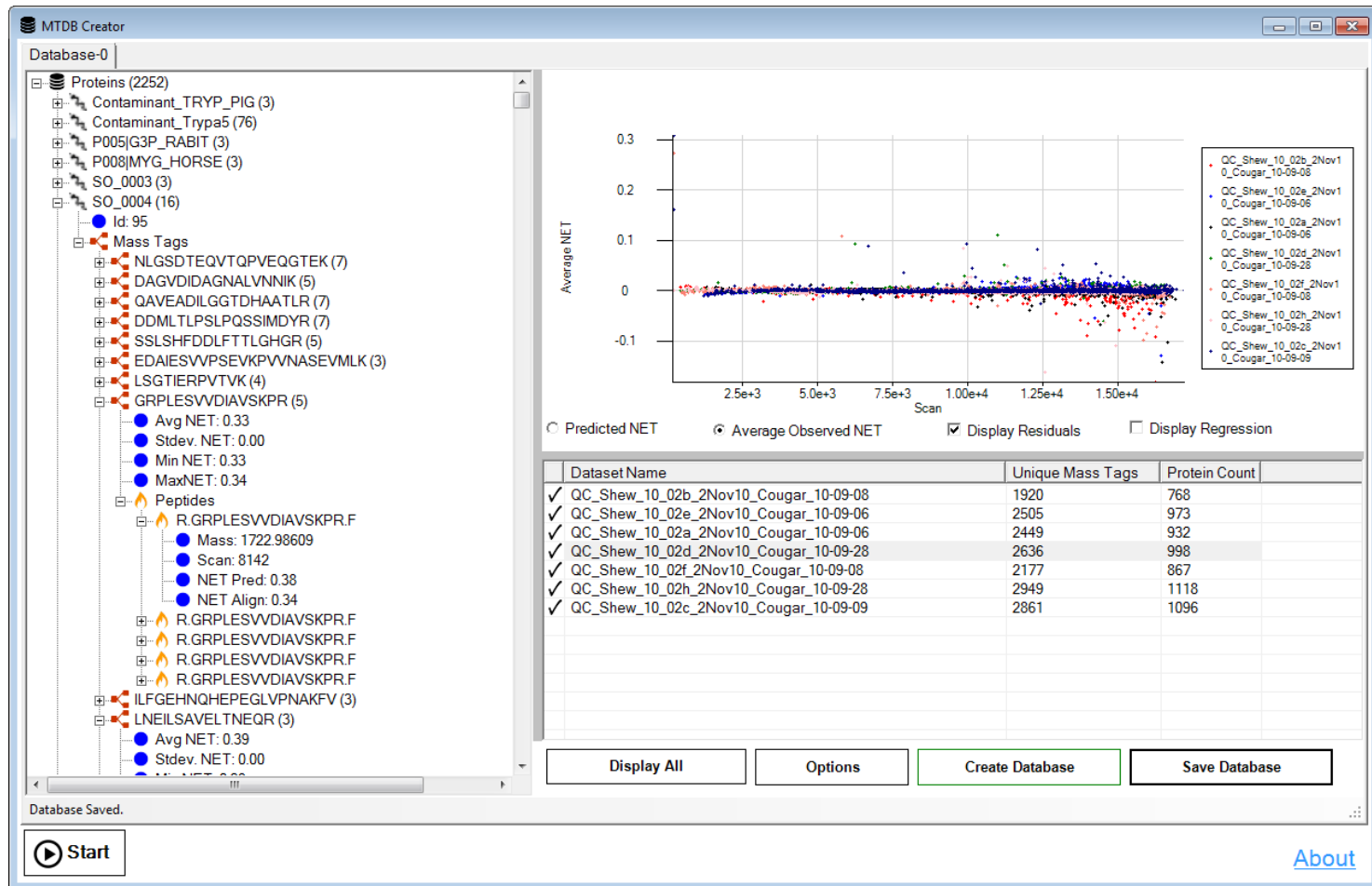
Start

About

# Save!



# Post Save



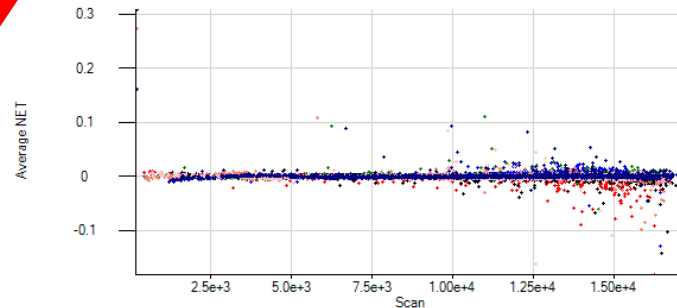
# Create another database?

Click Here To Start Another Database

The screenshot shows the MTDB Creator software interface. A red arrow points from the text "Click Here To Start Another Database" to the "Start" button at the bottom left. The interface displays a tree view of a database structure on the left, a scatter plot of Average NET vs Scan in the center, and a table of dataset statistics on the right.

**Database Structure (Left Panel):**

- Proteins (2252)
  - Contaminant\_TRYP\_PIG (3)
  - Contaminant\_Trypa5 (76)
  - P005[G3P\_RABIT (3)
  - P008[MYG\_HORSE (3)
  - SO\_0003 (3)
  - SO\_0004 (16)
    - Id: 95
      - Mass Tags
        - NLGSDTEQVTQPVEQGTEK (7)
        - DAGVIDDAGNALVNNIK (5)
        - QAVEADILGGTDHAATLR (7)
        - DDMLTLPSPQSSIMDYR (7)
        - SSLSHFDDLFTTLGHGR (5)
        - EDAIESVVPSEVKPVVNAVSEVMLK (3)
        - LSGTIERPVTVK (4)
        - GRPLESVVDIAVSKPR (5)
        - Avg NET: 0.33
        - Stdev. NET: 0.00
        - Min NET: 0.33
        - Max NET: 0.34
      - Peptides
        - R.GRPLESVVDIAVSKPR.F
          - Mass: 1727.0609
          - Scan: 81
          - NET P: 0.38
          - NET Sign: 0.34
        - R.GRPLESVVDIAVSKPR.F
        - R.GRPLESVVDIAVSKPR.F
        - R.GRPLESVVDIAVSKPR.F
        - R.GRPLESVVDIAVSKPR.F
        - ILFCINQHEPEGLVPNAKFV (3)
        - LMILSAVELTNEQR (3)
        - Avg NET: 0.39
        - Stdev. NET: 0.00
        - Min NET: 0.33
        - Max NET: 0.34



☐ Predicted NET ☒ Average Observed NET ☒ Display Residuals ☐ Display Regression

Dataset Name	Unique Mass Tags	Protein Count
✓ QC_Shew_10_02b_2Nov10_Cougar_10-09-08	1920	768
✓ QC_Shew_10_02e_2Nov10_Cougar_10-09-06	2505	973
✓ QC_Shew_10_02a_2Nov10_Cougar_10-09-06	2449	932
✓ QC_Shew_10_02d_2Nov10_Cougar_10-09-28	2636	998
✓ QC_Shew_10_02f_2Nov10_Cougar_10-09-08	2177	867
✓ QC_Shew_10_02h_2Nov10_Cougar_10-09-28	2949	1118
✓ QC_Shew_10_02c_2Nov10_Cougar_10-09-09	2861	1096

Display All

Options

Create Database

Save Database

Start

About