

# **PERCEPTRON** *v1.0.0.0*

A Next Generation Top-Down Proteoform  
Identification and Characterization Platform

## **USER MANUAL**

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### 3. Introduction to PERCEPTRON

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This chapter introduces the PERCEPTRON platform along with a description of its features.

#### 3.1. About PERCEPTRON

PERCEPTRON is a freely available web-based proteoform identification pipeline for application in Top-Down Proteomics (TDP). TDP is an emerging experimental protocol for analysis of intact proteoforms. PERCEPTRON search pipeline brings together algorithms for: (i) intact mass tuning, (ii) *de novo* peptide sequence tag extraction, (iii) *in silico* spectral comparison, (iv) identification of post-translational modifications as well as truncated proteins, and (v) a novel composite scoring scheme for candidate protein scoring. PERCEPTRON achieves high performance by leveraging NVIDIA GPU technology coupled with Microsoft ASP.NET and ANGULAR frameworks. The search results obtained include a list of proteins, their scores and details on the matching information. This information can be visualized as well as downloaded. PERCEPTRON aims to fill the crucial void of open-source and open-architecture protein identification software for TDP data, besides employing state-of-the-art algorithms.

#### 3.2. Features

The salient features of the pipeline are summarized below:

- **Graphical User Interface (GUI)** - A set of rich and intuitive graphical user interface has been developed for setting up the search parameters as well as for integrating the main components of the engine.
- **Whole Protein Molecular Weight Estimation** - The protein identification begins with the tuning of precursor protein's monoisotopic MW (MS1) as guided by its fragmentation spectra (MS2). Relative abundances and mass/charge ( $m/z$ ) ratios are used to calculate the consensus MW that is then employed in the search and scoring process.
- **Peptide Sequence Tag Extractor** - Peptide sequence tag ladders (PST) are extracted from the spectra by enumerating successive peaks having MW differences equal to an amino acid and within the user specified mass tolerance. Protein database is then filtered for proteins reporting these PSTs. The length of PST ladders, cumulative mass off-sets and relative abundances are used in calculating the PST scores.
- ***In silico* fragmentation** – *In silico* fragments of candidate proteins are generated by the user selected fragmentation techniques. *In vitro* and *in silico* spectral comparisons are performed and scored.
- **Post-translational Modification (PTM) Search** - Support for predicting typical PTMs has been provided in the tool. Users can select and search variable and fixed PTMs of their choice along with blind-PTMs by simply selecting them from the GUI.
- **Multifactorial Composite Scoring System** - A multifactorial candidate protein scoring scheme incorporating the aforementioned algorithms has been developed. User customization of the parameters and weights in the scoring function is admitted via a GUI.
- **Single and Batch Search** – PERCEPTRON provides support for search in single as well as batch modes. Towards an automated processing of multiple spectral data files, a batch processing mode allows for the selection of multiple files from the folder by clicking the attach file button. The

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experimental spectra, search parameters and results are automatically stored in the project directory for further processing and visualization.



## 4. Getting Started

PERCEPTRON user manual, sample dataset and software issues database is available (under the MIT open license) at <https://perceptron.lums.edu.pk/>

To initiate use of PERCEPTRON, the user may choose to register and log in by clicking on “Log in” (Figure 1) or continue as a guest without registration.

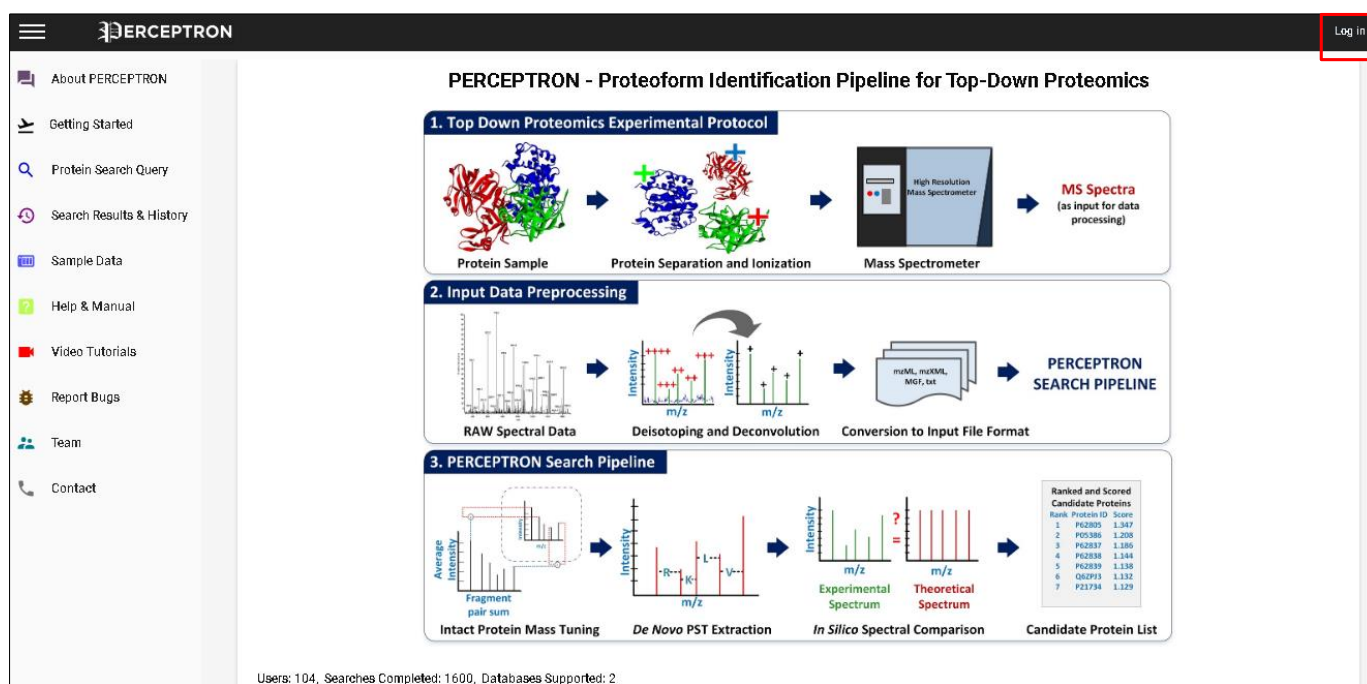
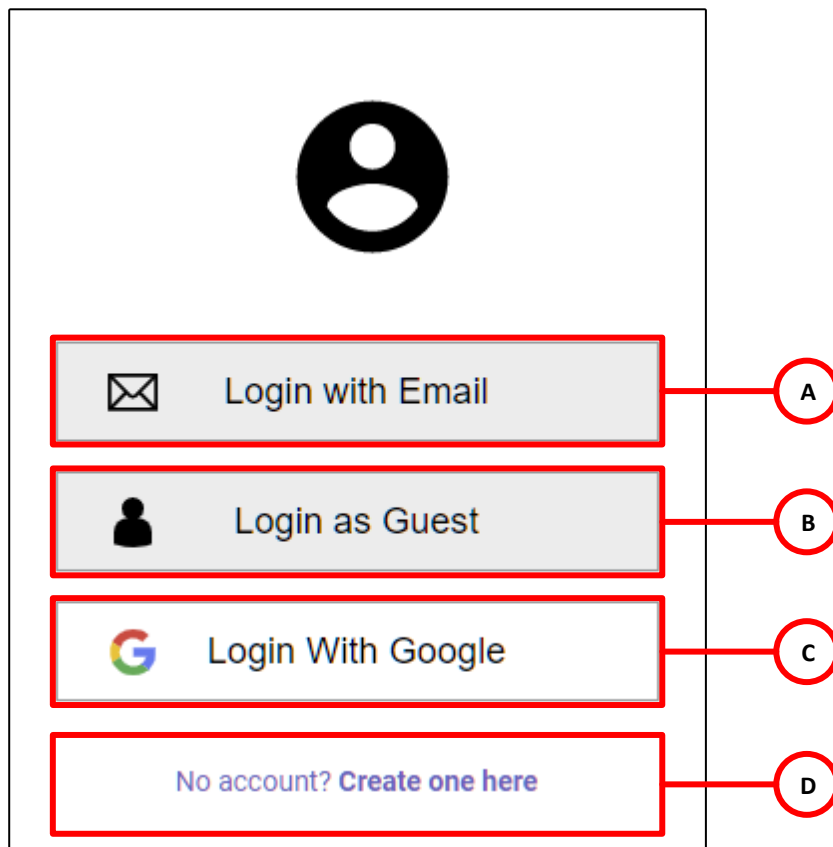


Figure 1. PERCEPTRON Homepage and Log in button

Click the ‘**Log in**’ button on the top right. A window will appear. Enter user credentials to proceed.



*Figure 2. PERCEPTRON Login options*

- A. User can create PERCPETRON account to login using an existing email account
- B. Enables user to login as a guest\* without the need to create a PERCEPTRON user account to perform search in PERCEPTRON
- C. User can login using an existing google account to use PERCEPTRON
- D. Create a user account to perform search in PERCEPTRON

\*Note that results will not be saved on the server side in this case.

## 5. Graphical User Interfaces

This chapter presents the interface overview for user facilitation (Figure 3).

### 5.1 Window 1: PERCEPTRON Homepage

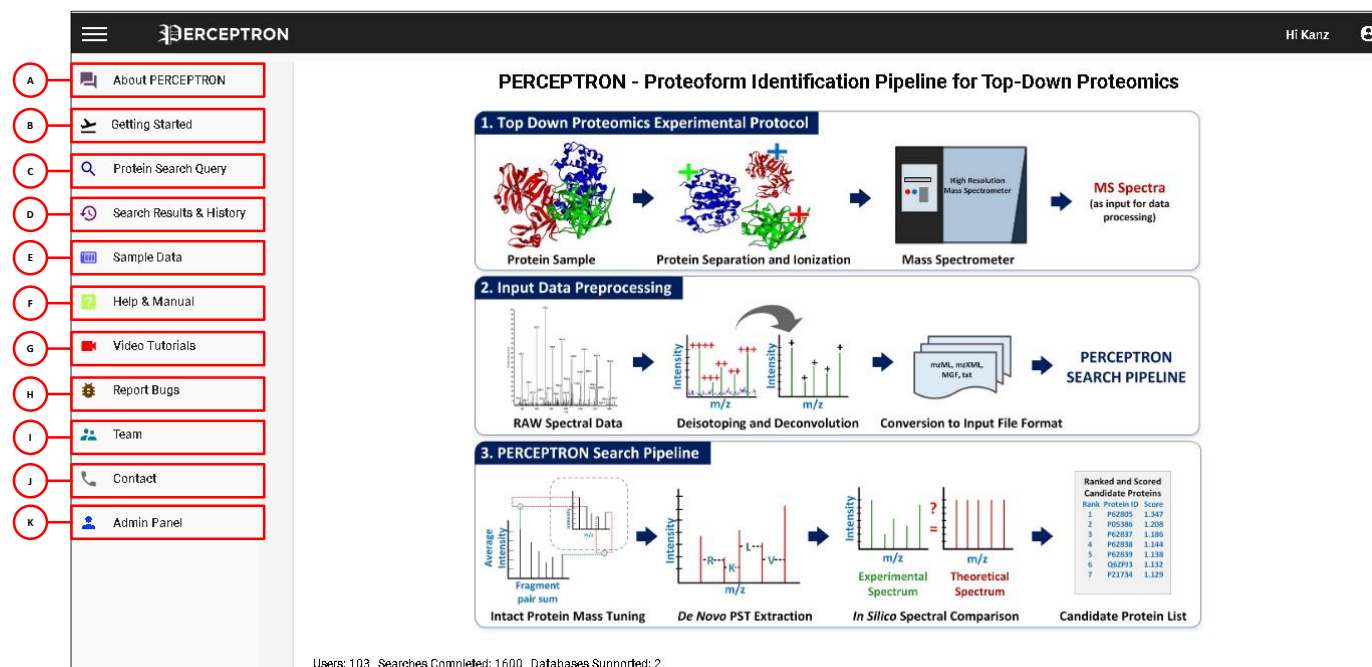


Figure 3. PERCEPTRON - Overview of User Interface

- A. About PERCEPTRON: A next-generation top-down proteoform search and identification platform
- B. Getting Started: Quick guide to proteoform search and identification using PERCEPTRON
- C. Protein Search Query: Job submission - Search top-down proteomics data files to identify and characterize proteoforms
- D. Search Results & History: View search results and history
- E. Sample Data: Sample top-down proteomics data for use with PERCEPTRON
- F. Help & Manual: Get assistance with using PERCEPTRON and download manual
- G. Video Tutorials: View step-by-step video tutorials demonstrating usage of PERCEPTRON
- H. Report Bugs: Report problems and issues here
- I. Team: PERCEPTRON project team members
- J. Contact: Contact us for further information
- K. Admin Panel: For updating or downloading protein database

## 5.2 Window 2: Protein Search Query

In order to start protein search, click on the ‘Protein Search Query’ tab and the following window (Figure 4) will appear.

### 5.2.1 Basic Parameters

Figure 4. PERCEPTRON - Overview of Basic Parameters

- A. In order to start protein search, user must enter the ‘Protein Search Title’ (for example: “MyProject”)
- B. Select protein database
- C. Browse and upload experimental data (.mzXML/ .MGF/ .txt)\* for Single mode; Peak-list files for Batch mode
- D. Enter the email address at which the link for downloading results will be sent. Note that users are notified about the availability of search results upon completion of the job
- E. Enter an FDR percentage to shortlist identified proteoforms at desired FDR cut off
- F. Provide the number of candidate protein hits to be received in results.

\*Note: File size must not exceed 60MB.

## 5.2.2 Set Experimental Parameters

The screenshot displays the PERCEPTRON web application interface. On the left is a sidebar with navigation links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, Contact, and Admin Panel. The main content area is titled 'Set Experimental Parameters' and contains several sections: 'Set Experimental Parameters' (with sub-sections for Mass Mode, Peptide Tolerance, Intact Mass Tolerance, Neutral Mass Loss, Tune Intact Protein Mass, Select Fragmentation Type, and Select Special Ions), 'Set De Novo Sequencing Parameters', 'Set Protein Modifications Parameters', and 'Set Scoring Components Weight \*'. Red boxes and lines highlight specific parameters and their corresponding labels A through I.

Labels and their corresponding parameters:

- A: Mass Mode (radio buttons for MH+ and M(Neutral))
- B: Peptide Tolerance (text input field)
- C: Slider Value (range input field)
- D: Select Fragmentation Type (dropdown menu)
- E: Filter Database using MS1 (checkbox)
- F: Intact Mass Tolerance (text input field)
- G: Neutral Mass Loss (text input field)
- H: Tune Intact Protein Mass (checkbox)
- I: Select Special Ions (dropdown menu)

Figure 5. PERCEPTRON - Overview of Experimental Parameters

- Select Mass Mode. MS data can only be provided in either m/z form with  $z = 1$  or neutral masses
- Select the tolerance value for Peptide and select its unit
- Select the 'slider value' to provide a range for tuning MS1 using 'Tune Intact Protein Mass' option
- Select the 'Fragmentation type' from drop down menu
- User can filter database by checking the option 'Filter Database using MS1'
- Set the tolerance value for Protein Mass and select its unit
- Provide the value of Neutral loss, if any
- Check the option 'Tune Intact Protein Mass' to allow for tuning of MS1 using MS2 data
- Choose the corresponding special ions for the type of fragmentation selected (i.e. a', b', y', z'', a\*, b\*, y\*, z' ions)

## 5.2.3 Set de novo Sequencing Parameters

The screenshot shows the PERCEPTRON web interface. The sidebar on the left contains links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, Contact, and Admin Panel. The main content area has a top section with 'Peptide Tolerance \*', 'Tune Intact Protein Mass' checkbox, 'Neutral Mass Loss' slider, 'Slider Value', 'Select Fragmentation Type \*', and 'Select Special Ions'. Below this is the 'Set De Novo Sequencing Parameters' section, which includes:
 

- A**: ☐ Enable PST Filtering
- B**: Tolerance For Each Hop (D8)
- C**: Set De Novo Sequencing Parameters (header)
- D**: Minimum Tag Length (dropdown)
- E**: Maximum Tag Length (dropdown)
- Overall tolerance for PST (dropdown)

 Below this section are 'Set Protein Modifications Parameters' and 'Set Scoring Components Weight \*' sections. At the bottom right are 'Reset' and 'Submit' buttons.

Figure 6. PERCEPTRON - Overview of De Novo Sequencing Parameters

- A. Check 'Enable PST Filtering' to filter PSTs
- B. Set the 'Tolerance for each Hop'
- C. Tags will be filtered above the minimum length of PST selected from the drop-down menu by the user
- D. Tags will be filtered below the maximum length of PST selected from the drop-down menu by the user
- E. Overall mass error tolerance shows error margin for the whole PST

**Note:** Input value for Minimum and Maximum Tag length should be different. Minimum Tag Length should be smaller than Maximum Tag Length.

## 5.2.4 Set Protein Modifications Parameters

The screenshot shows the 'Set Protein Modifications Parameters' section of the PERCEPTRON web application. The interface is divided into a sidebar on the left and a main content area on the right. The sidebar contains navigation links: 'About PERCEPTRON', 'Getting Started', 'Protein Search Query', 'Search Results & History' (A), 'Sample Data' (B), 'Help & Manual', 'Video Tutorials', 'Report Bugs', 'Team', 'Contact', and 'Admin Panel'. The main content area is titled 'Set Protein Modifications Parameters' and contains several input fields and dropdown menus. A red box labeled 'A' highlights the 'Handle Truncated Proteoforms' checkbox. A red box labeled 'B' highlights the 'Terminal Modification \*' dropdown menu. A red box labeled 'C' highlights the 'Blind-PTM Search' checkbox. A red box labeled 'D' highlights the 'PTM Tolerance \*' input field. A red box labeled 'E' highlights the 'Methionine Chemical Modifications' dropdown menu. A red box labeled 'F' highlights the 'Variable Modifications' dropdown menu. A red box labeled 'G' highlights the 'Cysteine Chemical Modifications' dropdown menu. A red box labeled 'H' highlights the 'Fixed Modifications' dropdown menu. The 'List of Modifications' section on the left lists various modifications: Acetylation\_A, Acetylation\_K, Acetylation\_S, Amidation\_F, Hydroxylation\_P, Methylation\_K, Methylation\_R, N\_Linked\_Glycosylation\_N, O\_Linked\_Glycosylation\_T, and O\_Linked\_Glycosylation\_S. The 'Set Scoring Components Weight \*' section is at the bottom. The 'Reset' and 'Submit' buttons are at the bottom right.

Figure 7. PERCEPTRON - Overview of Protein Modifications Parameters

- Check 'Handle Truncated Proteoforms' to allow search for truncated proteoforms.
- Allows the user to select specified terminal modifications. PERCEPTRON handles four cases: 1) None – No modification, 2) NME – N terminal methionine excision, 3) NME\_ACETYLTATION – N terminal acetylation with initiator methionine removed, and 4) M\_ACETYLTATION – N terminal methionine acetylation
- Select whether to perform Blind-PTM search and unknown modifications
- Set the tolerance value for Post Translational Modification (PTM) site selection
- Allows the user to select instrument specific modification on Methionine
- User can opt for required Variable 'Post translation Modifications' from the list of modifications
- Allows the user to select instrument specific modification on Cysteine
- Similarly, various 'Fixed Modifications' are also selected from the list

## 5.2.5 Set Scoring Components Weight

The screenshot displays the PERCEPTRON web application interface. The sidebar on the left contains navigation links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, Contact, and Admin Panel. The top header shows the PERCEPTRON logo and user information 'Hi! Kanz'. The main content area includes a 'Protein Search Title' field, an 'Enter your Email Address' field, a 'Select Database' dropdown, and an 'Upload Mass-Spectrometry Data' button with a file upload icon. Below these are sections for 'Set Experimental Parameters', 'Set De Novo Sequencing Parameters', 'Set Protein Modifications Parameters', and 'Set Scoring Components Weight\*'. The 'Set Scoring Components Weight\*' section is highlighted with a red box and labeled 'A'. It contains three sliders for 'Intact Protein Mass Score Weightage (%)', 'Peptide Sequence Tags Score Weightage (%)', and 'Spectral Comparisons Score Weightage (%)'. A red circle with the letter 'A' points to the third slider. Below the sliders, a note states: '\* Set weight for at least one of the components.' At the bottom right, there are 'Reset' and 'Submit' buttons.

Figure 8. PERCEPTRON - Overview of Scoring Component Weight

- A. Set the desired weights of Scoring Components towards computing scores by shifting the slider left or right accordingly



## 5.3 Window 3: Visualizing Search Results

User Search History				
Sr. #	Search Title	Creation Time	Status	
1	Default Run	2020/12/19 14:05:46	Completed	
2	MzXML_18122020	2020/12/18 15:02:56	Completed	
3	MGF_18122020	2020/12/18 14:39:55	Completed	
4	MzML_18122020	2020/12/18 14:39:24	Completed	
5	MzXML_18122020	2020/12/18 14:38:49	Completed	
6	CS1_Hela_batch	2020/12/18 14:19:33	Completed	
7	CS1_Hela_140s_single	2020/12/18 14:19:09	Completed	
8	CS2_ETD_17122020	2020/12/17 23:48:37	Completed	
9	Ecoli_ETD_CS2_batch	2020/12/16 18:18:17	Completed	
10	Hela_CS1_batchmode	2020/12/16 13:00:30	Completed	
11	Hela_CS1_single_140s	2020/12/16 01:08:14	Completed	
12	Hela_CS1_batch	2020/12/16 01:06:34	Completed	

Figure 9. User Search History window showing search results

User can view search history in ‘Search Results and History’ tab (Figure 9) with respective search titles. Latest search results are provided on the top. Click on the ‘Search Title’ to go to ‘Protein Spectral Matches’ which enlists the proteoforms identified from the search (Figure 10).

Protein Spectral Matches				
Sr. #	File Name	Protein ID	Protein Score	Molecular Weight
1	HELA_pk19_sw1_210sc_mono.txt	P62805	0.0696	11360.3815

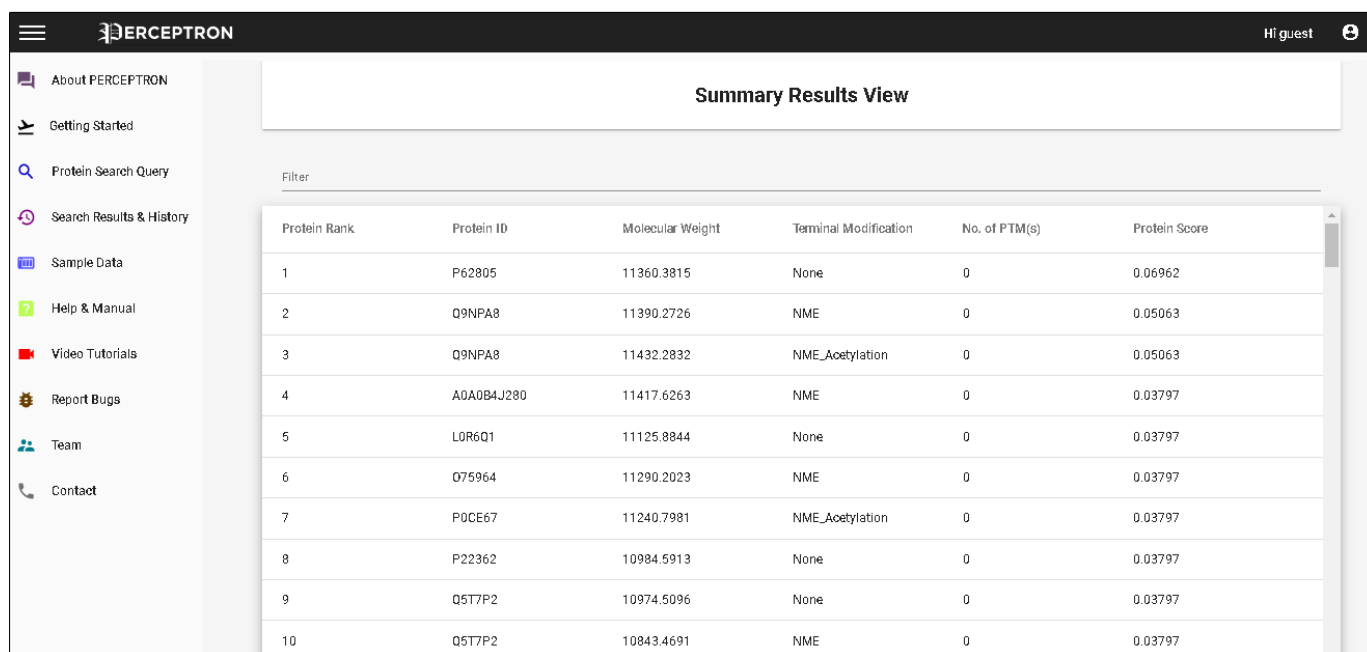
Items per page: 10 0 of 0

Figure 10. Protein spectral matches window showing results for the protein search query

Click on the results under ‘File Name’ to go to ‘Summary Results’ window (Figure 11). User can download results as a zip folder by clicking ‘Results Download.’

**Note:** Results are downloadable and kept on the server for 2 days. There is no way to retrieve the data older than 48 hours.

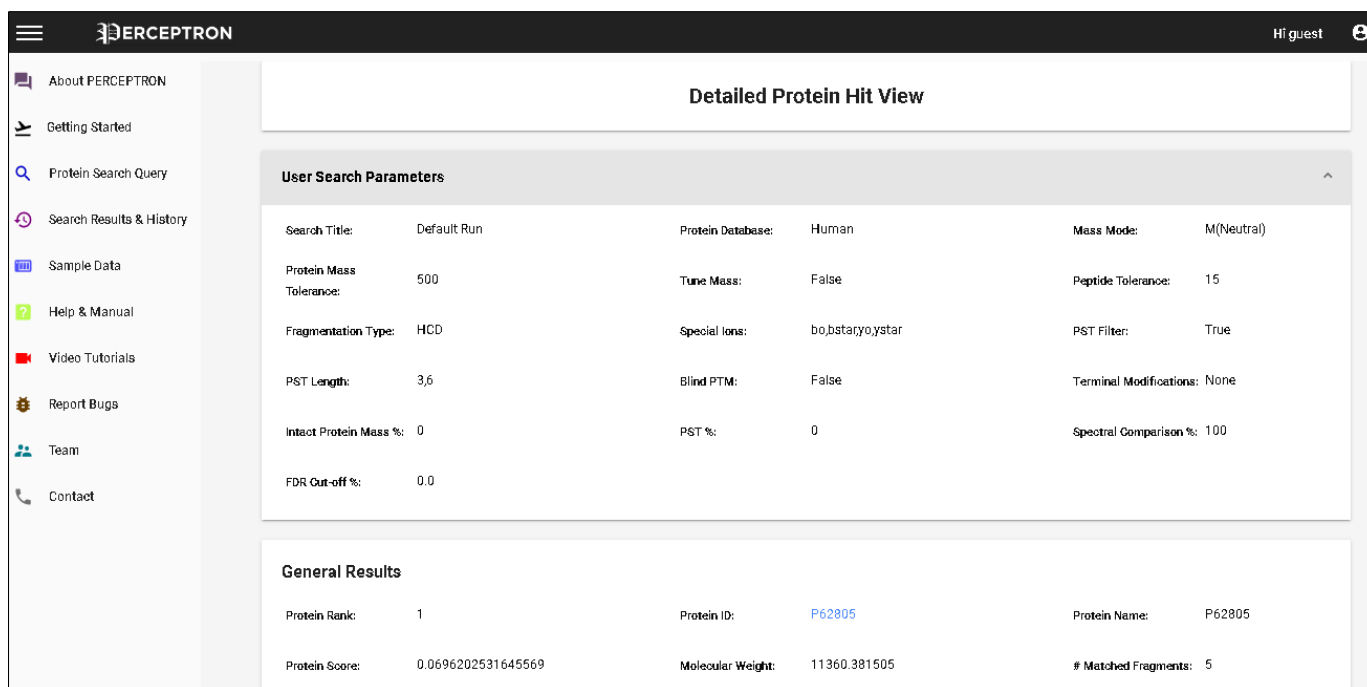
## 5.4 Window 4: Summary and Detailed Results View



Protein Rank	Protein ID	Molecular Weight	Terminal Modification	No. of PTM(s)	Protein Score
1	P62805	11360.3815	None	0	0.06962
2	Q9NPA8	11390.2726	NME	0	0.05063
3	Q9NPA8	11432.2832	NME_Acetylation	0	0.05063
4	A0A0B4J280	11417.6263	NME	0	0.03797
5	L0R6Q1	11125.8844	None	0	0.03797
6	Q75964	11290.2023	NME	0	0.03797
7	P0CE67	11240.7981	NME_Acetylation	0	0.03797
8	P22362	10984.5913	None	0	0.03797
9	Q5T7P2	10974.5096	None	0	0.03797
10	Q5T7P2	10843.4691	NME	0	0.03797

Figure 11. Summary Results window showing candidate proteins

Proteins found after the search are reported along with their Protein ID, Molecular Weight, Terminal Modifications, Number of Post-Translational Modifications (PTMs) and Protein Scores. User can click on any 'Protein ID' to see the details of the selected proteoform in 'Detailed Protein Hit View' (Figure 12).



User Search Parameters					
Search Title:	Default Run	Protein Database:	Human	Mass Mode:	M(Neutral)
Protein Mass Tolerance:	500	Tune Mass:	False	Peptide Tolerance:	15
Fragmentation Type:	HCD	Special Ions:	b,bstaryo,ystar	PST Filter:	True
PST Length:	3,6	Blind PTM:	False	Terminal Modifications:	None
Intact Protein Mass %:	0	PST %:	0	Spectral Comparison %:	100
FDR Cut-off %:	0.0				

General Results					
Protein Rank:	1	Protein ID:	P62805	Protein Name:	P62805
Protein Score:	0.0696202531645569	Molecular Weight:	11360.381505	# Matched Fragments:	5

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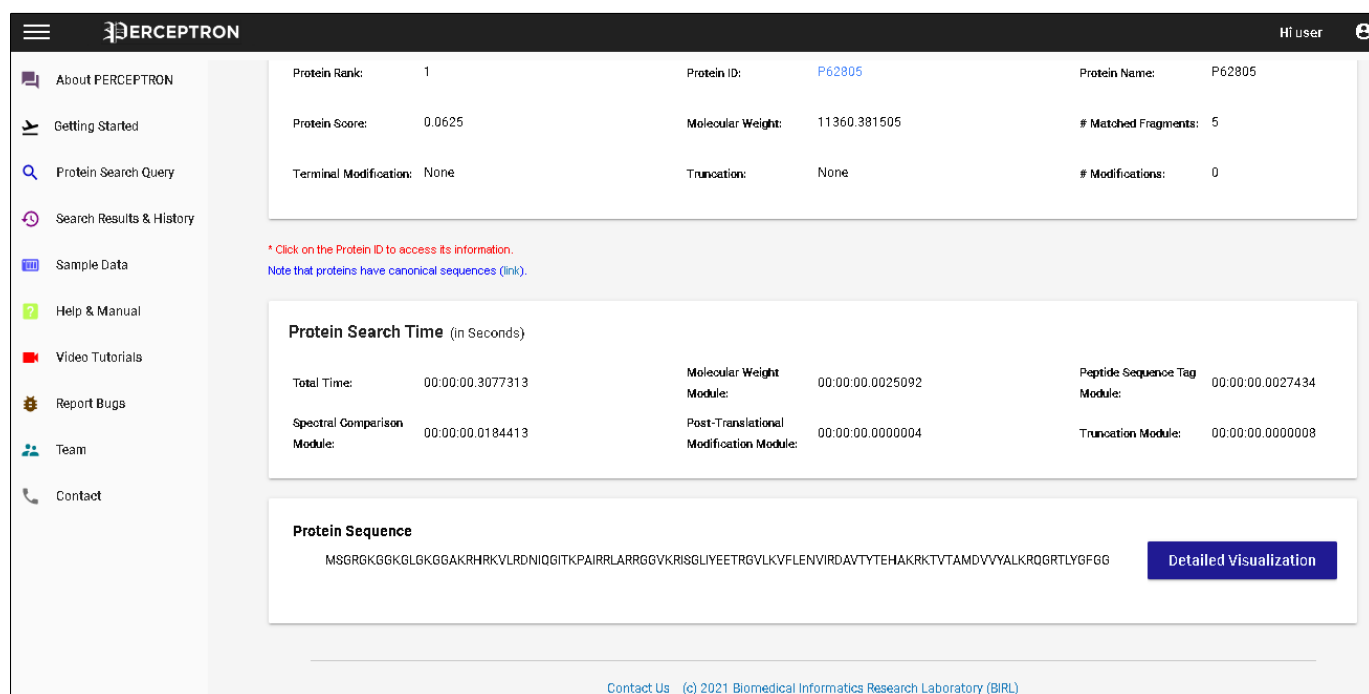


Figure 12. Detailed Results window showing search parameters and general results (top). Detailed Protein Hit View window showing Protein Search Time and Protein Sequence (bottom)

‘Detailed Protein Hit View’ window shows Search Parameters added while submitting protein search query. ‘General Results’ tab indicates an overview of search results. User can scroll down to view ‘Protein Search Time’ indicating runtimes for each algorithmic component. ‘Protein sequence’ shows the sequence of selected proteoform. PERCEPTRON offers visualization of search results. User can click ‘Detailed Visualization’ to visualize search results in detail (Figure 13-15).

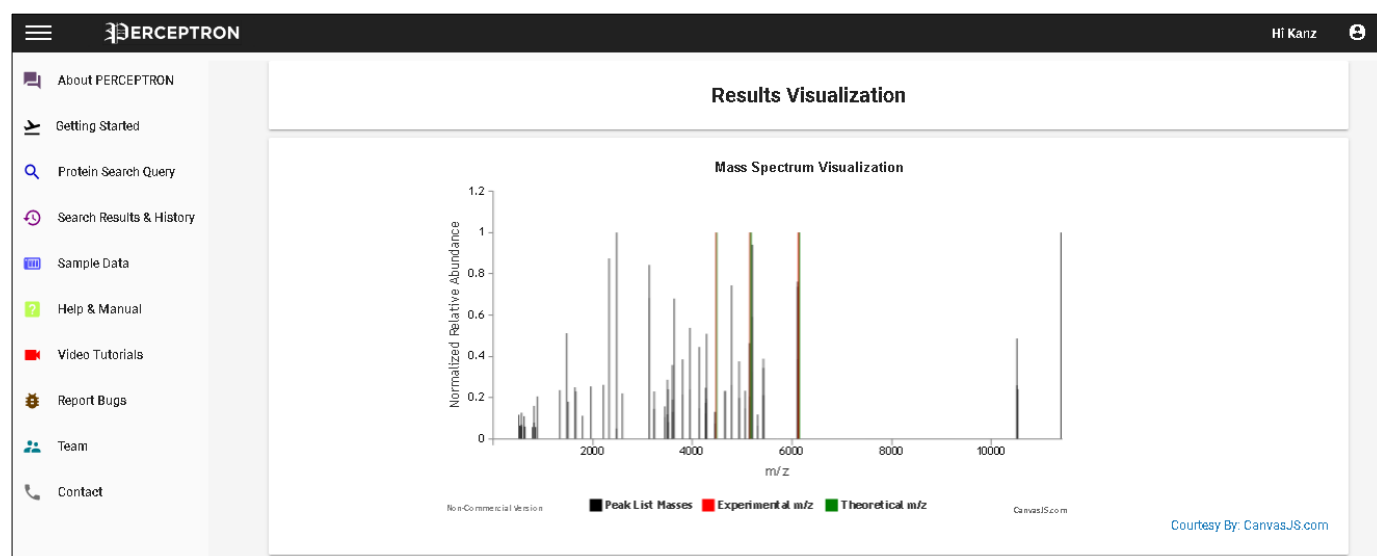


Figure 13. Detailed Results Visualization window with mass spectral visualization

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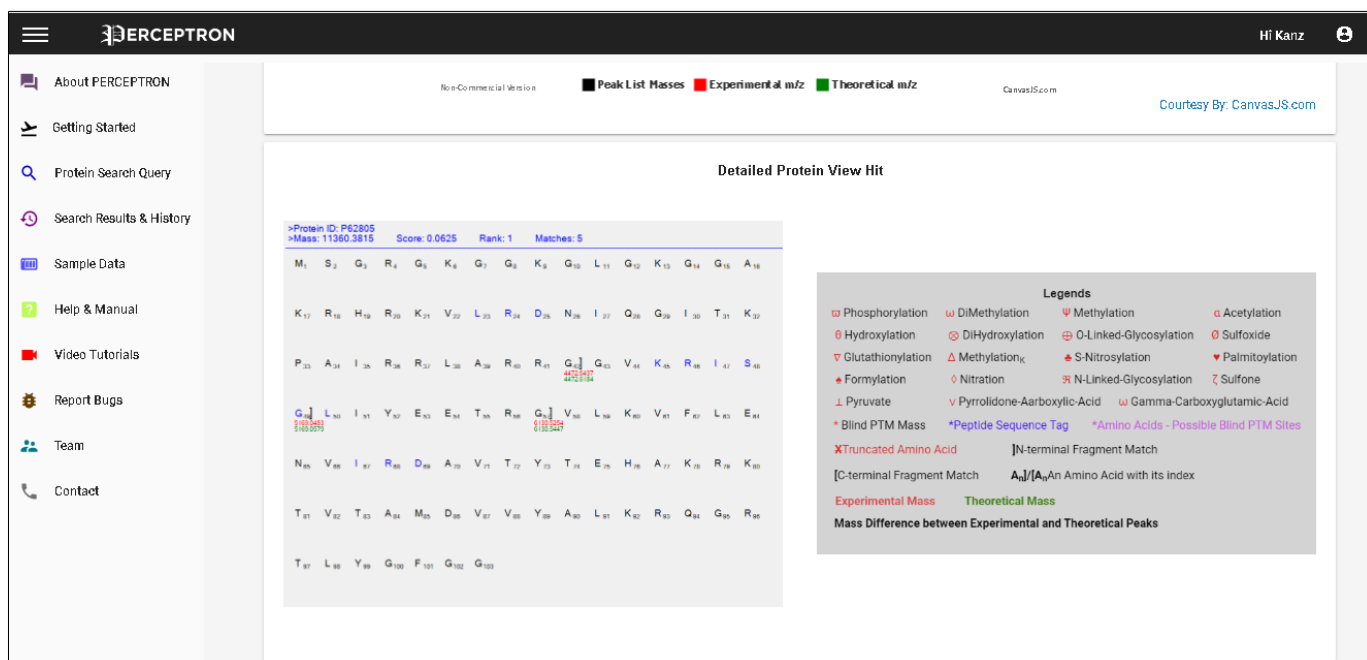


Figure 14. Detailed Results Visualization window with Detailed Protein Hit View (left) and Legends (right)

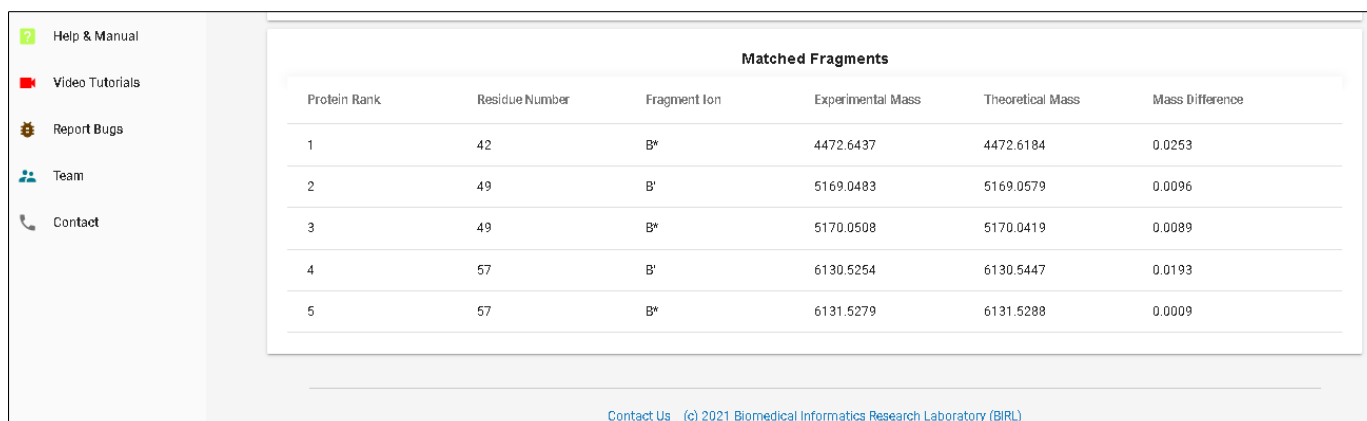


Figure 15. Detailed Results Visualization window with Matched Fragments

## 6. Performing Proteoform Search

### 6.1 File Formats Conversion

PERCEPTRON provides support for plain text files (data in columns containing mass to charge ratios ( $m/z$ ) and relative intensities), eXtensible Markup Language (XML) files with  $m/z$  and relative abundances (mzXML)<sup>1</sup>, Mass Spectrometry Markup Language (mzML)<sup>2,3</sup> and Mascot Generic Format (MGF)<sup>4</sup> data formats in both single and batch file processing modes.

#### 6.1.1 Raw to mzML File Format Conversion

Raw data files can be converted to mzML file format by using MS-Convert<sup>5</sup> (Figure 16).

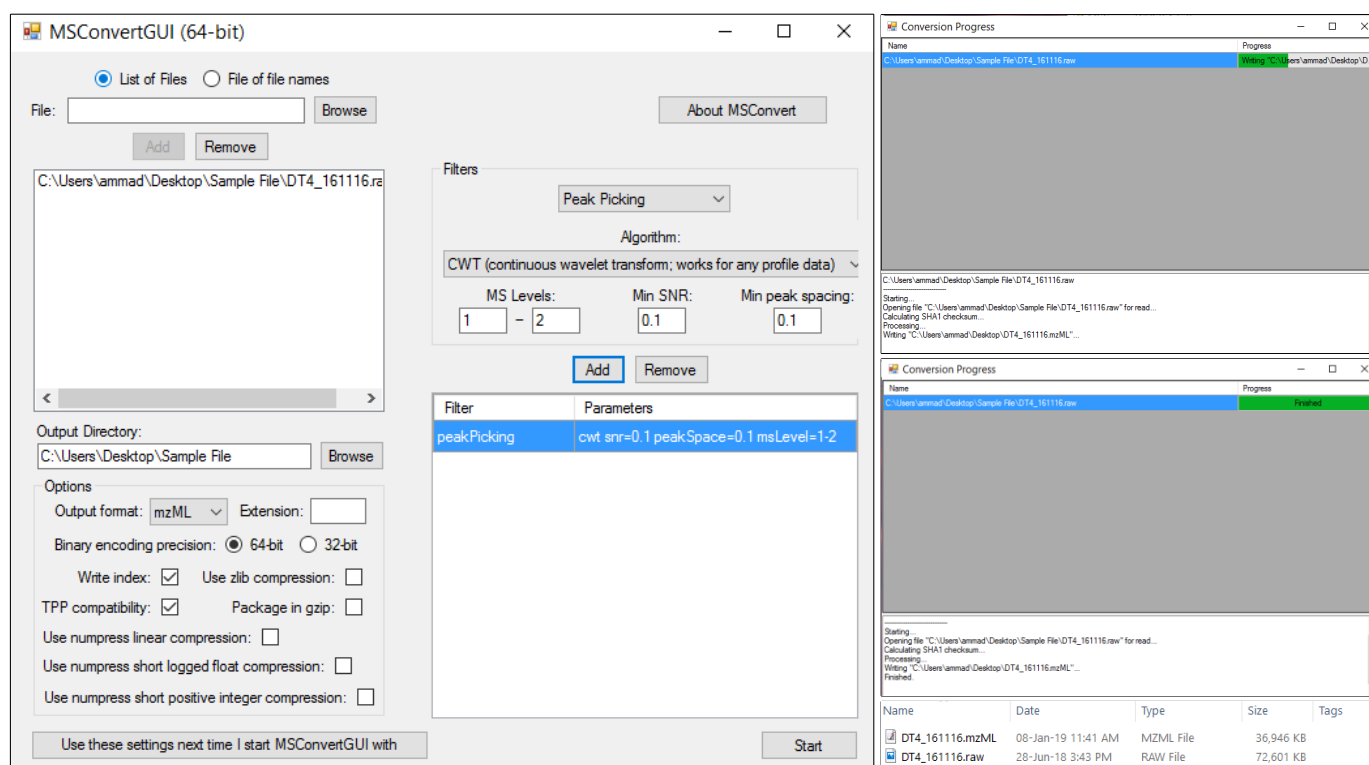


Figure 16. Conversion of raw to mzML

#### 6.1.2 Raw to mzXML File Format Conversion

User can convert raw data files to mzXML file format by using MS-Convert<sup>5</sup> (Figure 17).

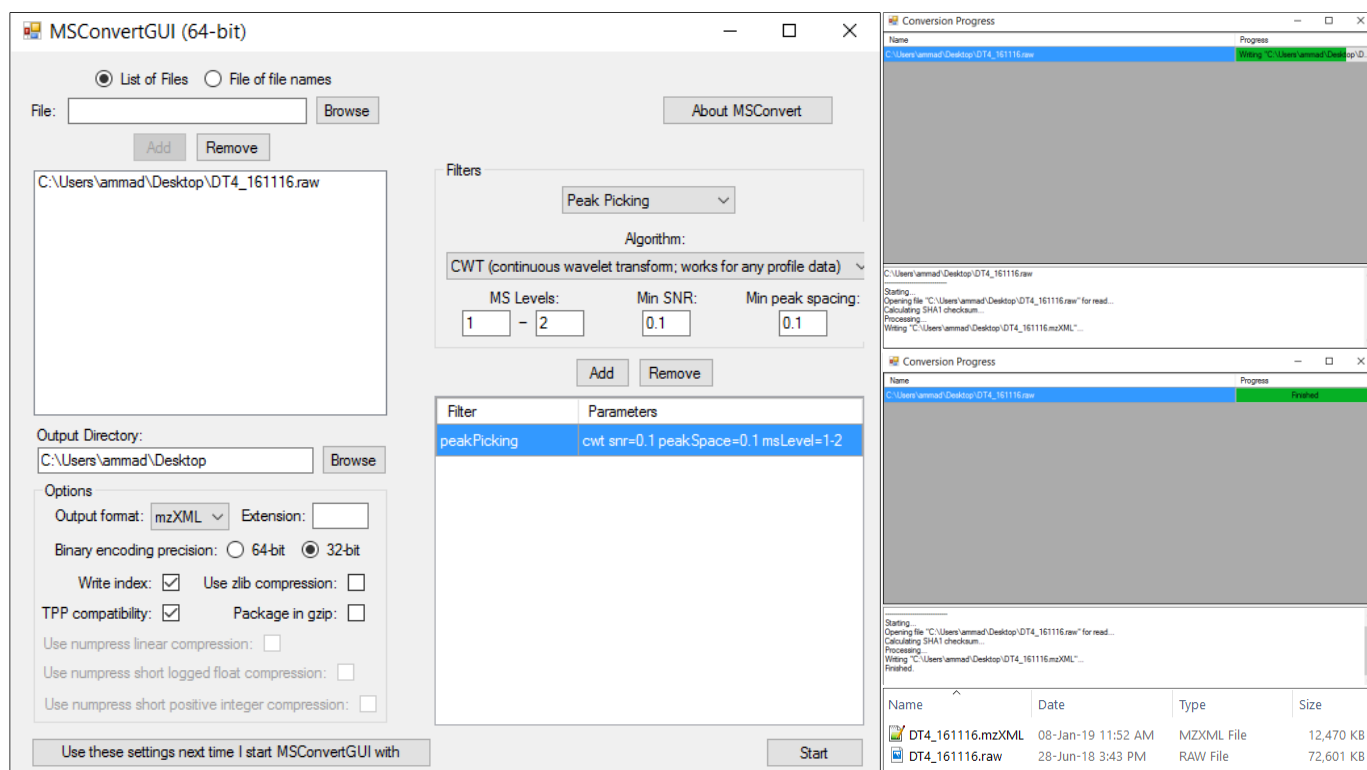


Figure 17. Conversion of raw to mzXML

### 6.1.3 MzXML to MGF File Format Conversion

User can convert mzXML files to MGF using MS-Decov<sup>6</sup> (Figure 18).

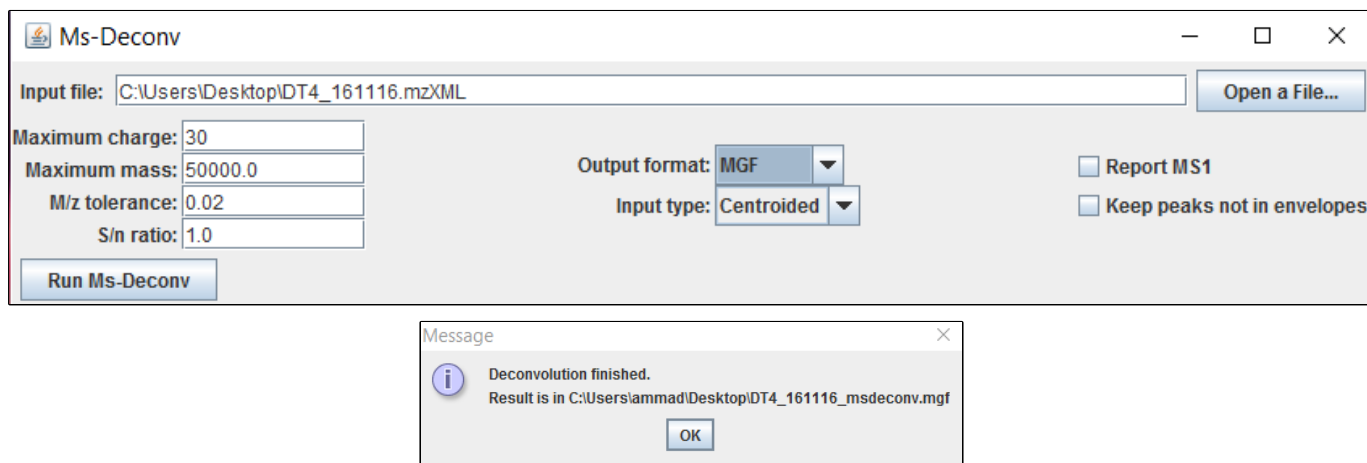


Figure 18. Conversion of mzXML to MGF

### 6.1.4 MGF to Flat Text File Format Conversion

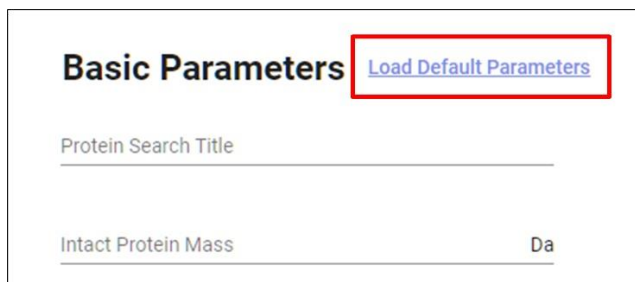
PERCEPTRON converts MGF files to flat text (peak list) using built-in custom file reader.

## 6.2 Search Parameters

PERCEPTRON can employ from the following set of search parameters including: (i) Default Parameters, and (ii) Selected parameters.

### How to load default Parameters?

To submit the job using default parameters, select 'Load Default Parameters' option in front of Basic Parameters (Figure 19).

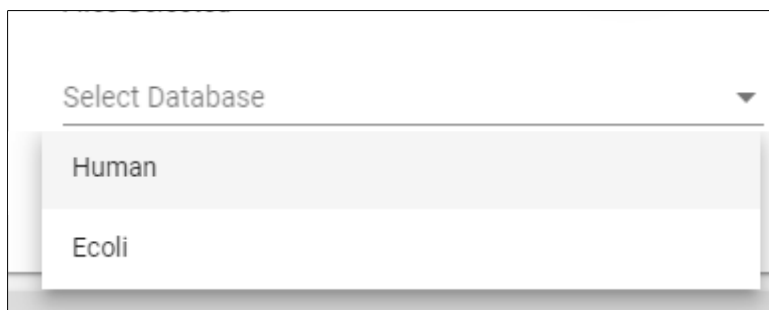


The image shows a web form titled "Basic Parameters". To the right of the title is a button labeled "Load Default Parameters", which is highlighted with a red rectangular box. Below the title, there are two input fields. The first is labeled "Protein Search Title" and has a horizontal line for text entry. The second is labeled "Intact Protein Mass" and has a horizontal line for text entry, followed by the unit "Da".

Figure 19. Load Default Parameters

## 6.3 Protein Databases

SwissProt database is included in PERCEPTRON by default. User can take any protein sequence from other databases (such as Uniprot) in '.fasta' format (Figure 20).



The image shows a dropdown menu with the label "Select Database" at the top. The menu is open, displaying two options: "Human" and "Ecoli". The "Human" option is highlighted with a light gray background.

Figure 20. Selecting Protein Database

## 6.4 Search Modes

The search modes are auto-selected based on the number of files that the user inputs. If one file is given as input, PERCEPTRON runs single search mode whereas if multiple files are given as input, the mode switches to batch mode.

- (i) Single Search Mode
- (ii) Batch Mode

Batch mode takes more processing time as it deals with larger data. The experimental spectra, search parameters and results are automatically stored in the project directory for further processing and visualization.

## 7. Results Visualization and Interpretation

This chapter presents an overview of interpreting results obtained using PERCEPTRON.

Sr. #	Search Title	Creation Time	Status
1	Default Run	2020/12/19 14:05:46	Completed
2	MzXML_18122020	2020/12/18 15:02:56	Completed
3	MGF_18122020	2020/12/18 14:39:55	Completed
4	MzXML_18122020	2020/12/18 14:39:24	Completed
5	MzXML_18122020	2020/12/18 14:38:49	Completed
6	CS1_Hela_batch	2020/12/18 14:19:33	Completed
7	CS1_Hela_140s_single	2020/12/18 14:19:09	Completed
8	CS2_ETD_17122020	2020/12/17 23:48:37	Completed
9	Ecoli_ETD_CS2_batch	2020/12/16 18:18:17	Completed
10	Hela_CS1_batchmode	2020/12/16 13:00:30	Completed
11	Hela_CS1_single_140so	2020/12/16 01:08:14	Completed
12	Hela_CS1_batch	2020/12/16 01:06:34	Completed

1. 'User Search History' in 'Search Results and History' tab shows search results with 'Search Title.' User can go to 'Protein Spectral Matches' by clicking the 'Search Title.'

Sr. #	File Name	Protein ID	Protein Score	Molecular Weight
1	HELA_pk19_sw1_210sc_mono.txt	P62805	0.0696	11360.3815

2. In 'Protein Spectral Matches,' user can download results by clicking 'Results Download' option provided on top right. The results along with search parameters will be downloaded as a '.zip' folder.
3. File name indicates the data file used for performing protein search. User can view the top-ranked proteoform identified (Protein ID) along with its protein score and molecular weight. By clicking the 'Protein ID,' user can go to 'Summary Results View.'

**Note:** 'Detailed Visualization' feature is not provided for proteoform search in batch mode. For batch mode, users can only download results as a .zip folder using the 'Results Download' option.



Protein Rank	Protein ID	Molecular Weight	Terminal Modification	No. of PTM(s)	Protein Score
1	P62805	11360.3815	None	0	0.06962
2	Q9NPA8	11390.2726	NME	0	0.05063
3	Q9NPA8	11432.2832	NME_Acetylation	0	0.05063
4	A0A0B4J280	11417.6263	NME	0	0.03797
5	L0R6Q1	11125.8844	None	0	0.03797
6	Q75964	11290.2023	NME	0	0.03797
7	P0CE67	11240.7981	NME_Acetylation	0	0.03797
8	P22362	10984.5913	None	0	0.03797
9	Q5T7P2	10974.5096	None	0	0.03797
10	Q5T7P2	10843.4691	NME	0	0.03797

- ‘Summary Results View’ shows the list of proteoforms identified from the data file provided by the user. Clicking the ‘Protein ID’ leads user to ‘Detailed Protein Hit View.’

User Search Parameters					
Search Title:	Default Run	Protein Database:	Human	Mass Mode:	M(Neutral)
Protein Mass Tolerance:	500	Tune Mass:	False	Peptide Tolerance:	15
Fragmentation Type:	HCD	Special Ions:	bo,bstaryo,ystar	PST Filter:	True
PST Length:	3,6	Blind PTM:	False	Terminal Modifications:	None
Intact Protein Mass %:	0	PST %:	0	Spectral Comparison %:	100
FDR Cut-off %:	0.0				

General Results			
Protein Rank:	1	Protein ID:	P62805
Protein Score:	0.0696202531645569	Molecular Weight:	11360.381505
		Protein Name:	P62805
		# Matched Fragments:	5

- ‘Detailed Protein Hit View’ has ‘User Search Parameters’ on top.
- Below search parameters panel is ‘General Results’ which gives user details of the selected proteoform.

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**PERCEPTRON** Hi user

**Protein Rank:** 1 **Protein ID:** [P62805](#) **Protein Name:** P62805

**Protein Score:** 0.0625 **Molecular Weight:** 11360.381505 **# Matched Fragments:** 5

**Terminal Modification:** None **Truncation:** None **# Modifications:** 0

\* Click on the Protein ID to access its information.  
Note that proteins have canonical sequences ([link](#)).

**Protein Search Time** (in Seconds)

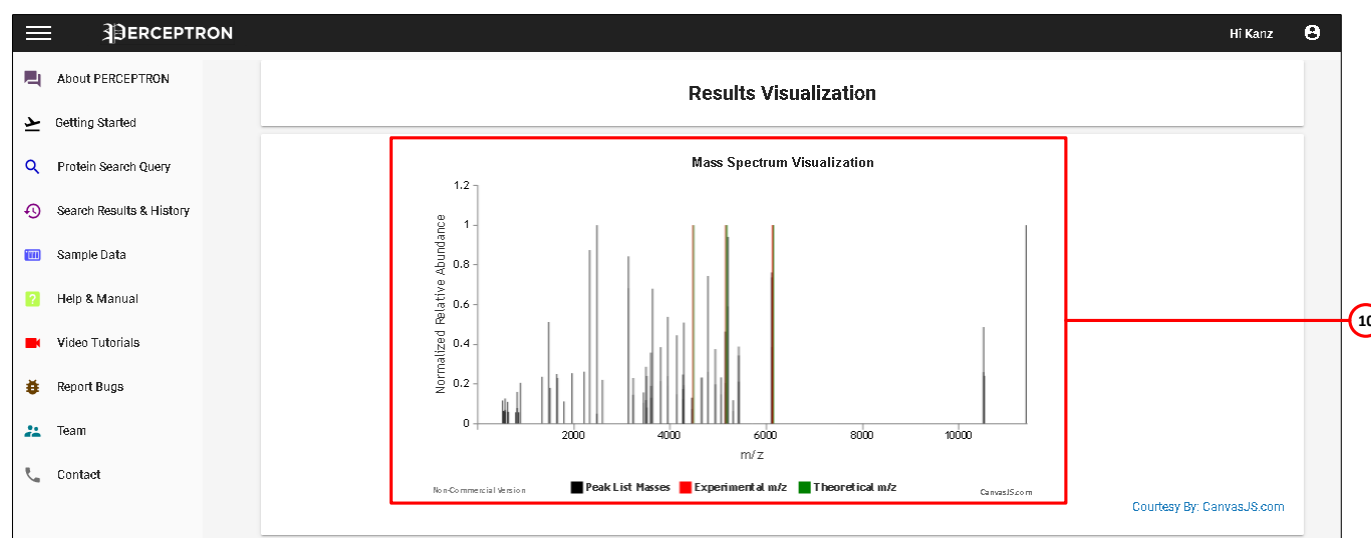
Total Time:	00:00:00.3077313	Molecular Weight Module:	00:00:00.0025092	Peptide Sequence Tag Module:	00:00:00.0027434
Spectral Comparison Module:	00:00:00.0184413	Post-Translational Modification Module:	00:00:00.0000004	Truncation Module:	00:00:00.0000008

**Protein Sequence**  
MSGRGKGGKGLGKGGAKRHRKVLRDNIQGITKPAIRRLARRGGVKRISGLIYEETRGVLKVFLENVIRDVITYTEHAKRKTVTAMDVVYALKRQGRITLYGFGG

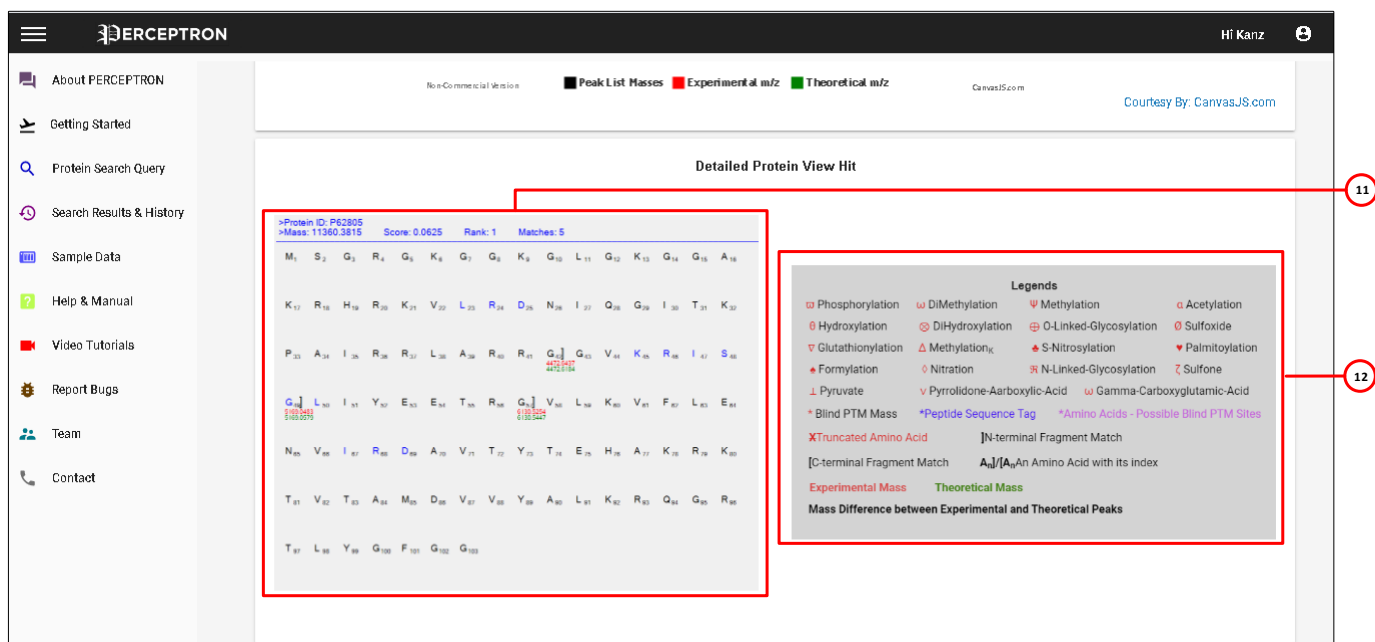
[Detailed Visualization](#)

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7. User can scroll down to see 'Protein Search Time' panel below 'General Results' indicating total time taken for processing protein query. Additionally, these runtimes have been split for highlighting time taken by each algorithmic component.
8. 'Protein Sequence' panel shows the sequence of the selected proteoform.
9. User can visualize search results in detail by clicking 'Detailed Visualization' button provided on bottom right.



10. 'Mass Spectrum Visualization' on 'Results Visualization' page shows Experimental Spectrum superimposed with Theoretical Spectrum highlighting peaks matched during spectral comparison. User can hover the cursor over to find peak list masses.



**Detailed Protein Hit View**

Protein ID: P62805  
 Mass: 11360.3815  
 Score: 0.0625  
 Rank: 1  
 Matches: 5

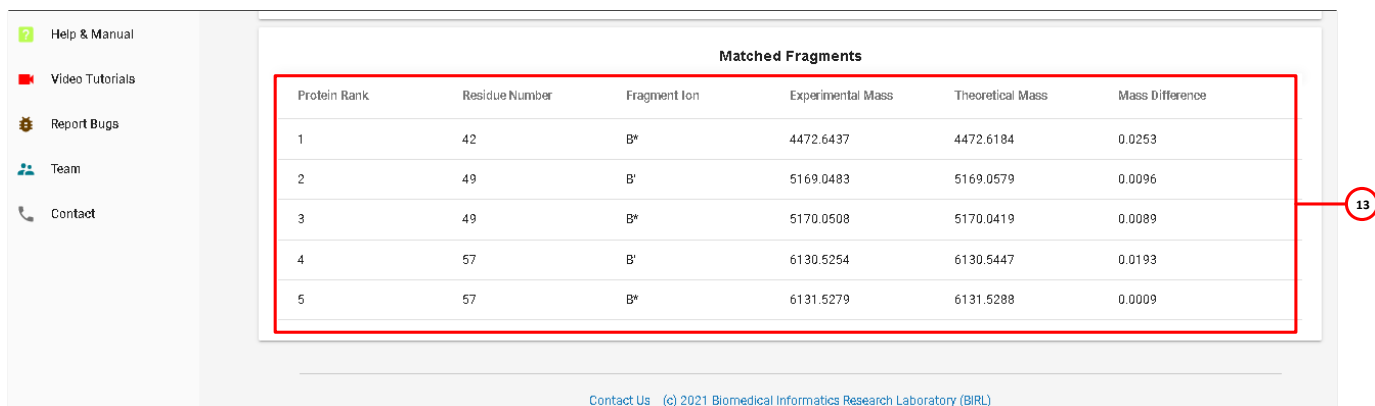
Sequence: M<sub>1</sub> S<sub>2</sub> G<sub>3</sub> R<sub>4</sub> G<sub>5</sub> K<sub>6</sub> G<sub>7</sub> G<sub>8</sub> K<sub>9</sub> G<sub>10</sub> L<sub>11</sub> G<sub>12</sub> K<sub>13</sub> G<sub>14</sub> G<sub>15</sub> A<sub>16</sub>  
 K<sub>17</sub> R<sub>18</sub> H<sub>19</sub> R<sub>20</sub> K<sub>21</sub> V<sub>22</sub> L<sub>23</sub> R<sub>24</sub> D<sub>25</sub> N<sub>26</sub> I<sub>27</sub> Q<sub>28</sub> G<sub>29</sub> I<sub>30</sub> T<sub>31</sub> K<sub>32</sub>  
 P<sub>33</sub> A<sub>34</sub> I<sub>35</sub> R<sub>36</sub> R<sub>37</sub> L<sub>38</sub> A<sub>39</sub> R<sub>40</sub> R<sub>41</sub> G<sub>42</sub> G<sub>43</sub> V<sub>44</sub> K<sub>45</sub> R<sub>46</sub> I<sub>47</sub> S<sub>48</sub>  
 G<sub>49</sub> L<sub>50</sub> I<sub>51</sub> Y<sub>52</sub> E<sub>53</sub> E<sub>54</sub> T<sub>55</sub> R<sub>56</sub> G<sub>57</sub> V<sub>58</sub> L<sub>59</sub> K<sub>60</sub> V<sub>61</sub> F<sub>62</sub> L<sub>63</sub> E<sub>64</sub>  
 N<sub>65</sub> V<sub>66</sub> I<sub>67</sub> R<sub>68</sub> D<sub>69</sub> A<sub>70</sub> V<sub>71</sub> T<sub>72</sub> Y<sub>73</sub> T<sub>74</sub> E<sub>75</sub> H<sub>76</sub> A<sub>77</sub> K<sub>78</sub> R<sub>79</sub> R<sub>80</sub>  
 T<sub>81</sub> V<sub>82</sub> T<sub>83</sub> A<sub>84</sub> M<sub>85</sub> D<sub>86</sub> V<sub>87</sub> V<sub>88</sub> Y<sub>89</sub> A<sub>90</sub> L<sub>91</sub> K<sub>92</sub> R<sub>93</sub> Q<sub>94</sub> G<sub>95</sub> R<sub>96</sub>  
 T<sub>97</sub> L<sub>98</sub> Y<sub>99</sub> G<sub>100</sub> F<sub>101</sub> G<sub>102</sub> G<sub>103</sub>

**Legends**

- Phosphorylation
- Hydroxylation
- Glutathionylation
- Formylation
- Pyruvate
- Blind PTM Mass
- Truncated Amino Acid
- DiMethylation
- DiHydroxylation
- Methylation<sub>ox</sub>
- Nitration
- Pyrrolidone-Aarboxylic-Acid
- Peptide Sequence Tag
- N-terminal Fragment Match
- C-terminal Fragment Match
- Methylation
- O-Linked-Glycosylation
- S-Nitrosylation
- N-Linked-Glycosylation
- Gamma-Carboxyglutamic-Acid
- Amino Acids - Possible Blind PTM Sites
- Acetylation
- Sulfoxide
- Palmitoylation
- Sulfone

Experimental Mass (red)  
 Theoretical Mass (green)  
 Mass Difference between Experimental and Theoretical Peaks

11. User can scroll down to find detailed results. Left panel in ‘Detailed Protein Hit View’ shows complete information of the selected proteoform. These details include:
  - i. Sequence of the proteoform containing one-letter symbols for amino acid residues along with the number at bottom right indication the position of the respective residue within the proteoform sequence
  - ii. Molecular weight of the proteoform selected from the list of identified proteoforms
  - iii. Rank of the respective proteoform in the list of proteoforms identified
  - iv. Proteoform score computed by PERCEPTRON
  - v. Matched fragments along with experimental (in red) and theoretical (in green) fragment masses
  - vi. Post-translational modifications as well as other modifications (e. g. truncation)
12. ‘Legends’ is a key to help user understand ‘Detailed Protein Hit View.’



**Matched Fragments**

Protein Rank	Residue Number	Fragment Ion	Experimental Mass	Theoretical Mass	Mass Difference
1	42	B*	4472.6437	4472.6184	0.0253
2	49	B'	5169.0483	5169.0579	0.0096
3	49	B*	5170.0508	5170.0419	0.0089
4	57	B'	6130.5254	6130.5447	0.0193
5	57	B*	6131.5279	6131.5288	0.0009

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13. ‘Matched Fragments’ shows a list of theoretical fragments generated by PERCEPTRON’s algorithmic pipeline matched with experimental fragments which are originating from data file provided as an input during protein search.
  - (i) ‘Protein Rank’ indicates the rank of the protein within the list of identified proteoforms
  - (ii) ‘Residue Number’ is the location of residue within proteoform sequence at which the match for ‘fragment ion’ was obtained
  - (iii) ‘Fragment Ion’ indicates the type of fragment ion matched
  - (iv) ‘Experimental Mass’ is the mass of experimental fragment from data file
  - (v) ‘Theoretical Mass’ is the mass of *in silico* fragment generated by PERCEPTRON
  - (vi) ‘Mass Difference’ is the difference between the masses of experimental and theoretical fragments

## 8. Video Tutorials

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Several video tutorials have been developed for employment of PERCEPTRON in protein search. These tutorials are available as a playlist at: [https://www.youtube.com/playlist?list=PLaNVq-kFOn0Z\\_7b-iL59M\\_CeV06JxEXmA](https://www.youtube.com/playlist?list=PLaNVq-kFOn0Z_7b-iL59M_CeV06JxEXmA)

## 9. Requirements for in-house Deployment

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### 4.1. Hardware Requirements

For in-house deployment of PERCEPTRON, the hardware requirement includes a graphical processing unit (GPU) that supports CUDA TOOLKIT 7.0.

### 4.2. Software Requirements

Compilation and software build of PERCEPTRON requires the following software:

- Windows Server 2012 R2
- Visual Studio 2013
- Angular 1.7.4
- Node.js 8.11.1
- SQL Server Management Studio (17.6 or 17.9.1)
- CUDA TOOLKIT 7.0
- CUDAFy.NET.1.29.5576.13786
- Microsoft Windows Server v6.2
- .NET Framework 4.5

### 4.3. Testing the Deployment

The freely available public deployment of PERCEPTRON is hosted on a Dell Power Edge R730, 2 x Intel Xeon E5-2620, 160 GB RAM (16GBx10) and an NVIDIA Tesla K40C (2880 Cores). Following Windows versions are compatible with PERCEPTRON:

- Windows 8.1
- Windows 7
- Win Server 2012 R2
- Win Server 2008 R2

## 10. Building PERCEPTRON for in-house Deployment

### 10.1 PERCEPTRON Application Programming Interface (API)

Open 'PerceptronAPI' from the folder **PERCEPTRON\_CPU** in visual studio (Figure 21). In the Solution Explorer, click on 'PerceptronAPI'. Go to 'App\_Start' and open 'WebApiConfig.cs'.

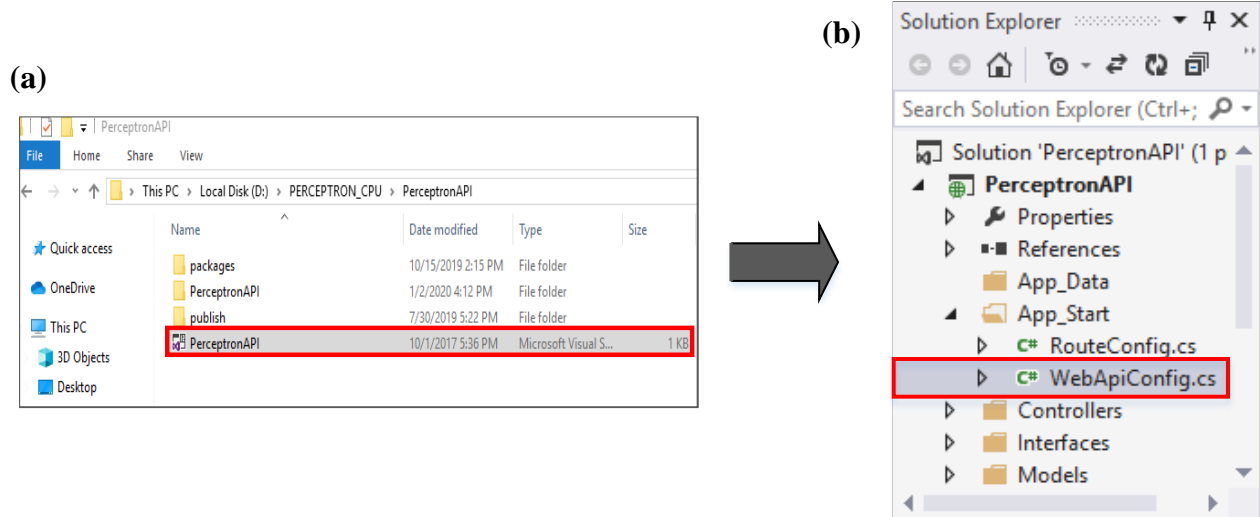


Figure 21. Building PERCEPTRON API. (a) Opening solution PerceptronAPI.sln; (b) Opening WebApiConfig.cs from Solution Explorer of Visual Studio

Next, search 'config.filters' using **CTRL+F** (Figure 22). Comment out the statement that includes: **config.Filters.Add(new RequireHttpsAttribute())** by typing '//' before the start of the statement.

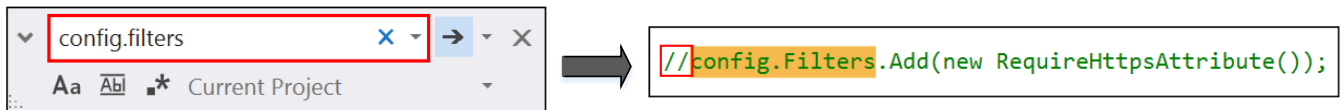


Figure 22. Searching for a statement in PERCEPTRON API solution

Open SQL Server Management Studio. Copy the given server name from SQL Server Pop Up (Figure 23).

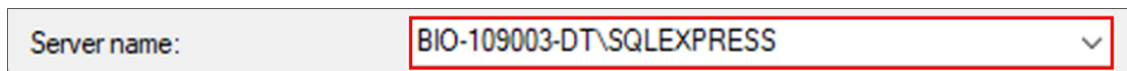


Figure 23. Copying Server Name from SQL Server Management Studio

In Visual Studio, open 'Web.config' from the Solution Explorer (Figure 24). Press **CTRL+F** to search item. Type server name, e.g. 'CHIRAGH-II' and press **ENTER**. Replace this server name with the name copied

in Figure 23. Copying Server Name from SQL Server Management Studio, e.g., **BIO-109003-DT\SQLEXPRESS**.

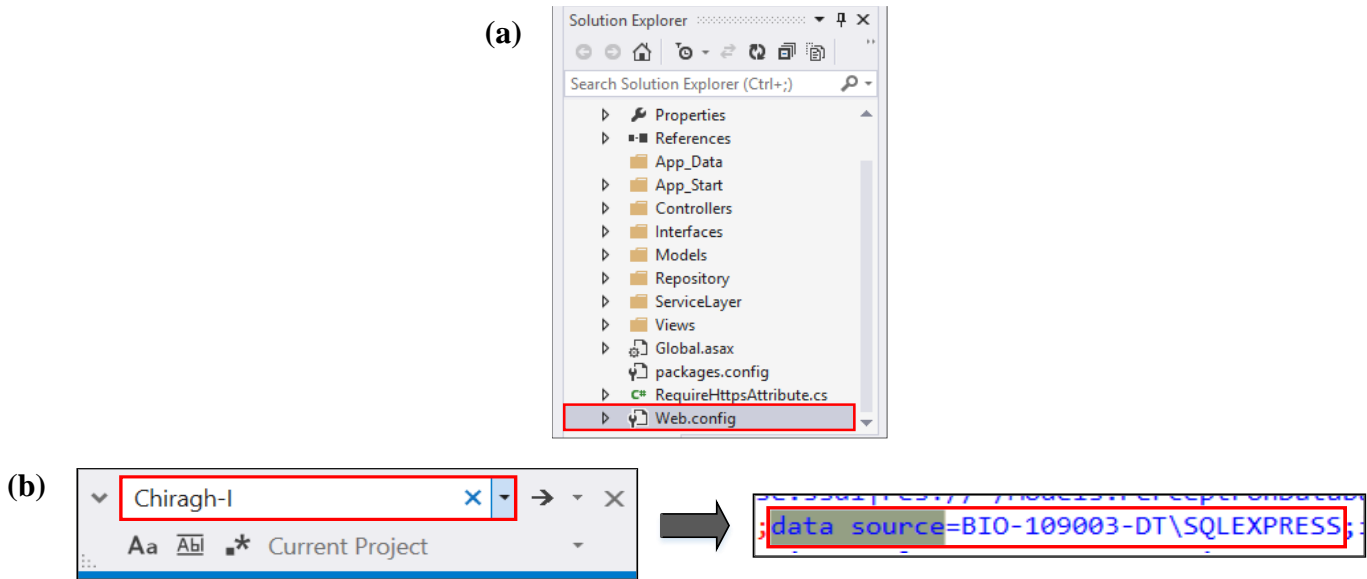


Figure 24. (a) Opening Web.config from Solution Explorer of Visual Studio (b) Changing data source (Server Name) in Web.config

Press **ENTER** again to change the name in *Sqlatabase.cs* (in Repository Folder) as well (Figure 25). Replace the given name for all occurrences of ‘**Server**’ in *Sqlatabase.cs* with the server name from SQL Pop Up. In each case, add ‘@’ right before ‘**Server**.’

```
using (var db = new PerceptronDatabaseEntities())
{
    var sqlConnection1 =
        new SqlConnection(
            @"Server=BIO-109003-DT\SQLEXPRESS; Database=
            PerceptronDatabase; Integrated Security=SSPI;")
}
```

Figure 25. Changing server name in *Sqlatabase.cs*

In dropdown menu of **BUILD**, select ‘**Build Solution.**’ Next, select ‘**Publish PerceptronAPI**’ under the same menu (Figure 26).

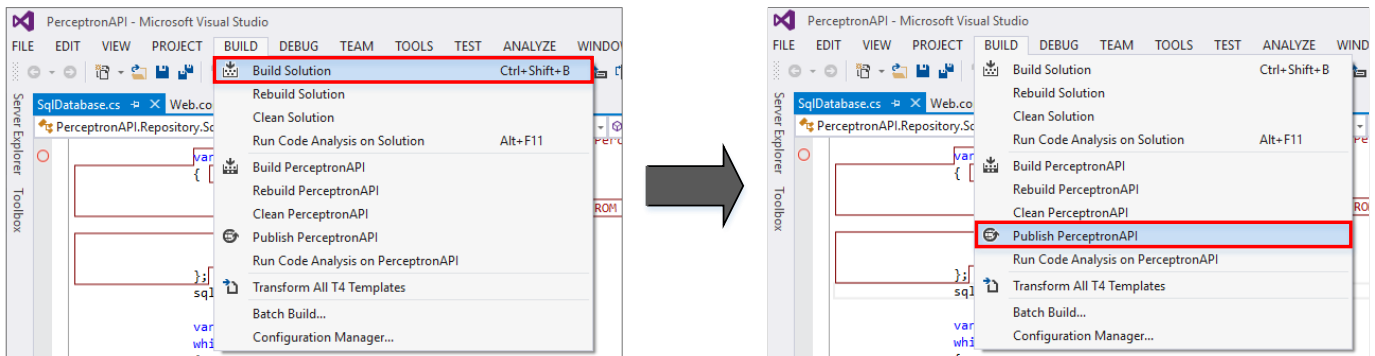


Figure 26. Building PERCEPTRON API

In Profile, select ‘**PERCEPTRON**’ (Figure 27). In Connection, go to Target Location and ensure the following pathway: ‘**C:\inetpub\wwwroot\PerceptronAPI**’. In Settings, set Configuration to ‘**Debug**’.

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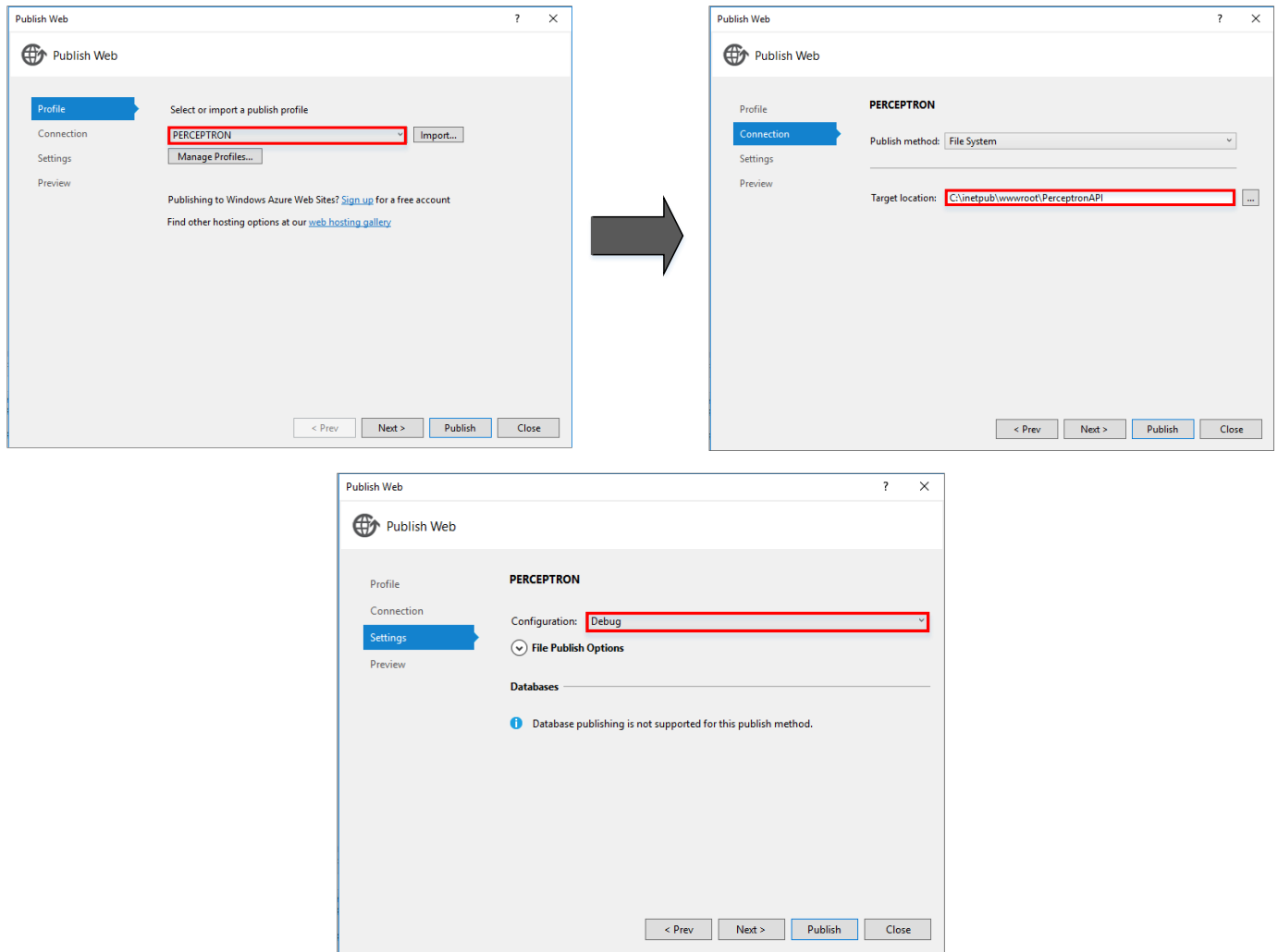


Figure 27. Steps to build PERCEPTRON API

Open the following path (Figure 28) and make a folder in it by the name 'App\_Data'.

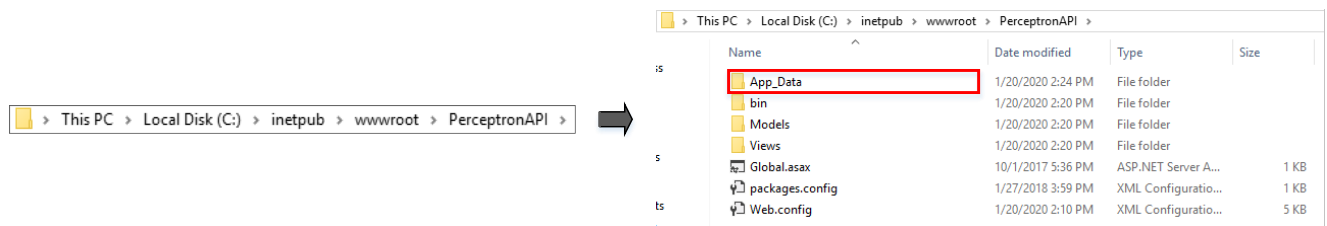
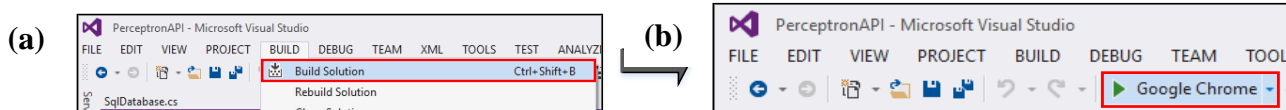
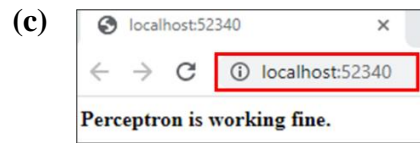


Figure 28. Publishing Perception API

From the dropdown menu of **BUILD**, select '**Build Solution**' (Figure 29). Run on '**Google Chrome**' and save the URL obtained.







*Figure 29. Steps to build PERCEPTRON API. (a) Building PERCEPTRON API solution file (PerceptronAPI.sln); (b) Run PerceptronAPI; (c) Google chrome page with URL localhost:52340 displaying the message “PERCEPTRON is working fine”*

Message in Figure 29 i.e., “PERCEPTRON API is working fine” ensures that PERCEPTRON API has been successfully built and is running fine.

## 10.2 PERCEPTRON Front-End

Open Visual Studio Code. From '**File**' dropdown menu, select '**Open Folder**' (Figure 30). Select the folder '**PerceptronFrontEnd**' and click on '**Select Folder.**'

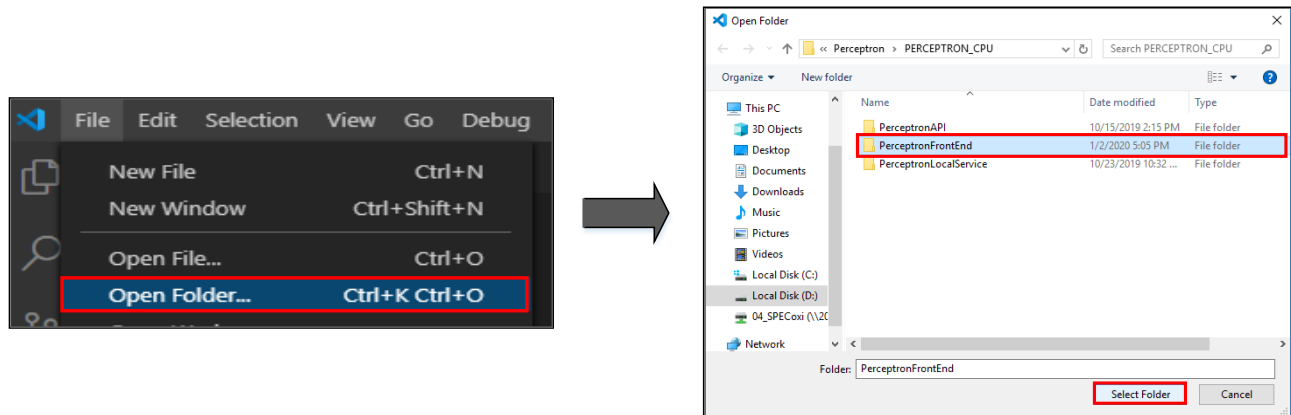
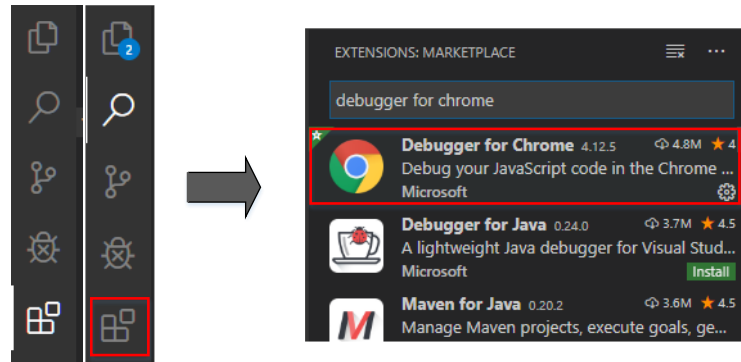


Figure 30. Opening PerceptronFrontEnd folder in Visual studio code

### 10.3 Connecting PERCEPTRON API to PERCEPTRON Front-End

In Visual Studio Code, click on the ‘**Extensions**’ icon (as indicated below in Figure 31) and type ‘**Debugger for Chrome**’ in the search bar. Select the one shown below.



Click ‘**Install**’ to install the debugger.

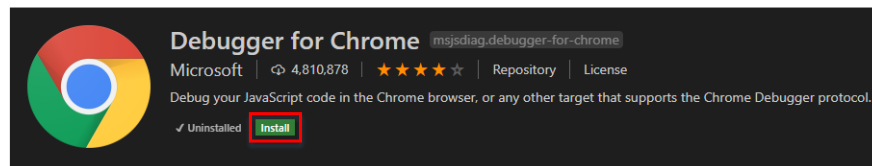
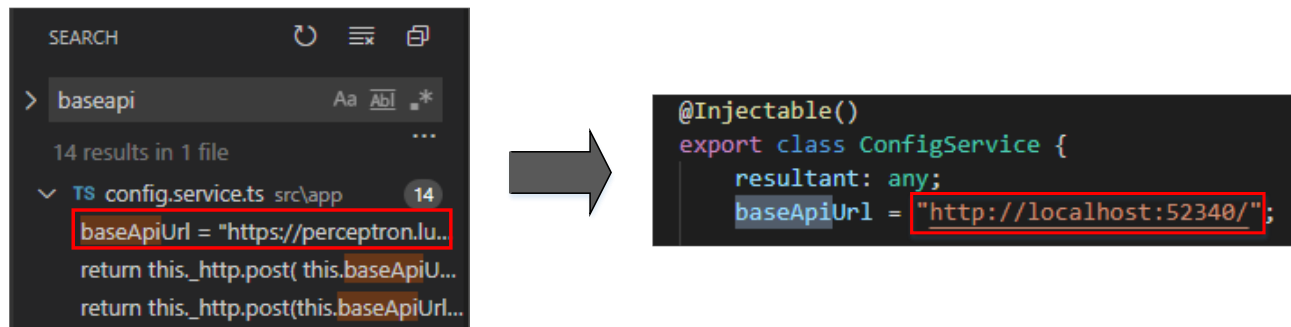


Figure 31. Installing extension in VS Code

Next, type ‘**baseAPI**’ in the search bar and select the one shown below (Figure 32). Replace the given URL with the one saved before in Figure 29. Steps to build PERCEPTRON API. (a) Building PERCEPTRON API solution file (PerceptronAPI.sln); (b) Run PerceptronAPI; (c) Google chrome page with URL localhost:52340 displaying the message “PERCEPTRON is working fine”



Type '**ng build**' in Terminal. A new folder by the name of ‘**dist**’ will form in the same directory.

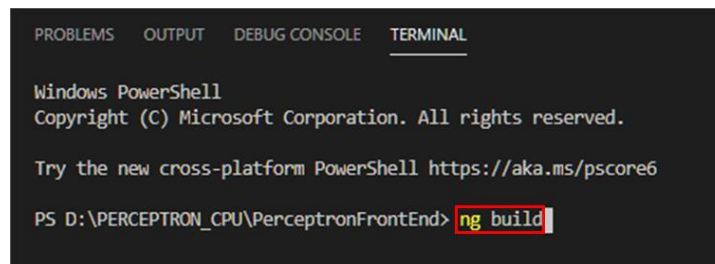



Figure 32. Building Perceptron Front-End

At bottom in Terminal Window, click on the icon  located at right side to clear Terminal and then open 'New Terminal' from **Toolbox**. Type 'ng serve' and press **ENTER**. Open the link (<http://localhost:4200/>) provided in Figure 33 by pressing CTRL button + left mouse button.

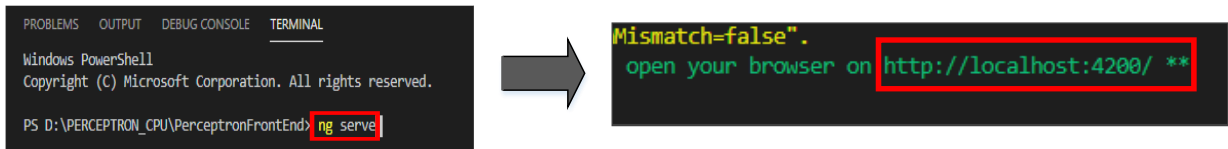
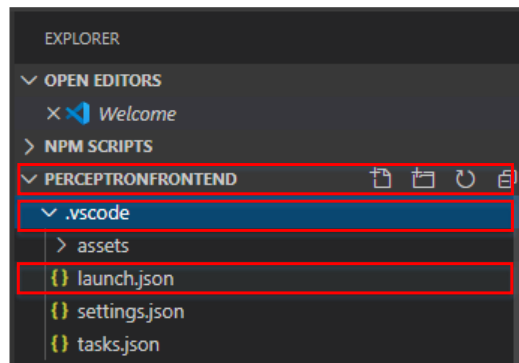
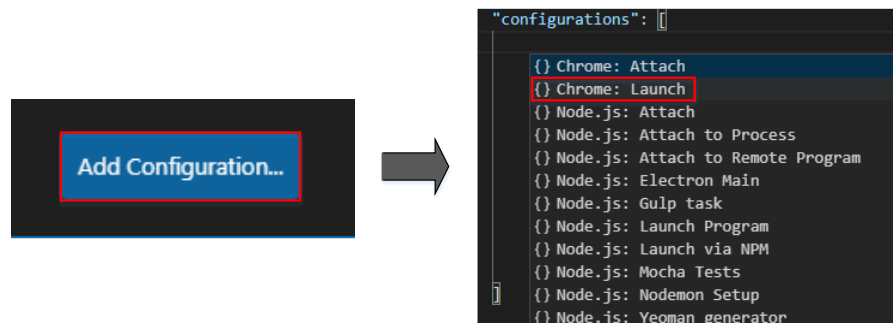


Figure 33. Hosting Perceptron Front-End on system with default URL

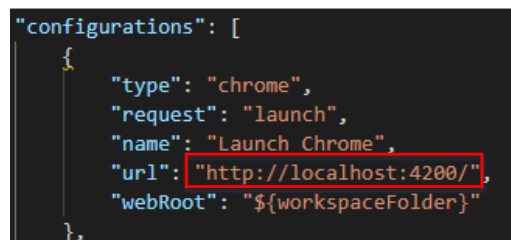
In Explorer, select 'PERCEPTRONFRONTEND'. Click on '.vscode' and open 'launch.json'.



Click 'Add Configuration' icon on the bottom right corner and select 'Chrome: Launch' from the dropdown menu that appears



Replace the URL acquired in Figure 33. Hosting Perceptron Front-End on system with default URL.



In the Toolbox, go to 'Debug' and select 'Start Debugging' (Figure 34). In the Pop Up that appears, click 'Debug Anyway' and then 'Open launch.json'.

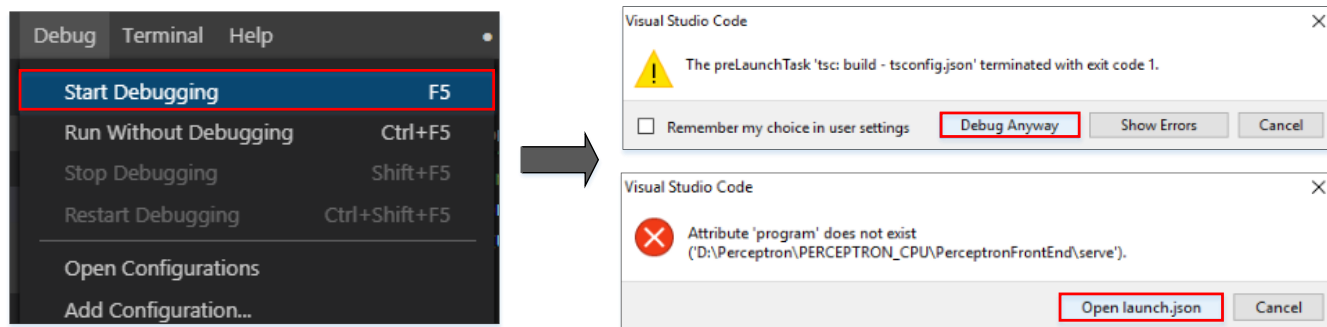


Figure 34. Steps to build PERCEPTRON Front-End

## 10.4 PERCEPTRON Local Service

Open SQL Server Management Studio. Copy the given server name from SQL Server Pop Up (Figure 35).

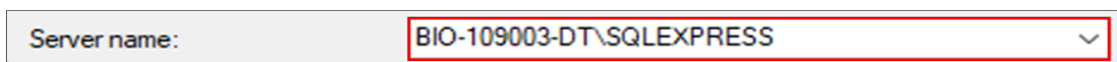


Figure 35. Copying Server Name from SQL Server Management Studio

Open 'PerceptronLocalService.sln' from the folder **PERCEPTRON\_CPU** in visual studio (Figure 36). In the Solution Explorer, select 'App.config'.



Figure 36. Building Perceptron Local Service. (a) Opening PerceptronLocalService.sln; (b) Opening App.config from Solution Explorer of Visual Studio

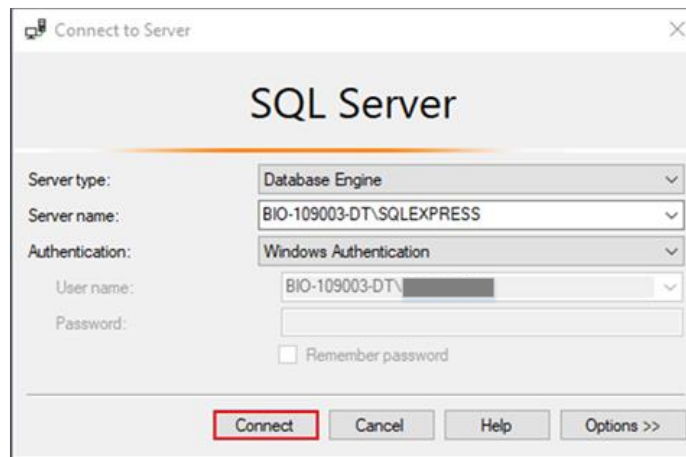
Press **CTRL+F** to search server name (Figure 37). Type '**CHIRAGH-I**' and press **ENTER**. Replace this server name with the name copied in Figure 35. Copying Server Name from SQL Server Management Studio, e.g., **BIO-109003-DT\SQLEXPRESS**. Replace the given name for all occurrences of '**Data Source**' in App.config with the server name from SQL Pop Up.



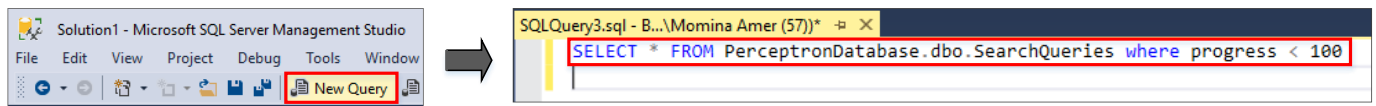
Figure 37. Changing data source value (Server Name) in App.config

Send a Protein Search Query on local host (see Section 5.2)

Open SQL Server Management Studio and click on '**Connect**' (Figure 38).



Select 'New Query' and type 'SELECT \* FROM PerceptronDatabase.dbo.SearchQueries where progress < 100' in the window that appears.



In SQL, click on 'Execute'.

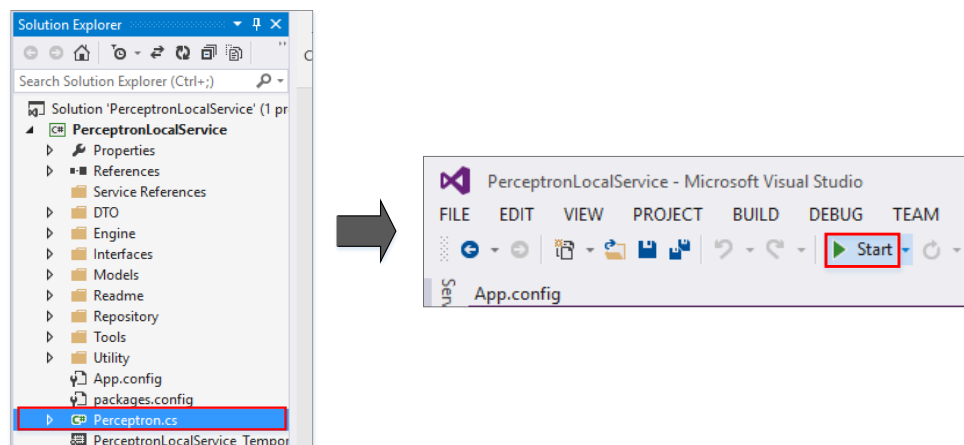


The query will show up in the Results Window.

Results		Messages			
QueryId	UserId	Progress	CreationTime	Email	
1	1ec2fba3-d044-43fc-ba87-15edc62fdd6d	0	01/21/2020 18:55:20	NULL	

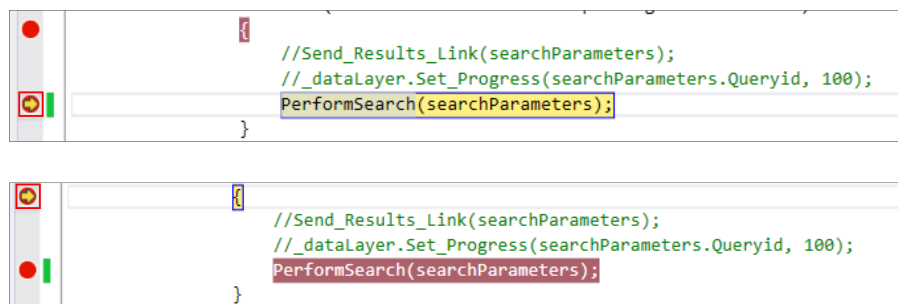
Figure 38. Steps to execute Protein Search Query

In Visual Studio, open 'PerceptronLocalService.sln'. Go to Solution Explorer and select 'Perceptron.cs'. Click 'Start' to run it (Figure 39).



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Click **‘Continue’** twice to step over the breakpoints.



On the locally hosted PERCEPTRON, click on **‘Search Results & History’** to see the results of your query.

Sr. #	File Name	Protein ID	Protein Score	Molecular Weight	Truncation	Spectral Matches	No. of Modifications	Total Search Time
1	\\App_Data\\HEL A_pk13_sw1_6 6sc_mono.txt	Q4VC39	0.2316	11397.7953	No	1	1	

*Figure 39. Testing Perceptron Local Service*



## 11. Step-by-Step Guide to in-house Deployment

### 11.1 Installing Visual Studio Code (VS Code)

Users can download VS Code setup using the following link:

<https://code.visualstudio.com/download>

Click **'64 bit'** in front of **User Installer** (Figure 40) to download the setup. Run the downloaded .exe file.

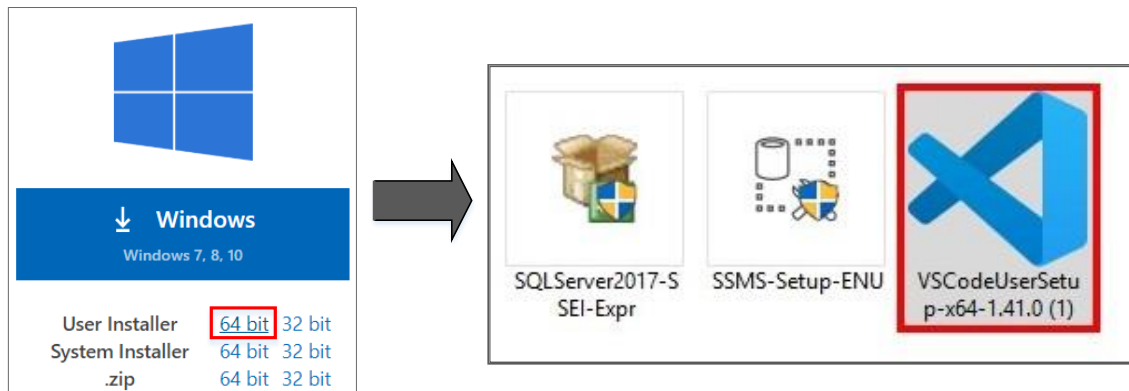


Figure 40. Downloading Visual Studio Code (VS Code) setup

Accept license terms and choose a destination folder to download Visual Studio Code setup (Figure 41).

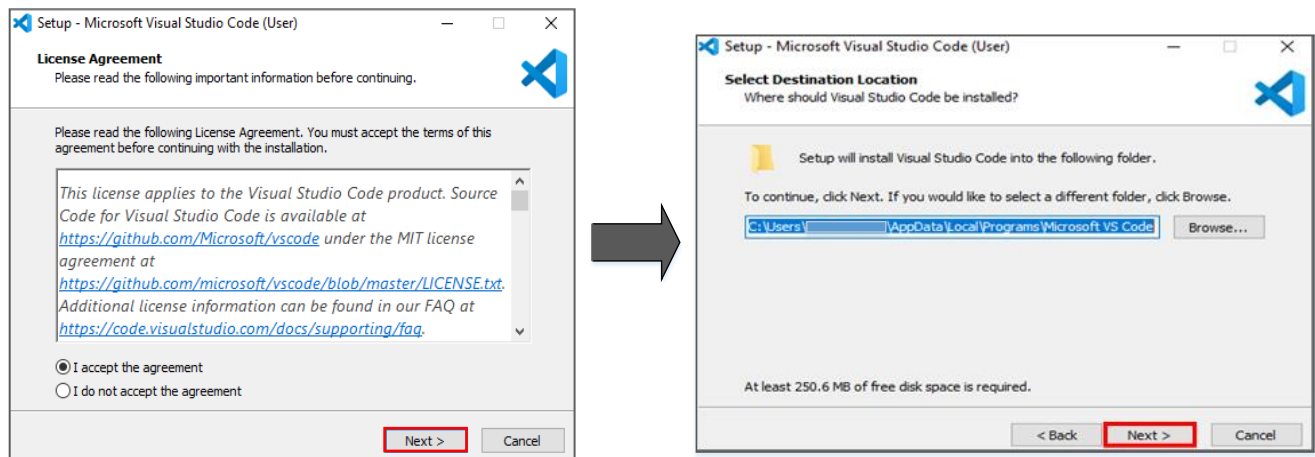
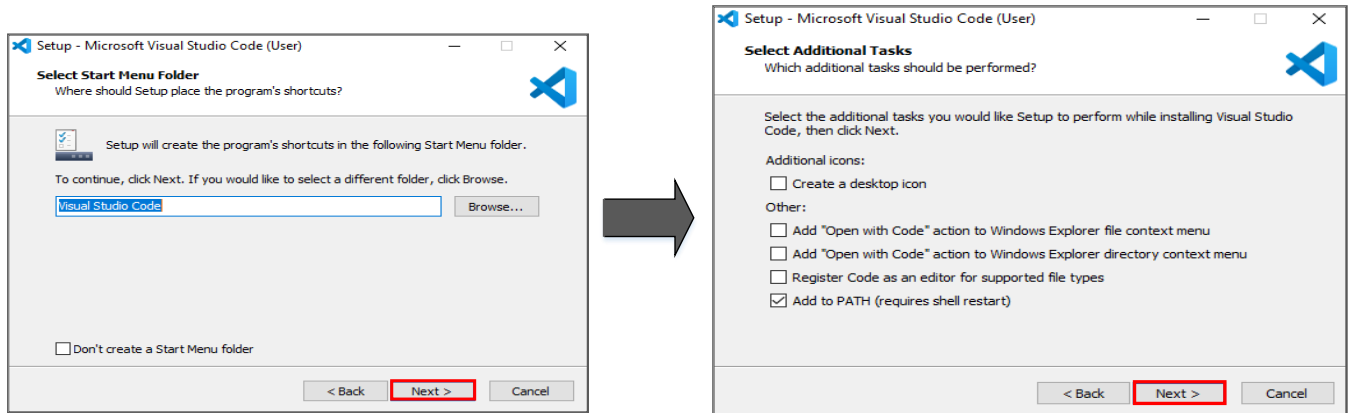


Figure 41. Choosing destination folder to download VS Code setup

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Click **'Next'** then select **'Add to PATH.'** Click **'Next'** to proceed (Figure 42).



Click **'Install'** to begin installation. Click **'Finish'** to complete installation.

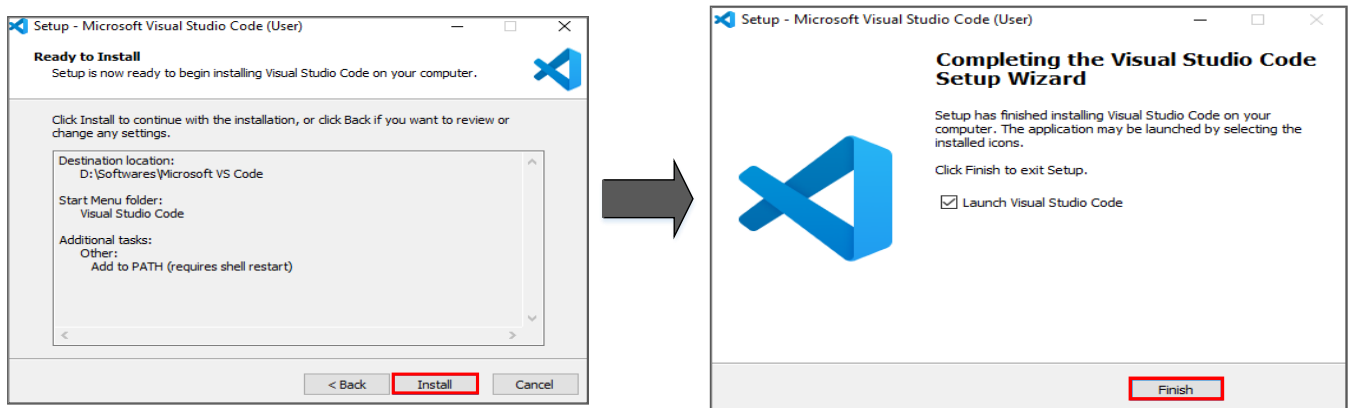


Figure 42. Steps to install Visual Studio Code setup

## 11.2 Installing SQL Server Management Studio (SSMS)

Users can download SSMS setup (version 17.6 or version 17.9.1) using the following link:

<https://docs.microsoft.com/en-us/sql/ssms/release-notes-ssms?view=sql-server-ver15#additional-downloads>

Click **‘Download’** to download the setup (Figure 43). Run the downloaded .exe file.

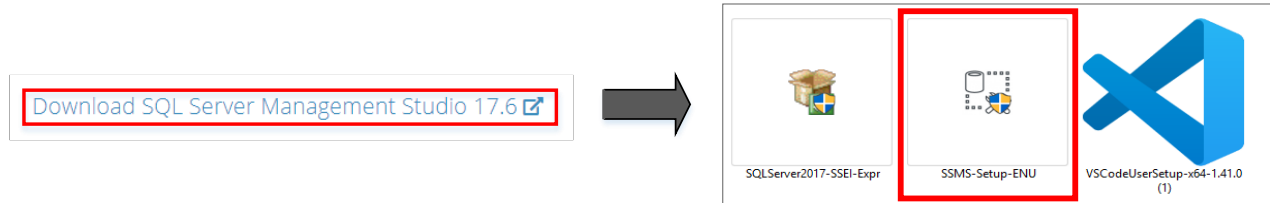


Figure 43. Downloading SQL Server Management Studio (SSMS) setup

Click **‘Install’** to begin installation (Figure 44). Click **‘Close’** to complete installation.

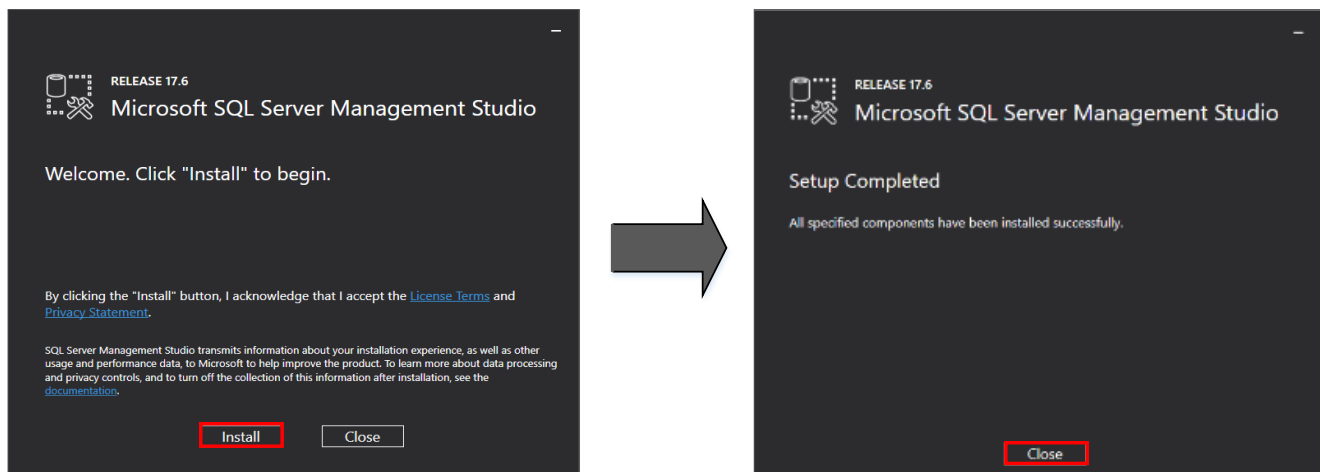


Figure 44. Steps to install SQL Server Management Studio (SSMS)

### 11.3 Installing Node.js.8.11.1

Users can download the setup using the following link:

<http://www.npackd.org/p/org.nodejs.NodeJS64/8.11.1>

Click on **‘Download Node.js 64 bit 8.11.1’** (Figure 45) to download node.js setup. Click on **‘Run’** to proceed with downloading the .exe file.

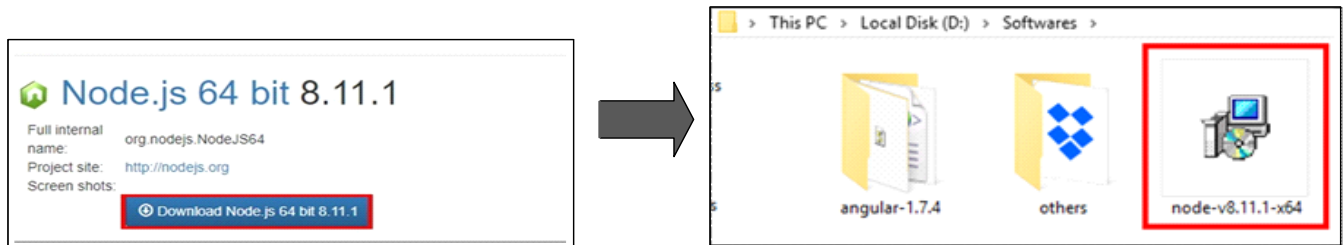
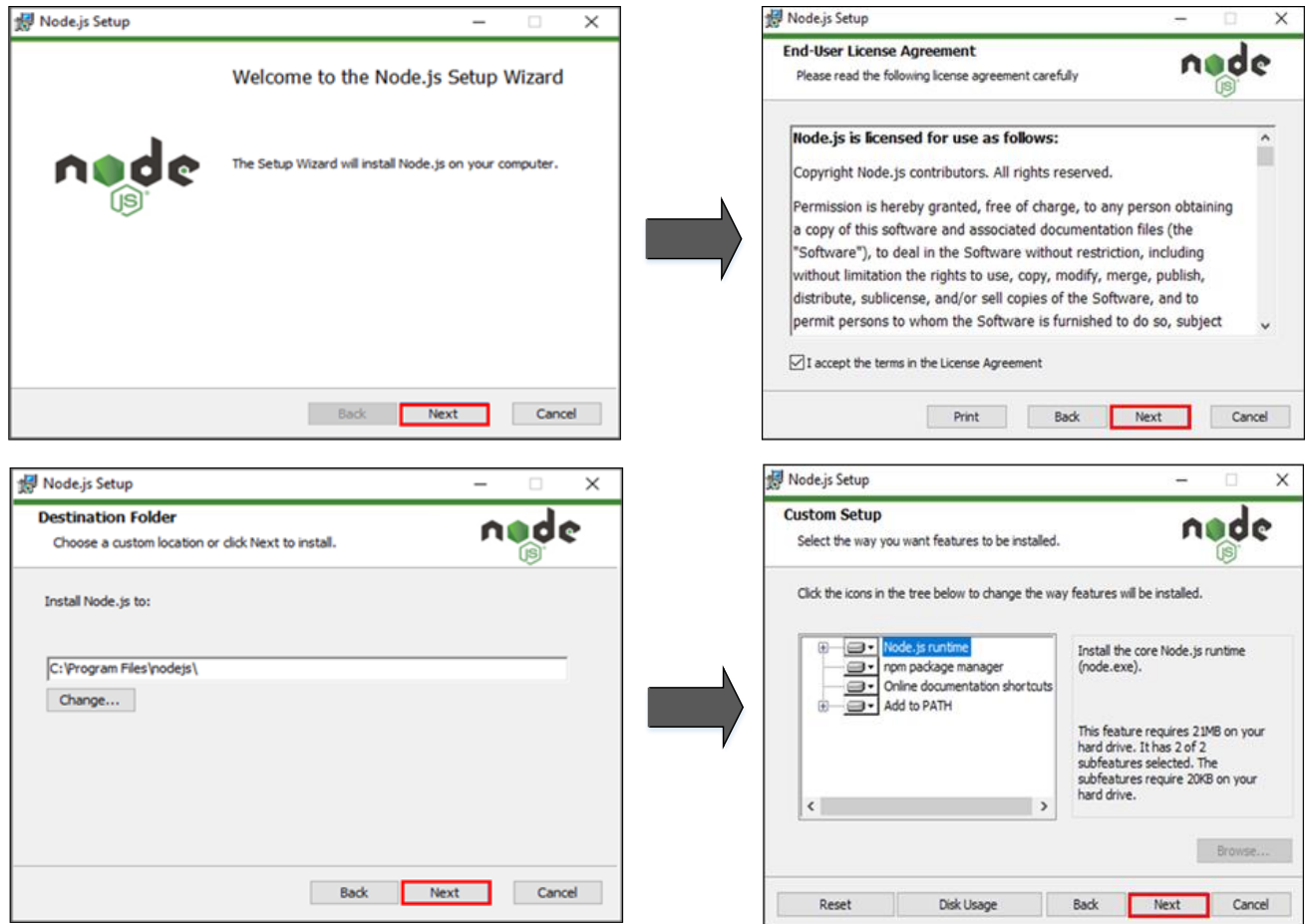
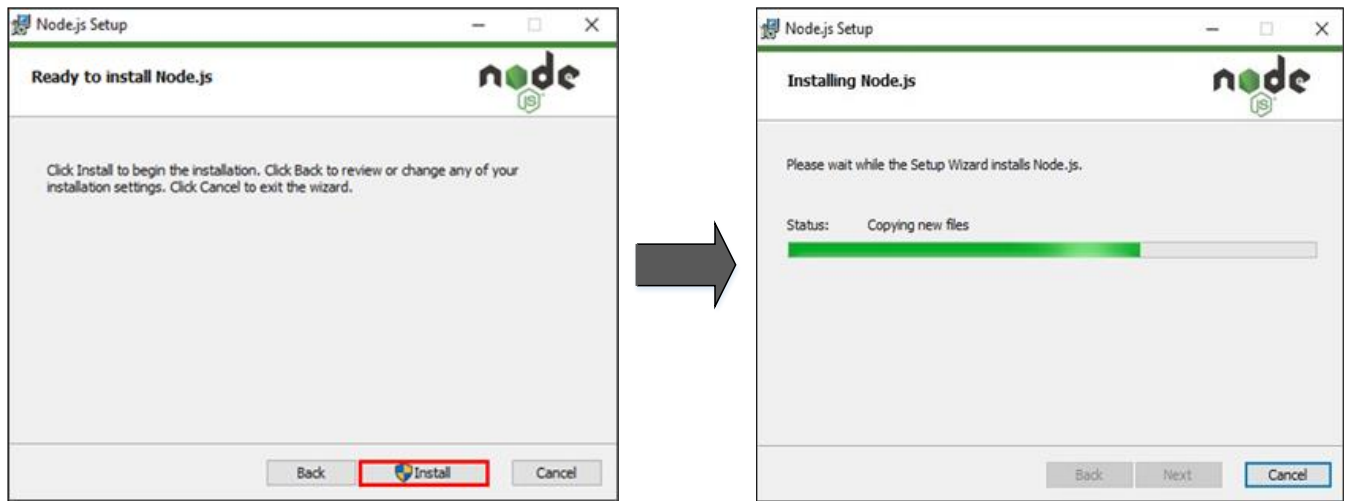


Figure 45. Downloading Node.js (version 8.11.1) setup

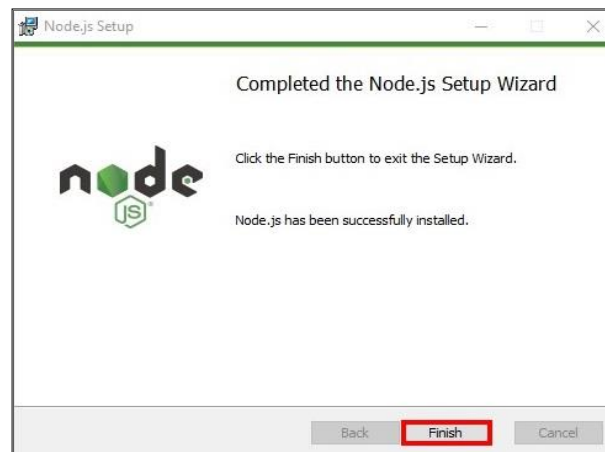
Click **‘Next’** and accept license terms to proceed (Figure 46).



Click **‘Install’** to begin installation.



Click '**Finish**' to complete installation.



*Figure 46. Steps to install Node.js setup*

## 11.4 Installing SQL 2017

Users can download Structured Query Language (SQL) 2017 setup using the following link:

<https://www.microsoft.com/en-pk/download/details.aspx?id=55994>

Select a language and click **‘Download’** (Figure 47).

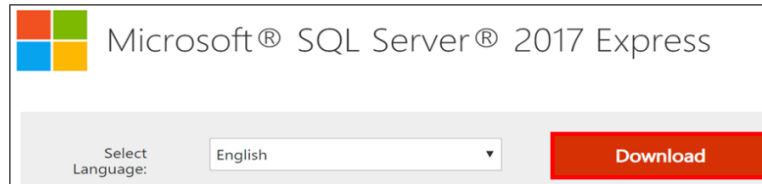
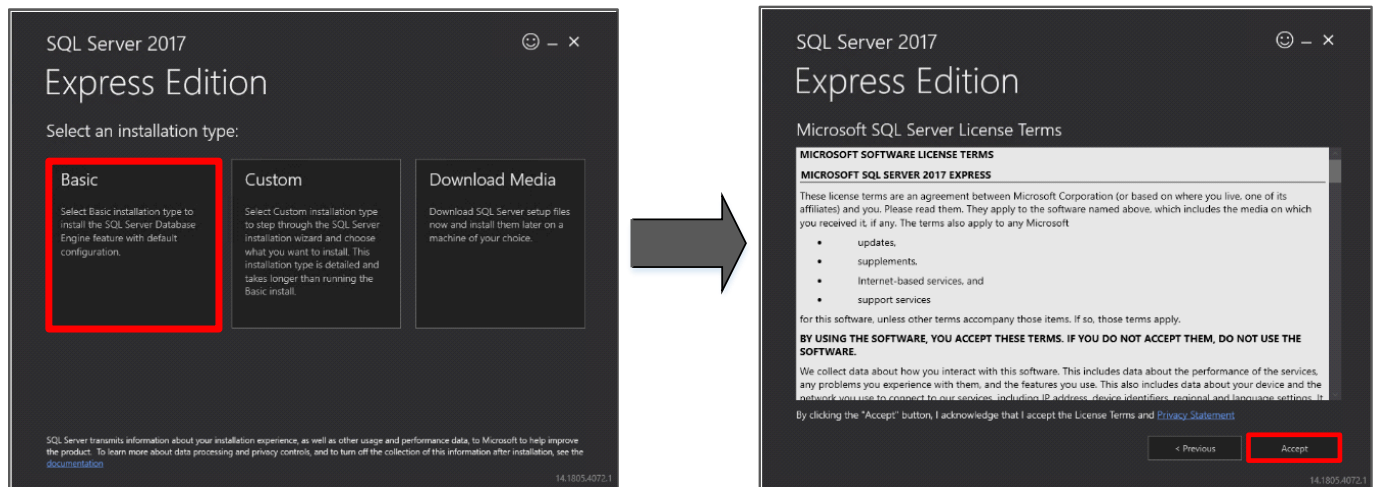


Figure 47. Downloading SQL 2017 setup

Select **‘Basic’** and then click **‘Accept’** to accept license terms (Figure 48).



Allow installation to proceed. Click **‘Close’** to complete installation.

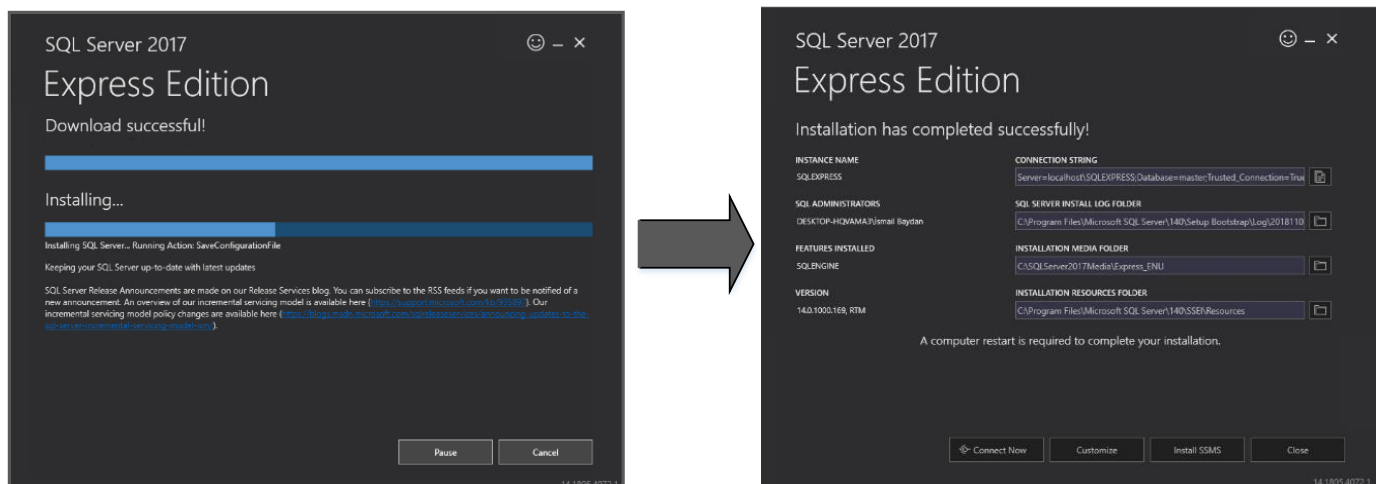


Figure 48. Steps to install SQL 2017 setup

## 11.5 Installing Angular 1.7.4

Users can download Angular 1.7.4 as a zip file using the following link:

<https://code.angularjs.org/1.7.4/>

Open the link and select the .zip file for installing Angular 1.7.4 (Figure 49). Extract the contents in the file.

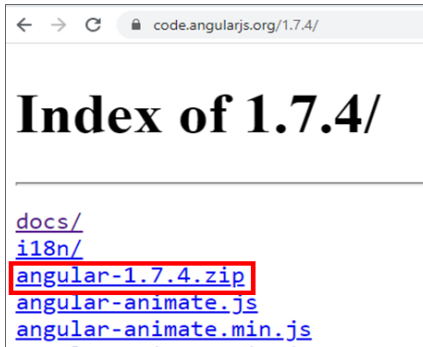
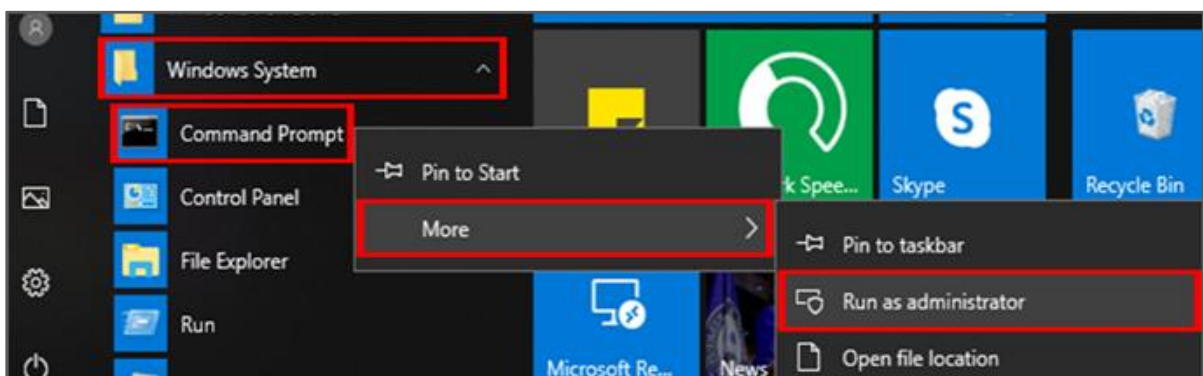
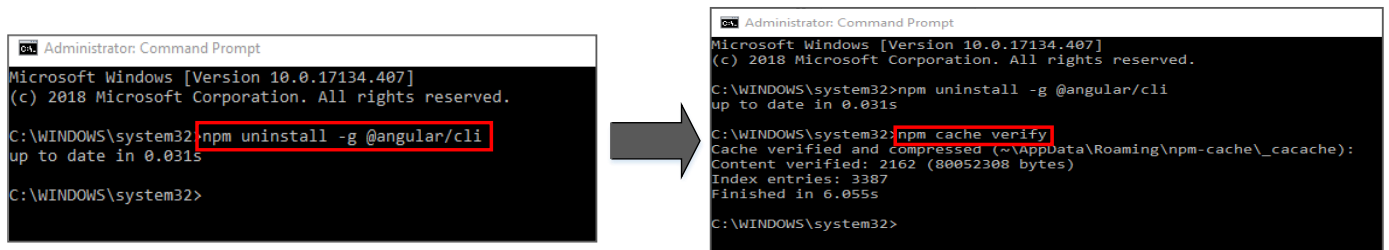


Figure 49. Downloading Angular 1.7.4 setup

Next, open Command Window by selecting ‘**Windows System**’ (Figure 50). Right click on ‘**Command Prompt**,’ then select ‘**More**’ and click ‘**Run as administrator**.’



Type '**npm uninstall -g @angular/cli**' in Command Window and press **ENTER**. Next, type '**npm cache verify**' and press **ENTER** again.



Type '**npm install -g @angular/cli@1.7.4**' and press **ENTER** to install. Type '**ng -v**' and press **ENTER** to ensure successful installation.

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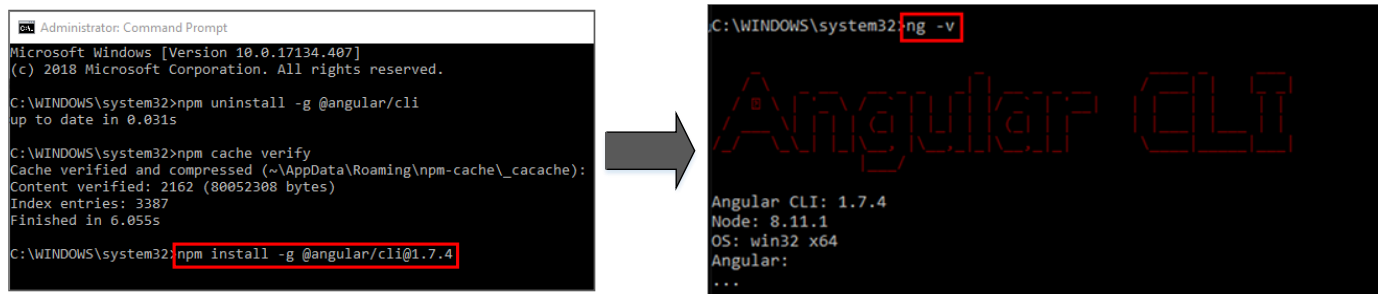


Figure 50. Steps to install Angular 1.7.4



## 11.6 Importing Files into SQL Server

First, open SQL Server Management Studio (Figure 51).

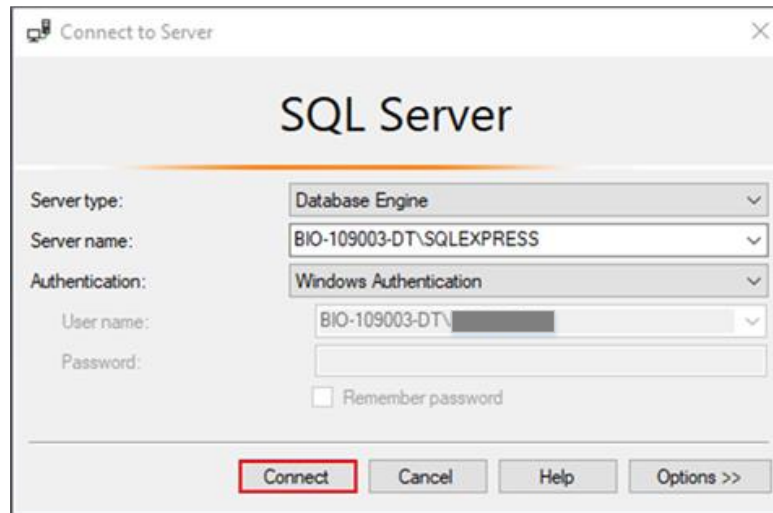



Figure 51. SQL Server Management Studio Pop Up

1. Click **'Connect'**
2. Right click **'Databases'** on left plane (Object Explorer)
3. Click **'Restore Databases'**
4. Choose **'Device'**, click , and add your **.bak** file
5. Click **'OK'**, and then **'OK'** again

## 11.7 Importing PERCEPTRON Database using SQL File

Download sql file of PERCEPTRON Database provided on Github by following the link:  
<https://github.com/BIRL/PERCEPTRON/blob/master/Code/DatabaseSchema/PerceptronDatabase.sql>.

Click on “Raw” to save the sql file (Figure 52).

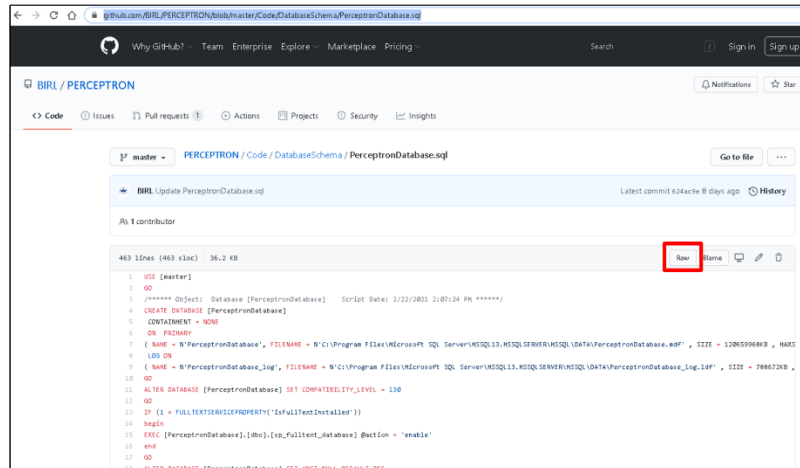


Figure 52. Downloading SQL File from GitHub

Open Microsoft SQL Server Management Studio (SSMS). Click on “File”, “Open” and “File” (Figure 53) to open ‘PERCEPTRONDatabase.sql’ file in SSMS.

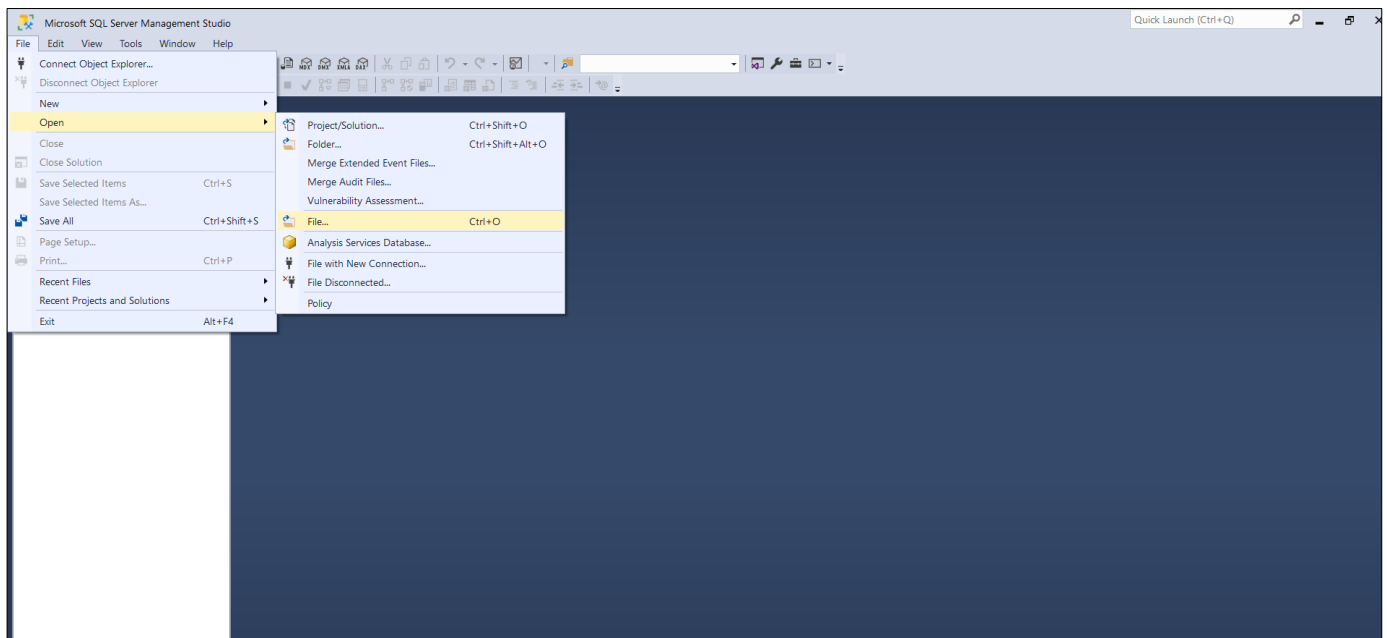


Figure 53. Steps to add SQL file downloaded from GitHub

Change file paths and size information, as required e.g., file path: “C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA...” and file size: 10240 KB (Figure 54) and click “**Execute**” in toolbar.

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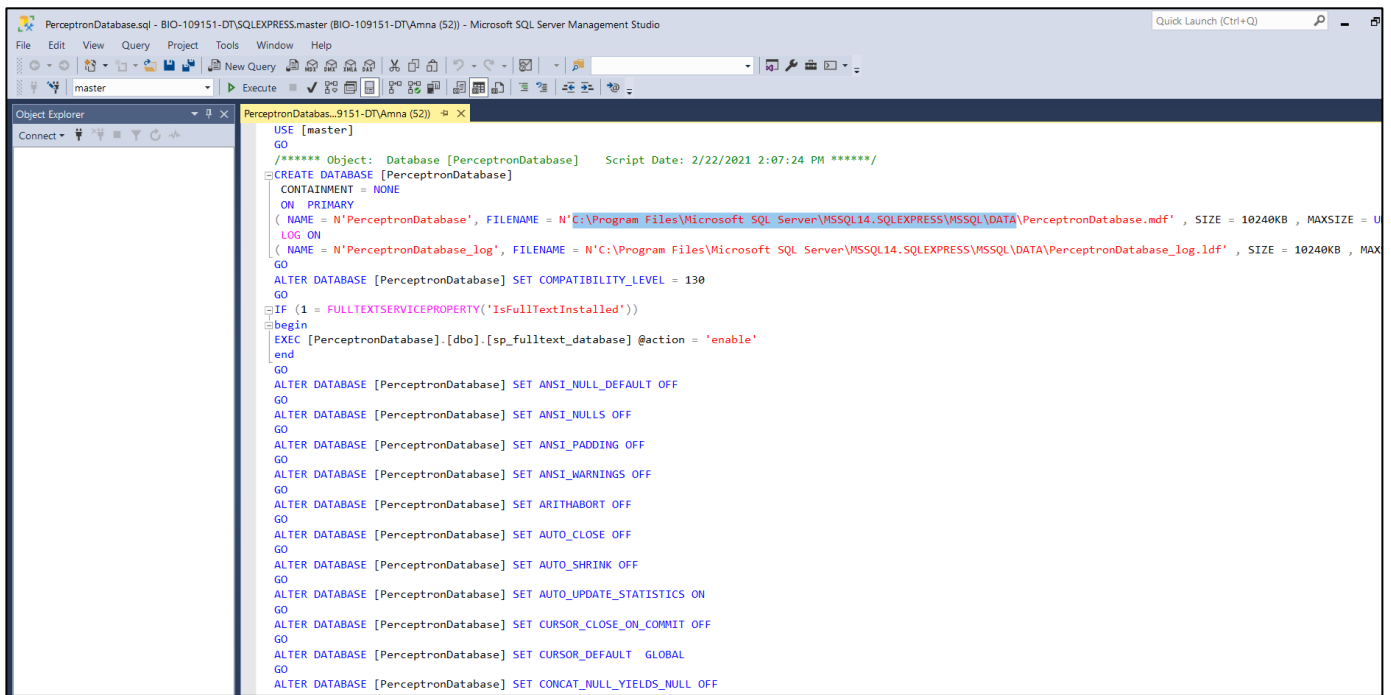


Figure 54. Steps to execute SQL file

Upon successful execution, “PERCEPTRONDatabase” will appear in Databases panel on left (Figure 55).

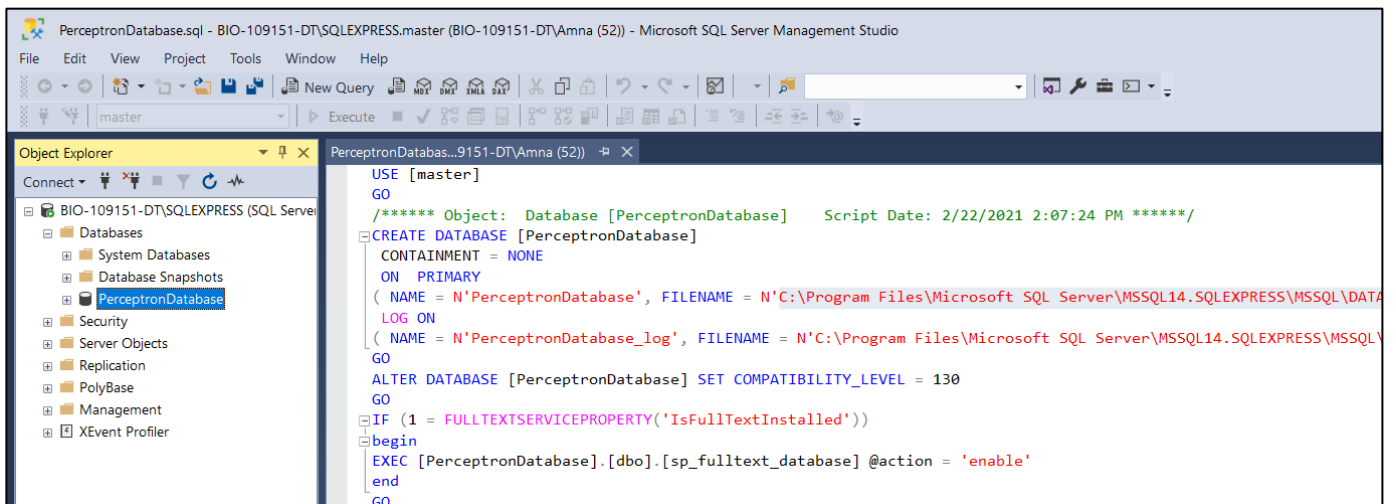


Figure 55. Importing PERCEPTRON Database using SQL File

## 12. References

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