

PERCEPTRON

V 1.0.0.0

A Next Generation Top-Down Proteoform
Identification and Characterization Platform

USER MANUAL

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3. Introduction to PERCEPTRON

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

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allows for the selection of multiple files from the folder by clicking the attach file button. The 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.

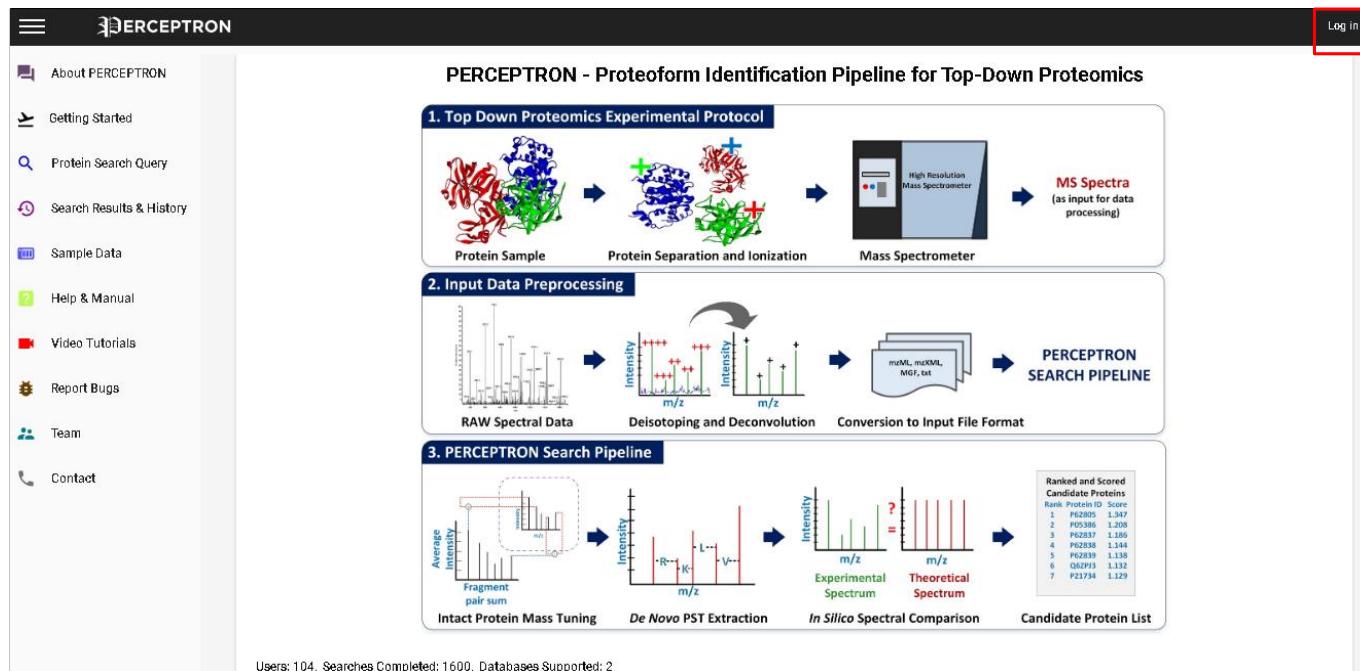


Figure 1. PERCEPTRON Homepage and Log in button

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

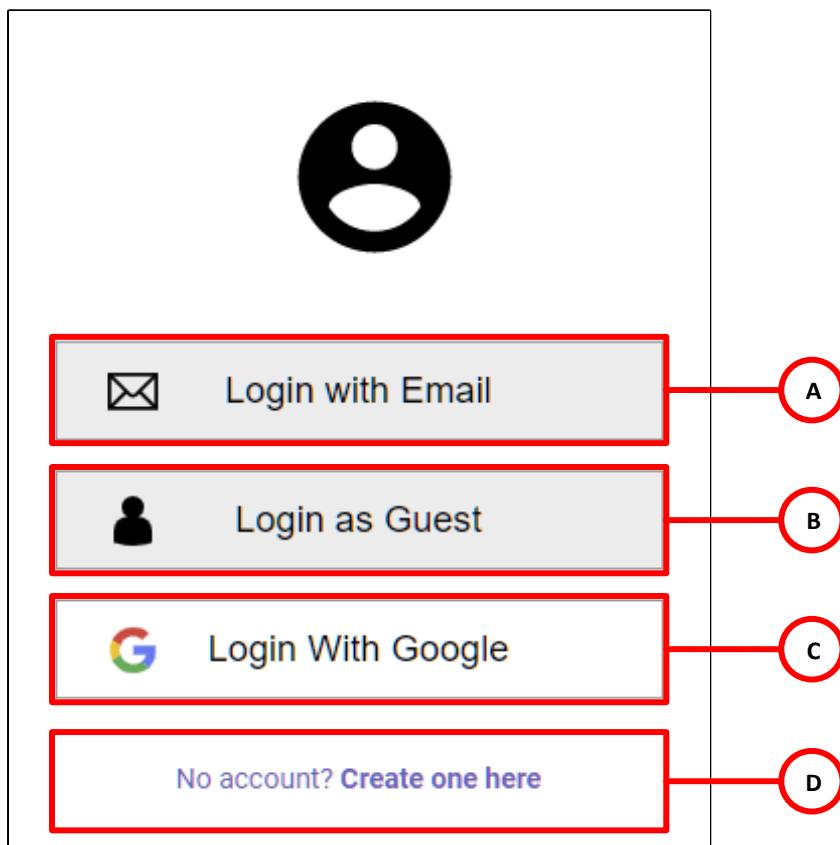


Figure 2. PERCEPTRON Login options

- 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

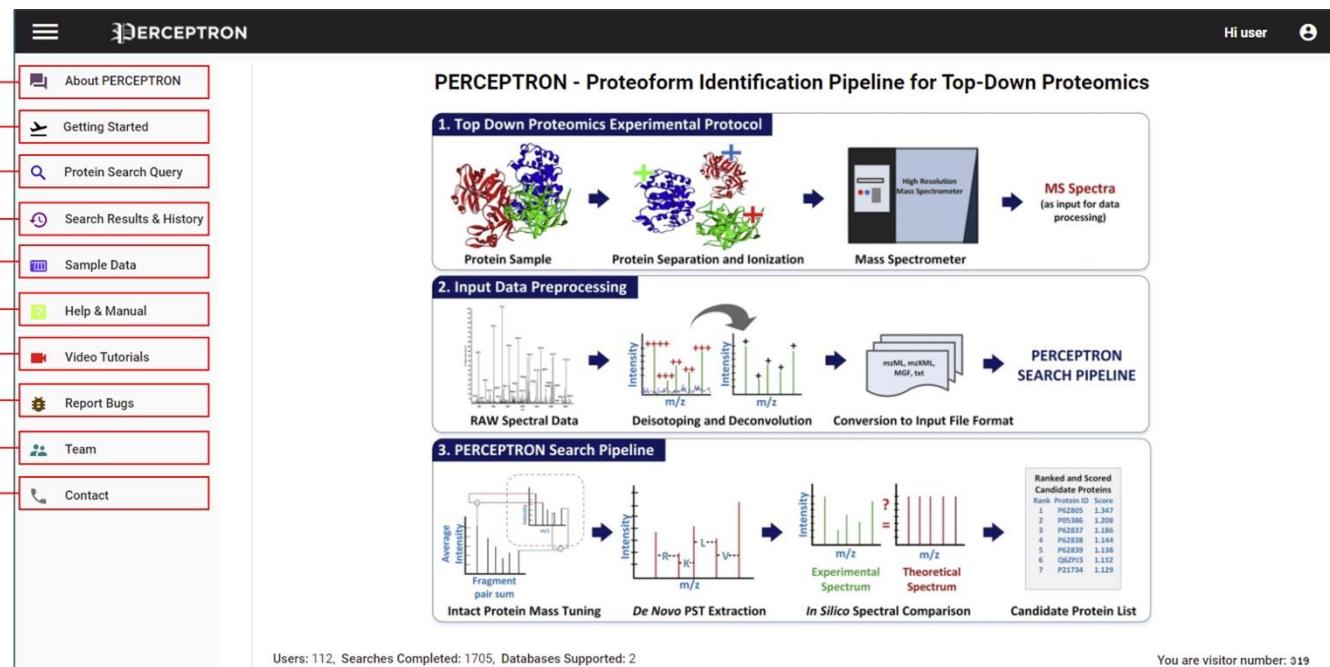


Figure 3. PERCEPTRON - Overview of User Interface

- About PERCEPTRON: A next-generation top-down proteoform search and identification platform
- Getting Started: Quick guide to proteoform search and identification using PERCEPTRON
- Protein Search Query: Job submission - Search top-down proteomics data files to identify and characterize proteoforms
- Search Results & History: View search results and history
- Sample Data: Sample top-down proteomics data for use with PERCEPTRON
- Help & Manual: Get assistance with using PERCEPTRON and download manual
- Video Tutorials: View step-by-step video tutorials demonstrating usage of PERCEPTRON
- Report Bugs: Report problems and issues here
- Team: PERCEPTRON project team members
- Contact: Contact us for further information

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. Click “Load Default Parameters” to set search parameters of Case Study I as default* parameters
- B. In order to start protein search, user must enter the ‘Protein Search Title’ (for example: “MyProject”)
- C. Select protein database
- D. Browse and upload experimental data (.mzML/ .mzXML/ .MGF/ .txt)** for Single mode; Peak-list files*** for Batch mode
- E. 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
- F. Enter an FDR percentage to shortlist identified proteoforms at desired FDR cut off
- G. Provide the number of candidate protein hits to be received in results

Note:

* Search parameters are dataset-specific. Search parameters for dataset employed in Case Study I (Histone H4 Proteoforms) have been set as default search parameters. For more details, please visit <https://perceptron.lums.edu.pk/index.html#/repository>

** File size must not exceed 60MB.

*** Compress peak-list files as a zipped format (.zip) to upload for batch mode search.

5.2.2 Set Experimental Parameters

The screenshot shows the 'Set Experimental Parameters' section of the PERCEPTRON web application. On the left sidebar, there are links labeled A through D. The main area contains several input fields and checkboxes. Red circles labeled E through I point to specific controls: E points to the 'Mass Mode' radio buttons; F points to the 'Intact Mass Tolerance' slider; G points to the 'Neutral Mass Loss' slider; H points to the 'Tune Intact Protein Mass' checkbox; and I points to the 'Select Special Ions' dropdown.

Left Sidebar:

- A: About PERCEPTRON
- B: Getting Started
- C: Protein Search Query
- D: Search Results & History
- E: Sample Data
- F: Help & Manual
- G: Video Tutorials
- H: Report Bugs
- I: Team
- J: Contact

Top Right:

- Hi user
- Upload Mass-Spectrometry Data * (with a warning message: Please select a data file/.zip file.)
- Receive Top 10 Results

Set Experimental Parameters:

- Mass Mode: * (radio buttons for MHH and M(Neutral))
- Peptide Tolerance * (text input: ppm)
- Slider Value (text input: 50 Da)
- Filter Database using MS1 (checkbox)
- Tune Intact Protein Mass (checkbox)
- Select Fragmentation Type * (dropdown menu)
- Intact Mass Tolerance * (slider from 0 to Da)
- Neutral Mass Loss (slider from 0 to Da)
- Select Special Ions (dropdown menu)

Bottom:

- Reset
- Submit

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 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 (highlighted with a red circle A), Report Bugs (highlighted with a red circle B), Team, and Contact. The main content area is titled 'Basic Parameters' and includes fields for 'Protein Search Title *', 'Enter your E-mail Address', 'FDR Cut-off' (set to 1%), 'Select Database *', 'Upload Mass-Spectrometry Data *' (with a note 'Please select a data file/zip file.'), 'Receive Top' (set to 10), and 'Results'. Below this is a section titled 'Set Experimental Parameters' with a dropdown menu. The 'Set De Novo Sequencing Parameters' section contains several input fields: a checkbox 'Enable PST Filtering' (highlighted with a red circle C), dropdown menus for 'Minimum Tag Length' and 'Maximum Tag Length' (highlighted with red circles D and E respectively), a dropdown for 'Tolerance for Each Hop' (highlighted with a red circle B), and a slider for 'Overall tolerance for PST'. At the bottom are 'Reset' and 'Submit' buttons.

Figure 6. PERCEPTRON - Overview of De Novo Sequencing Parameters

- Check 'Enable PST Filtering' to filter PSTs
- Set the 'Tolerance for each Hop'
- Tags will be filtered above the minimum length of PST selected from the drop-down menu by the user
- Tags will be filtered below the maximum length of PST selected from the drop-down menu by the user
- 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' page. On the left is a sidebar with links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main area has sections for 'Set De Novo Sequencing Parameters' and 'Set Protein Modifications Parameters'. Under 'Set Protein Modifications Parameters', there is a 'List of Modifications' dropdown containing: Acetylation_A, Acetylation_K, Acetylation_S, Amidation_F, Hydroxylation_P, Methylation_K, Methylation_R, N_Linked_Glycosylation_N, O_Linked_Glycosylation_T, O_Linked_Glycosylation_S. There are checkboxes for 'Handle Truncated Proteoforms' (circled A), 'Blind-PTM Search' (circled C), and 'Set Scoring Components Weight *'. There are dropdowns for 'PTM Tolerance * Units' (circled D), 'Methionine Chemical Modifications' (circled E), 'Variable Modifications' (circled F), and 'Cysteine Chemical Modifications' (circled G). At the bottom are 'Reset' and 'Submit' buttons.

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_ACETYLATION – N terminal acetylation with initiator methionine removed, and 4) M_ACETYLATION – 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 shows the PERCEPTRON web application interface. On the left is a sidebar with links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main area has sections for Protein Search Title, E-mail Address, FDR Cut-off, Select Database, Upload Mass-Spectrometry Data (with a note: "Please select a data file/.zip file."), and Receive Top Results. Below these are dropdown menus for Experimental Parameters, De Novo Sequencing Parameters, Protein Modifications Parameters, and Scoring Components Weight. The Scoring Components Weight section is highlighted with a red box and contains three sliders: Intact Protein Mass Score Weightage (%), Peptide Sequence Tags Score Weightage (%), and Spectral Comparisons Score Weightage (%). A circled letter 'A' points to the rightmost slider.

Figure 8. PERCEPTRON - Overview of Scoring Component Weight

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

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5.3 Window 3: Visualizing Search Results

The screenshot shows the 'User Search History' window. 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, and Contact. The main area is titled 'User Search History' and contains a table with 12 rows of search results. The columns are 'Sr. #', 'Search Title', 'Creation Time', and 'Status'. The data is as follows:

Sr. #	Search Title	Creation Time	Status
1	Default Run	2020/12/18 14:05:46	Error in Query
2	MzXML_18122020_take2	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_140sc	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).

The screenshot shows the 'Protein Spectral Matches' window. 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, and Contact. The main area is titled 'Protein Spectral Matches' and contains a table with 1 row of results. The columns are 'Sr. #', 'File Name', 'Protein ID', 'Protein Score', and 'Molecular Weight'. The data is as follows:

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

Below the table, there is a note: 'Note that proteins have canonical sequences ([link](#)).'. A 'Results Download' button is also present. At the bottom, there is a note: '* Click on the table row for corresponding candidate proteins list.' and footer links: 'Contact Us' and '(c) 2021 Biomedical Informatics Research Laboratory (BIRL)'.

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

The screenshot shows the 'Summary Results View' window of the PERCEPTRON application. On the left is a sidebar with links to various sections: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main area is titled 'Summary Results View' and contains a table with 10 rows of protein data. The columns are: Protein Rank, Protein ID, Molecular Weight, Terminal Modification, No. of PTM(s), and Protein Score. The data is as follows:

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	AOA0B4J280	11417.6263	NME	0	0.03797
5	L0R6Q1	11125.8844	None	0	0.03797
6	075964	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).

The screenshot shows the 'Detailed Protein Hit View' window of the PERCEPTRON application. On the left is a sidebar with links to various sections: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main area is titled 'Detailed Protein Hit View' and contains two sections: 'User Search Parameters' and 'General Results'.

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,bstar,y,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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The screenshot shows the PERCEPTRON search results interface. On the left is a sidebar with links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main content area displays search parameters and protein details. At the top, it shows 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, and # Modifications: 0. Below this, a note says "Click on the Protein ID to access its information. Note that proteins have canonical sequences (link)". Under "Protein Search Time (in Seconds)", it lists Total Time: 00:00:00.3077313, Spectral Comparison Module: 00:00:00.0184413, Molecular Weight Module: 00:00:00.0025092, Post-Translational Modification Module: 00:00:00.0000004, Peptide Sequence Tag Module: 00:00:00.0027434, and Truncation Module: 00:00:00.0000008. Under "Protein Sequence", it shows the sequence MSGRGKGGKGLGKGGAKRHRKVLRDNIQGITKPAIRRLARRGGVKRISGLIYEETRGVLKVFLENVIRDAVTYEHAKRKTVTAMDVVVYALKRQGRRTLGYFGG and a "Detailed Visualization" button.

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).

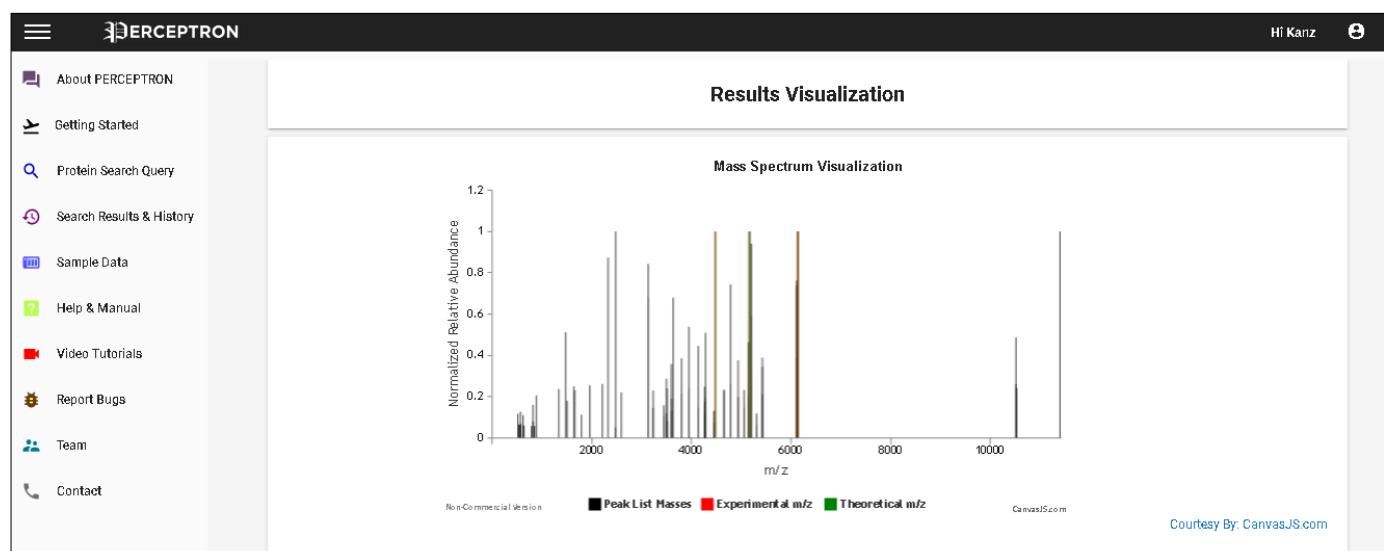


Figure 13. Detailed Results Visualization window with mass spectral visualization

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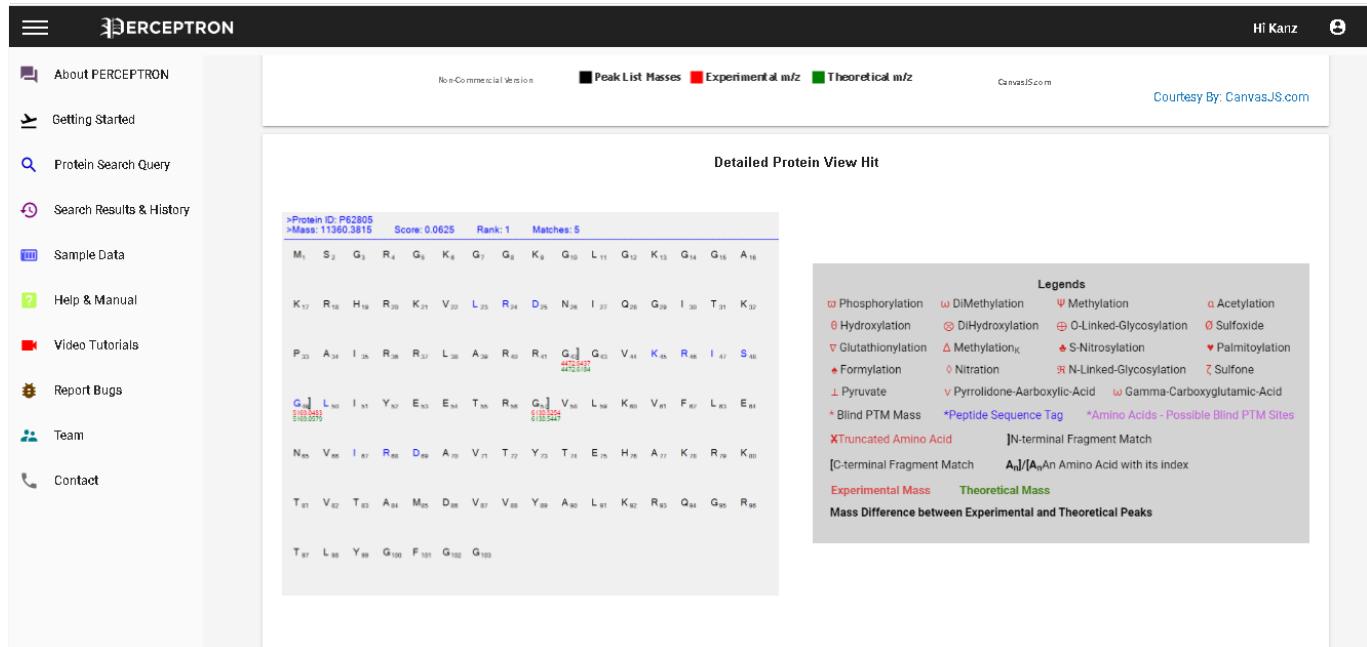


Figure 14. Detailed Results Visualization window with Detailed Protein Hit View (left) and Legends (right)

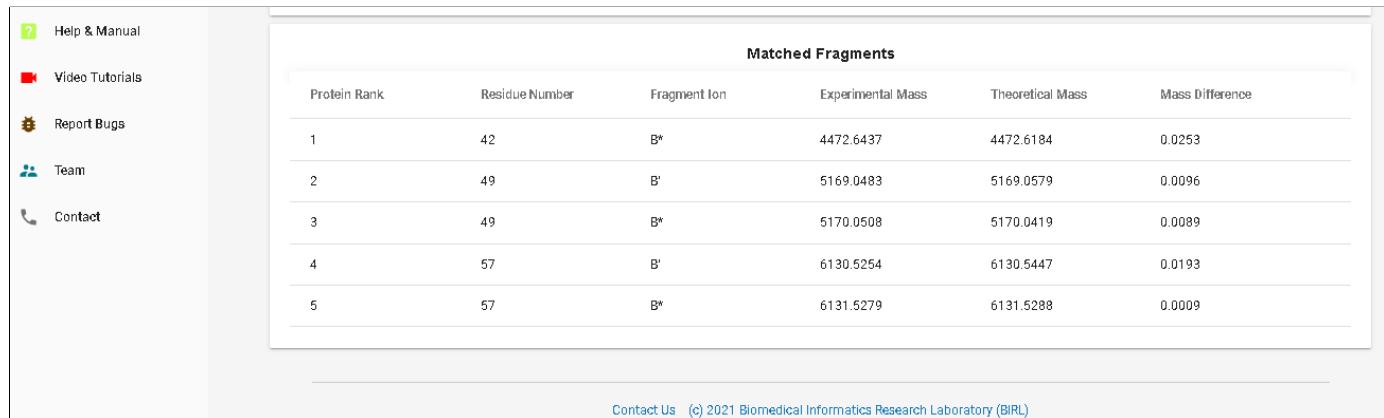


Figure 15. Detailed Results Visualization window with Matched Fragments

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)¹, Mass Spectrometry Markup Language (mzML)^{2,3} and Mascot Generic Format (MGF)⁴ 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-Convert⁵ (Figure 16).

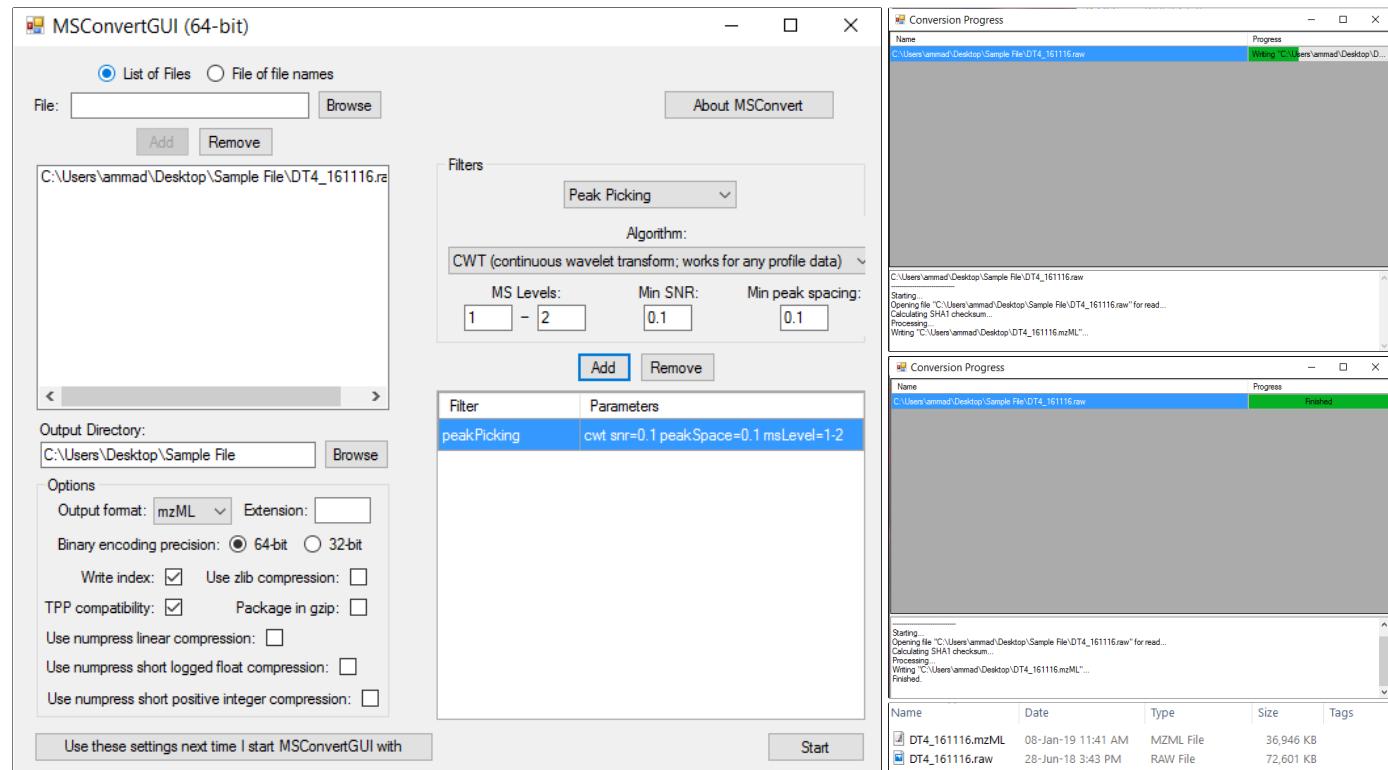


Figure 16. Conversion of raw to mzML

6.1.2 Raw to mzXML File Format Conversion

User can convert raw data files to mzXML file format by using MS-Convert⁵ (Figure 17).

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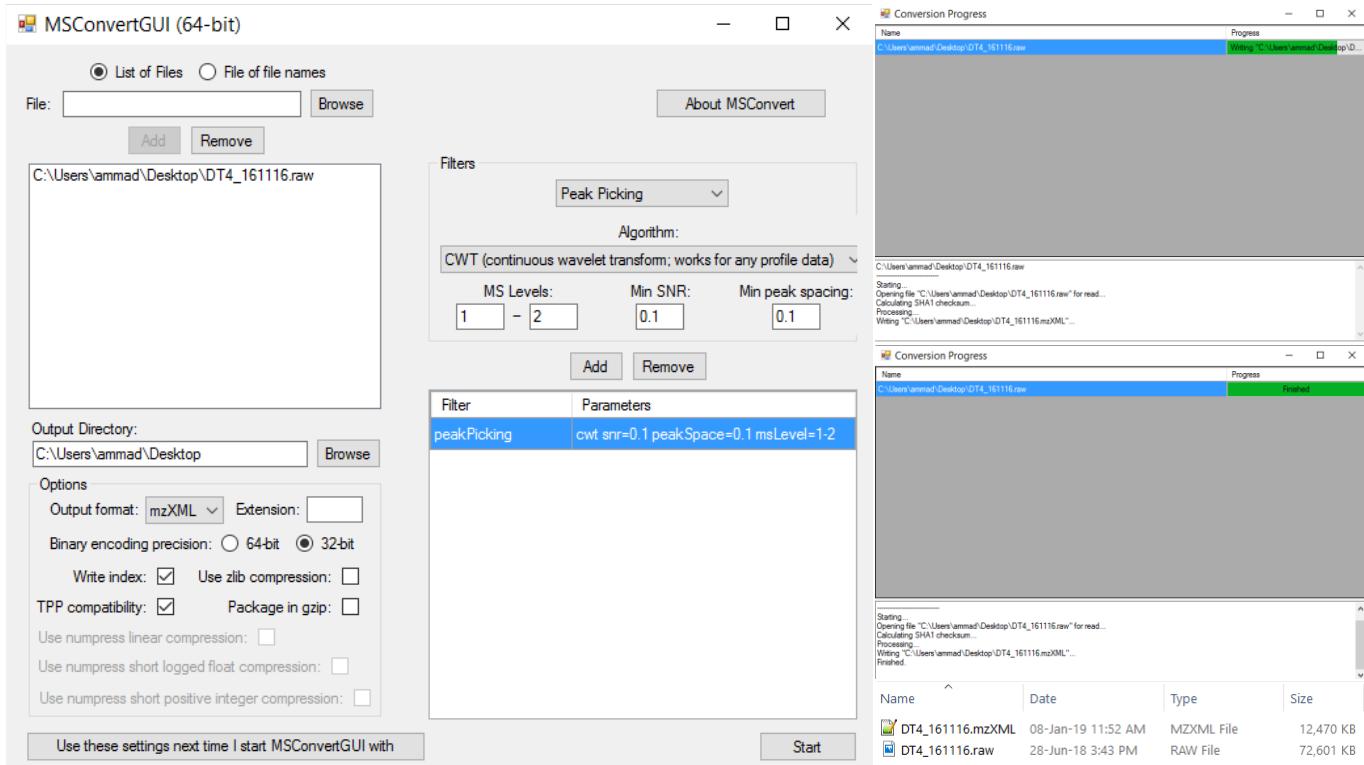


Figure 17. Conversion of raw to mzXML

6.1.3 MzXML to MGF File Format Conversion

User can convert mzXML files to MGF using MS-Decov⁶ (Figure 18).

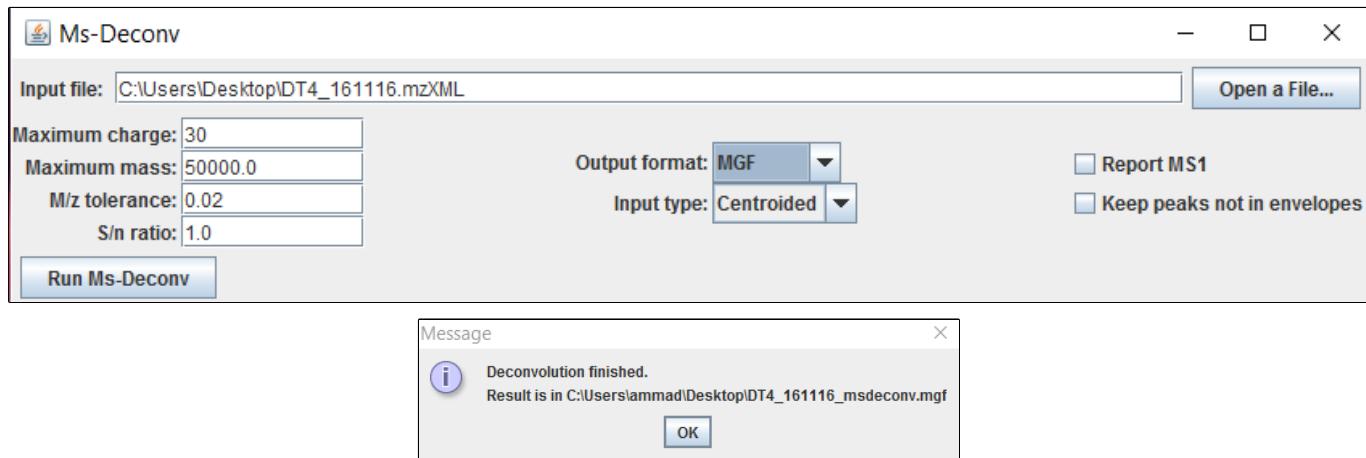


Figure 18. Conversion of mzXML to MGF

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).



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). For in-house deployment, users can add protein databases in .FASTA format within PERCEPTRON Local Service folder (path*: ... \PerceptronLocalService\PerceptronLocalService\ProteinDatabasesInFastaFormat\)

For in-house deployments please see the section 10 & 11.

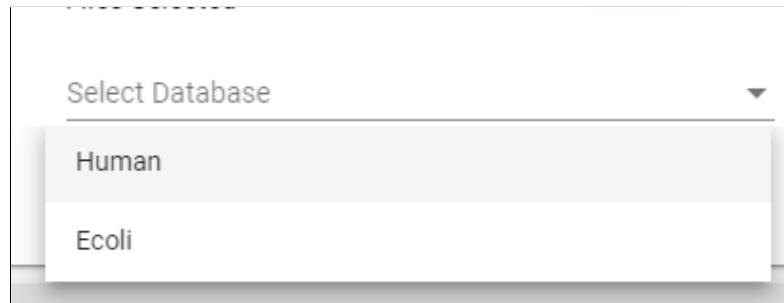


Figure 20. Selecting Protein Database from the drop-down menu

* Case Sensitive

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	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_140sc	2020/12/16 01:08:14	Completed
12	HeLa_CS1_batch	2020/12/16 01:06:34	Completed

- ‘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

- 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.
- 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.

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Summary 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

- ‘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.’

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:	b0,b1,b2,y0,y1,y2,y3	PST Filter:	True
PST Length:	3,6	Blind PTM:	False	Terminal Modifications:	None
Inexact 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

- ‘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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The screenshot shows the PERCEPTRON search results page. At the top, general protein information is displayed: 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, and # Modifications: 0. A note below states: "Click on the Protein ID to access its information. Note that proteins have canonical sequences (link)." To the left is a sidebar with links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact.

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

MSGRGKGGKGLGKGAKRHRKVLRDNQGITKPAIRRLARRGGVKRISGLIYEETRGVLKVFLENVIRDAVTYEHAKRKTVTAMDVVYALKRQGRTLYGFGG

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.

The screenshot shows the PERCEPTRON results visualization page. The main title is “Results Visualization”. Below it is a “Mass Spectrum Visualization” chart. The y-axis is “Normalized Relative Abundance” ranging from 0 to 1.2. The x-axis is “m/z” with major ticks at 2000, 4000, 6000, 8000, and 10000. The chart displays several vertical bars representing different mass peaks. A legend at the bottom indicates: Non-Commercial Version (grey), Peak List Masses (black), Experimental m/z (red), and Theoretical m/z (green). A red box highlights the “Mass Spectrum Visualization” chart. A red line with a circle labeled “10” points to the “Experimental m/z” legend entry. The bottom right corner of the visualization area contains the text “Courtesy By: CanvasJS.com”.

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.

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The screenshot shows the PERCEPTRON web application. On the left is a sidebar with links: About PERCEPTRON, Getting Started, Protein Search Query, Search Results & History, Sample Data, Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main area is titled 'Detailed Protein View Hit'. It displays a protein sequence with modifications highlighted in red. To the right is a legend box containing various post-translational modification symbols and their meanings. Numbered circles 11 and 12 point to the sequence and the legend respectively.

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:

- 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
- Molecular weight of the proteoform selected from the list of identified proteoforms
- Rank of the respective proteoform in the list of proteoforms identified
- Proteoform score computed by PERCEPTRON
- Matched fragments along with experimental (in red) and theoretical (in green) fragment masses
- Post-translational modifications as well as other modifications (e. g. truncation)

12. ‘Legends’ is a key to help user understand ‘Detailed Protein Hit View.’

The screenshot shows the PERCEPTRON web application. On the left is a sidebar with links: Help & Manual, Video Tutorials, Report Bugs, Team, and Contact. The main area is titled 'Matched Fragments' and contains a table with columns: Protein Rank, Residue Number, Fragment Ion, Experimental Mass, Theoretical Mass, and Mass Difference. Numbered circle 13 points to the table.

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

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.

- ‘Protein Rank’ indicates the rank of the protein within the list of identified proteoforms
- ‘Residue Number’ is the location of residue within proteoform sequence at which the match for ‘fragment ion’ was obtained
- ‘Fragment Ion’ indicates the type of fragment ion matched
- ‘Experimental Mass’ is the mass of experimental fragment from data file
- ‘Theoretical Mass’ is the mass of *in silico* fragment generated by PERCEPTRON
- ‘Mass Difference’ is the difference between the masses of experimental and theoretical fragments

8. Video Tutorials

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

9. Requirements for in-house Deployment

4.1. Hardware Requirements

For in-house deployment of PERCEPTRON, the hardware requirement includes a graphical processing unit (GPU) that supports CUDA TOOLKIT e.g., NVIDIA GEFORCE GTX 1650 CUDA TOOLKIT 10.0.

4.2. Software Requirements

Compilation and software build of PERCEPTRON requires the following software:

- Windows 10
- Visual Studio 2017
- Angular 1.7.4
- Node.js 8.11.1
- SQL Server Management Studio (17.6 or 17.9.1)
- .NET Framework 4.8
- CUDA TOOLKIT versions 10.0 (for PERCEPTRON GPU)
- NVIDIA GeForce Graphics Driver 456.71 (Windows 10 x64)

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 10
- Win Server 2012 R2

10. Step-by-Step Guide to in-house Deployment

10.1 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 21) to download the setup. Run the downloaded .exe file.

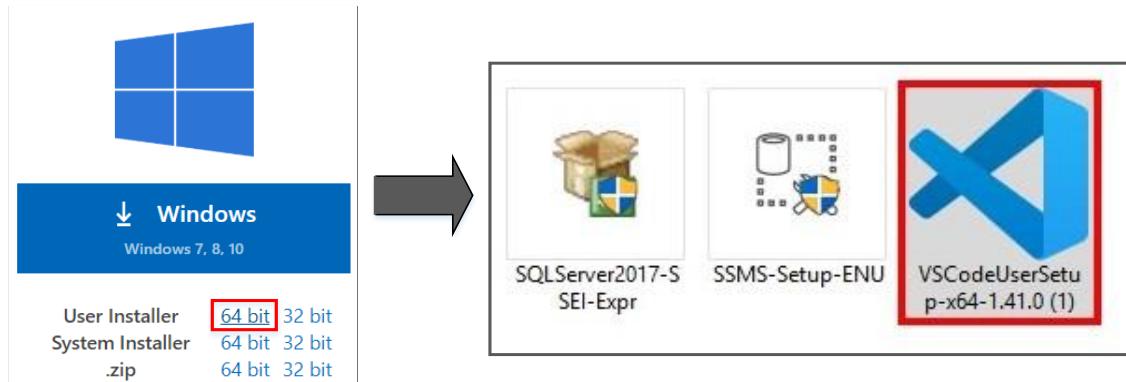


Figure 21. Downloading Visual Studio Code (VS Code) setup

Accept license terms and choose a destination folder to download Visual Studio Code setup (Figure 22).

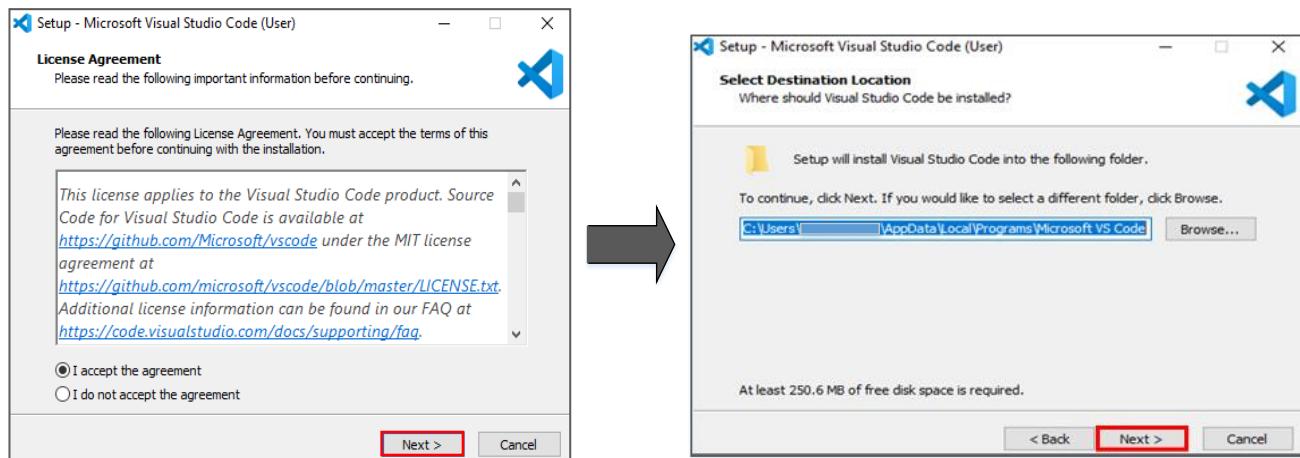
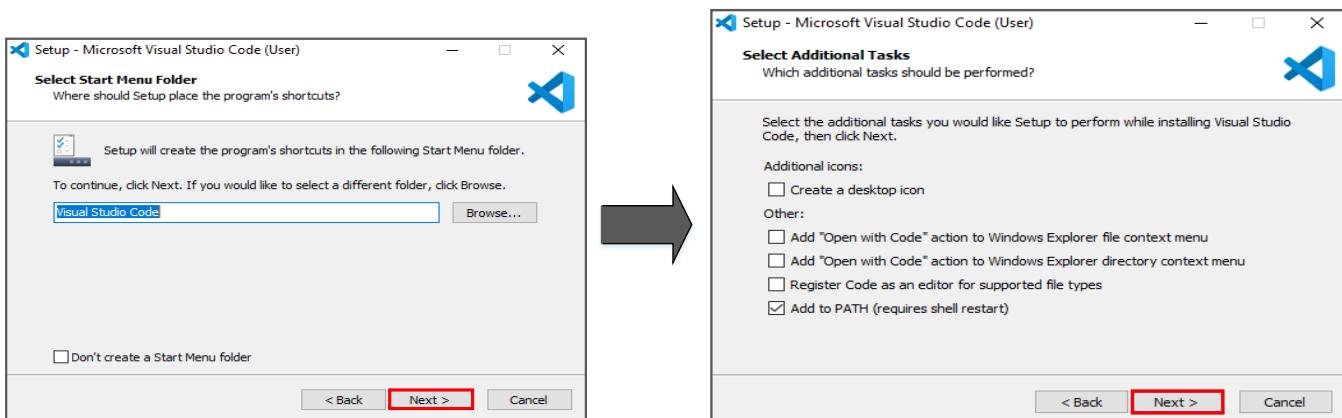


Figure 22. Choosing destination folder to download VS Code setup

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Click ‘Next’ then select ‘Add to PATH.’ Click ‘Next’ to proceed (Figure 23).



Click ‘Install’ to begin installation. Click ‘Finish’ to complete installation.

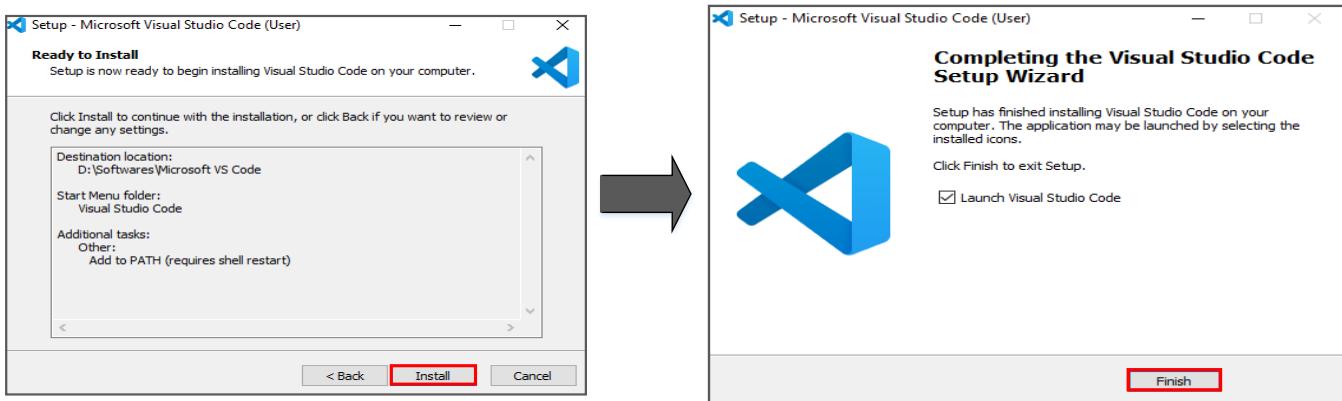


Figure 23. Steps to install Visual Studio Code setup

10.2 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 24). Run the downloaded .exe file.

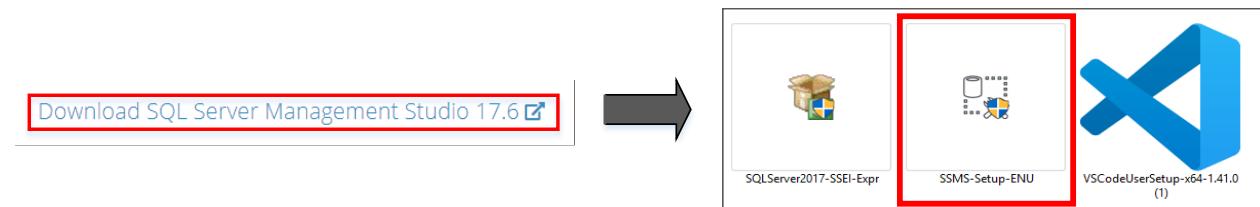


Figure 24. Downloading SQL Server Management Studio (SSMS) setup

Click ‘Install’ to begin installation (Figure 25). Click ‘Close’ to complete installation.

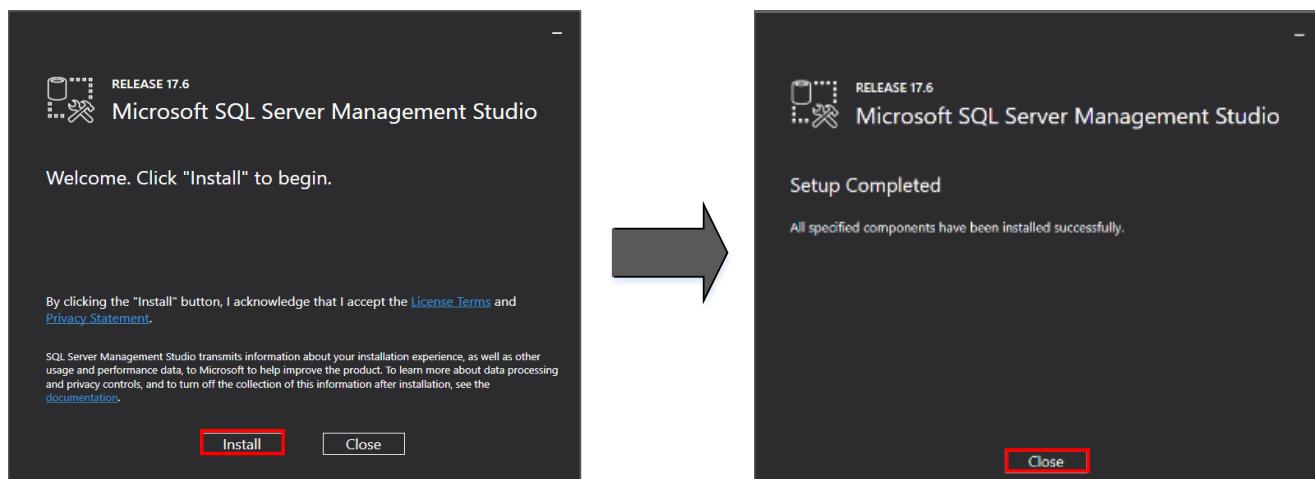


Figure 25. Steps to install SQL Server Management Studio (SSMS)

10.3 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 26) to download node.js setup. Run the .exe file for installation.

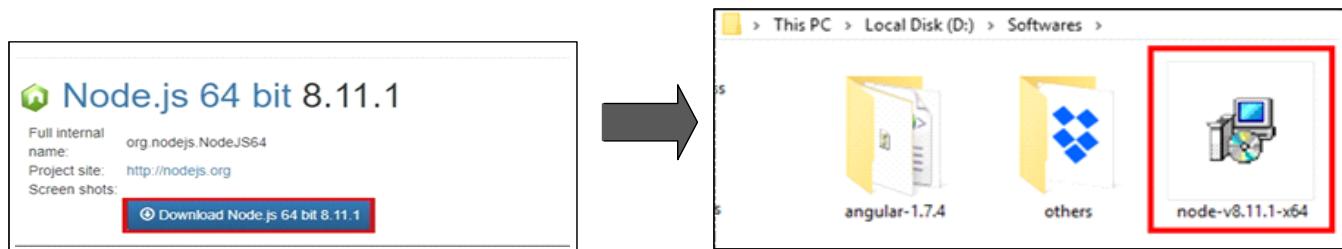
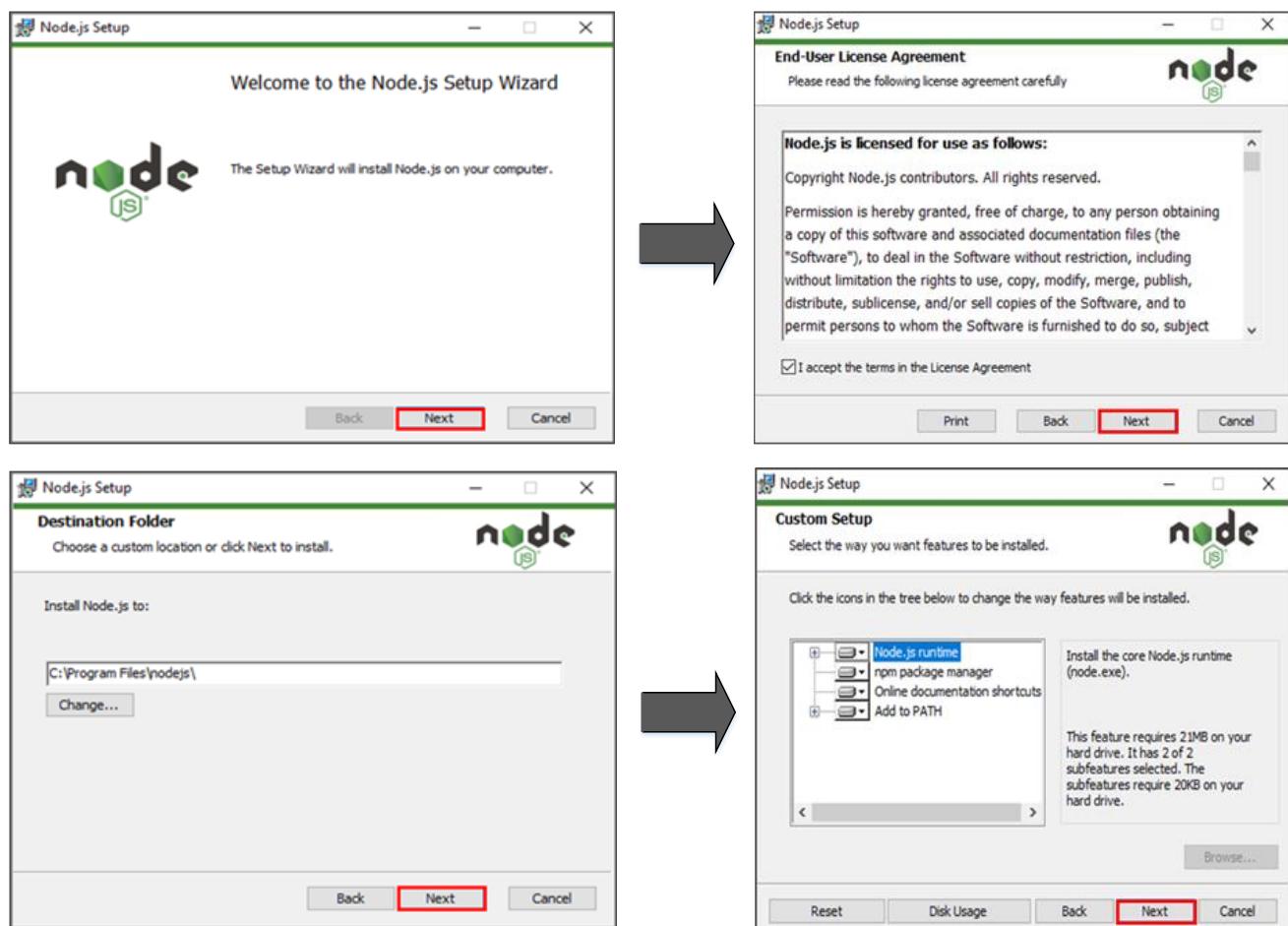


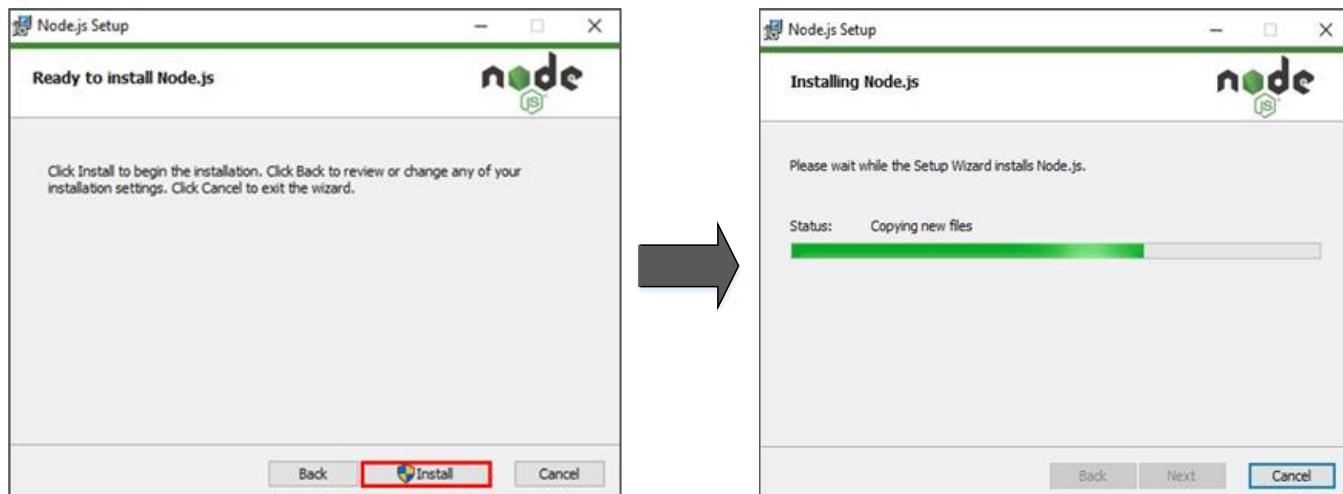
Figure 26. Downloading Node.js (version 8.11.1) setup

Click ‘Next’ and accept license terms to proceed (Figure 27).



Click ‘Install’ to begin installation.

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Click 'Finish' to complete installation.

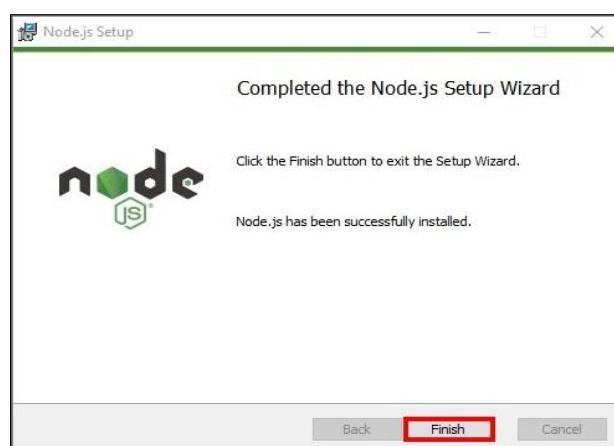


Figure 27. Steps to install Node.js setup

10.4 Installing SQL 2017

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

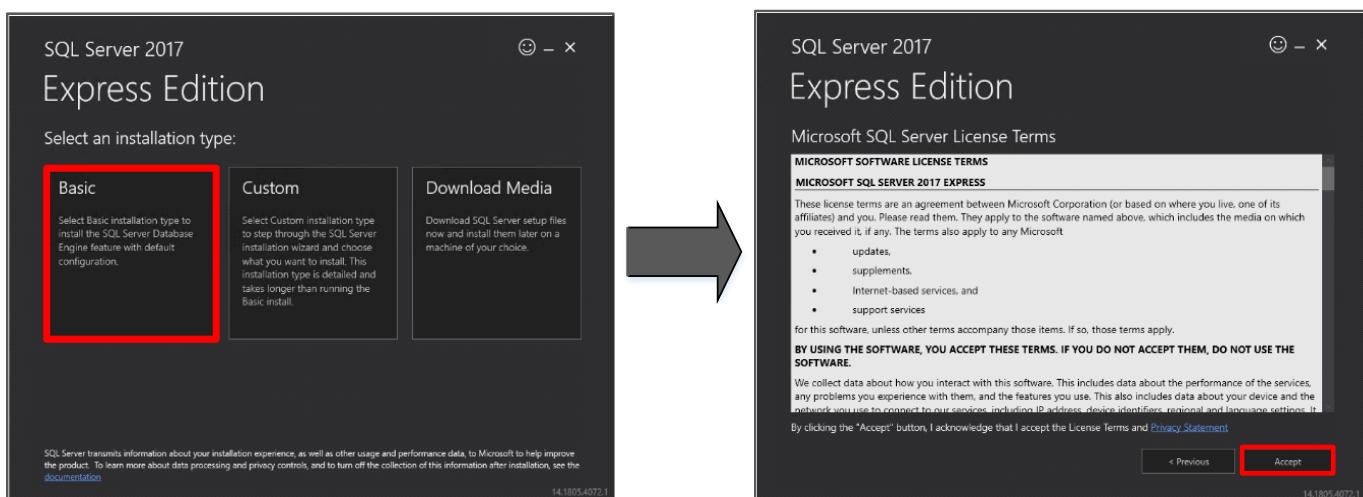
<https://www.microsoft.com/en-pk/download/details.aspx?id=55994>

Select a language and click ‘Download’ (Figure 28).



Figure 28. Downloading SQL 2017 setup

Select ‘Basic’ and then click ‘Accept’ to accept license terms (Figure 29).



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

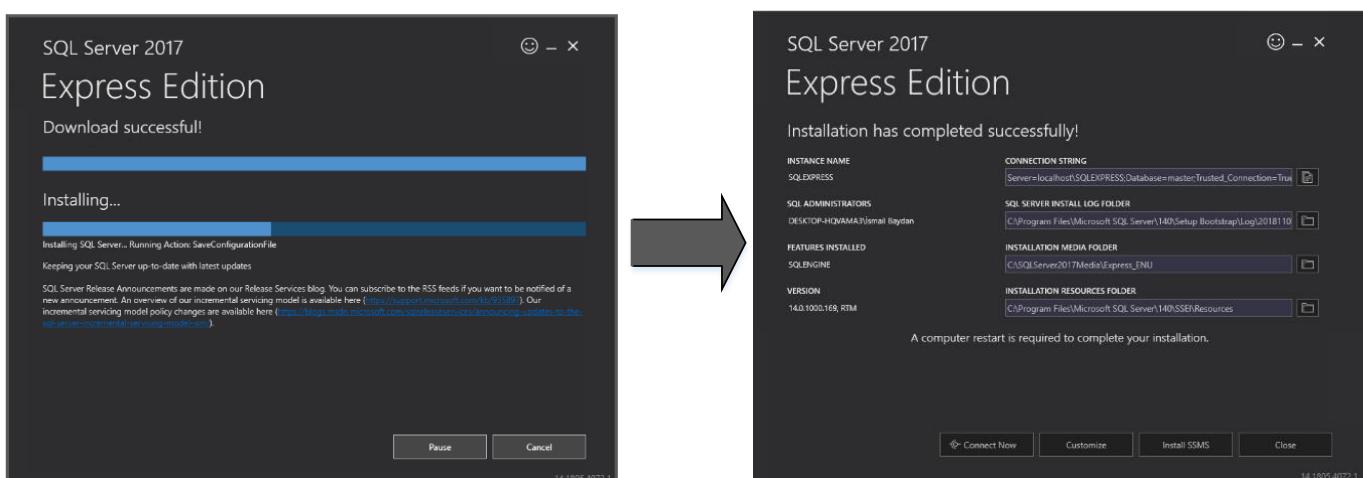


Figure 29. Steps to install SQL 2017 setup

10.5 Installing Angular 1.7.4

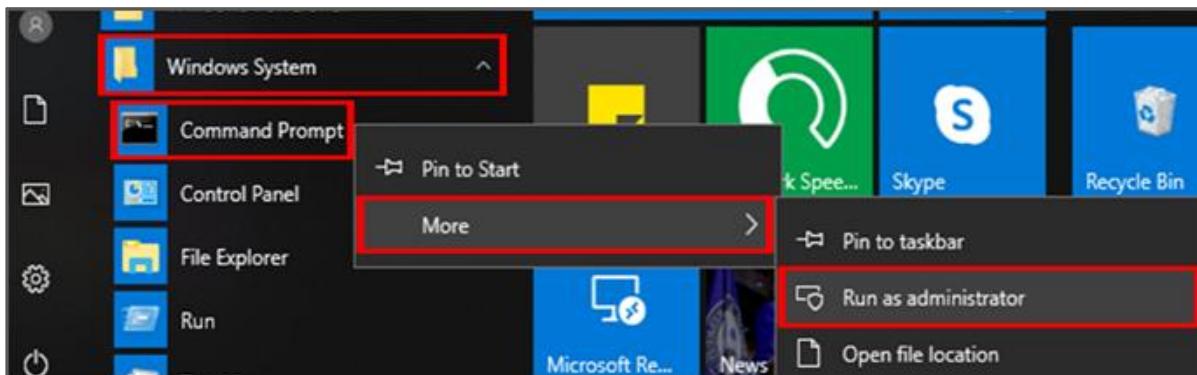
Users can download Angular 1.7.4 as a zip file using the following link: <https://code.angularjs.org/1.7.4/>

Open the link and select the .zip file for installing Angular 1.7.4 (Figure 30). Extract the contents in the file.



Figure 30. Downloading Angular 1.7.4 setup

Next, open Command Window by selecting ‘Windows System’ (Figure 31). 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.

```
Administrator: Command Prompt
Microsoft Windows [Version 10.0.17134.407]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\WINDOWS\system32>npm uninstall -g @angular/cli
up to date in 0.031s

C:\WINDOWS\system32>
```

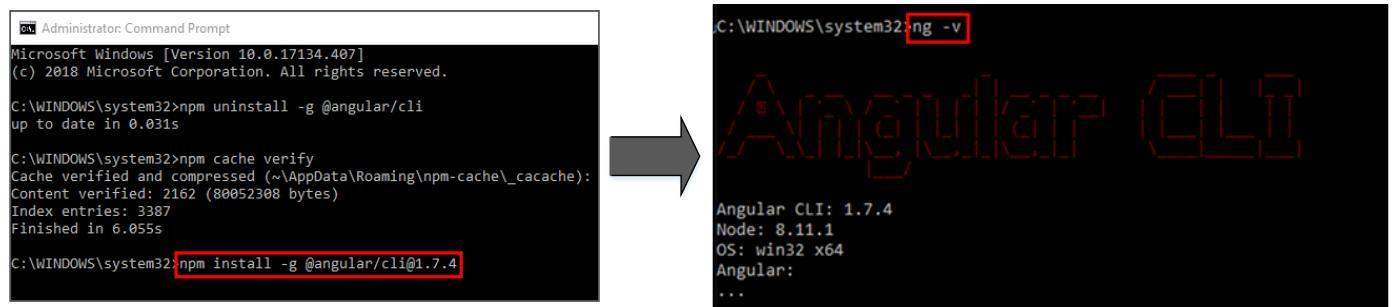
```
Administrator: Command Prompt
Microsoft Windows [Version 10.0.17134.407]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\WINDOWS\system32>npm cache verify
Cache verified and compressed (~\AppData\Roaming\npm-cache\_cacache):
Content verified: 2162 (80052308 bytes)
Index entries: 3387
Finished in 6.055s

C:\WINDOWS\system32>
```

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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```
Administrator: Command Prompt
Microsoft Windows [Version 10.0.17134.407]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\WINDOWS\system32>npm uninstall -g @angular/cli
up to date in 0.031s

C:\WINDOWS\system32>npm cache verify
Cache verified and compressed (~\AppData\Roaming\npm-cache\_cacache):
Content verified: 2162' (80052308 bytes)
Index entries: 3387
Finished in 6.055s

C:\WINDOWS\system32>npm install -g @angular/cli@1.7.4
```

C:\WINDOWS\system32>**ng -v**

Angular CLI: 1.7.4
Node: 8.11.1
OS: win32 x64
Angular:
...

Figure 31. Steps to install Angular 1.7.4

10.6 Adding 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 32).

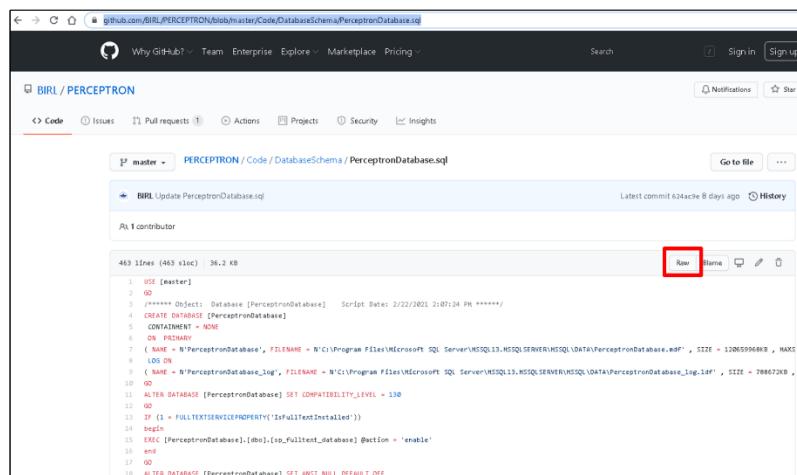


Figure 32. Downloading SQL File from GitHub

Open Microsoft SQL Server Management Studio (SSMS). Click on “File”, “Open” and “File” (Figure 33) to open ‘PerceptronDatabase.sql’ file in SSMS.

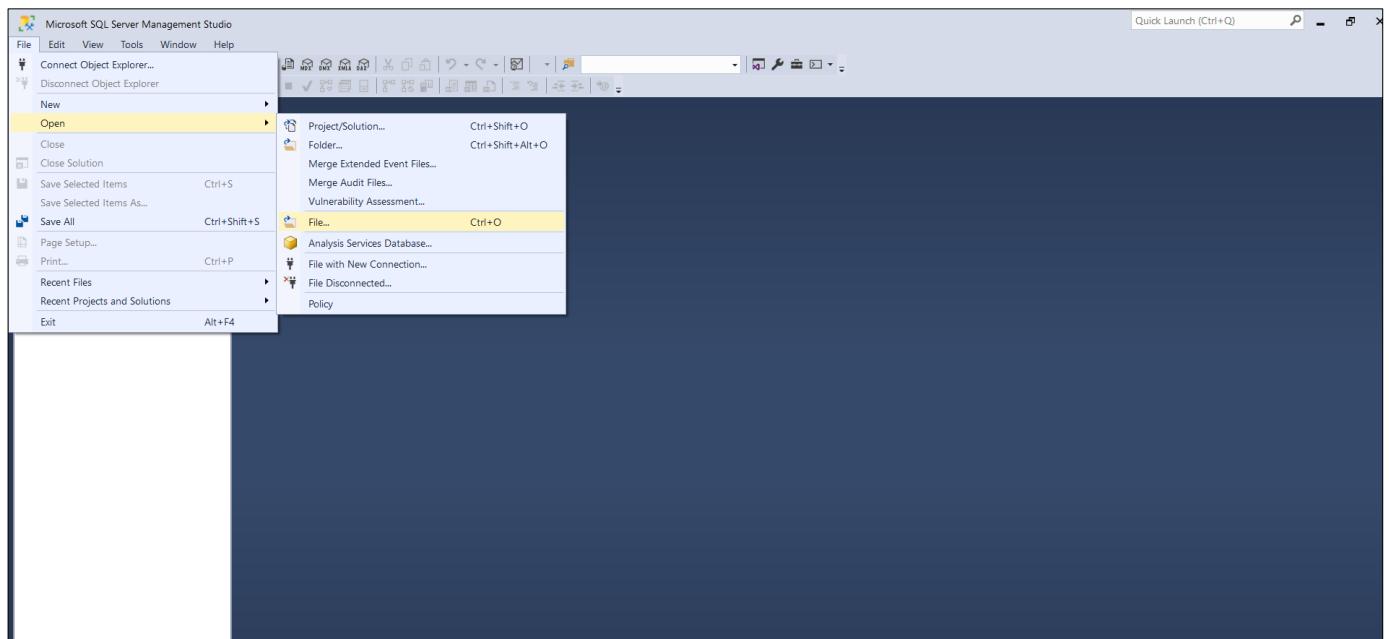
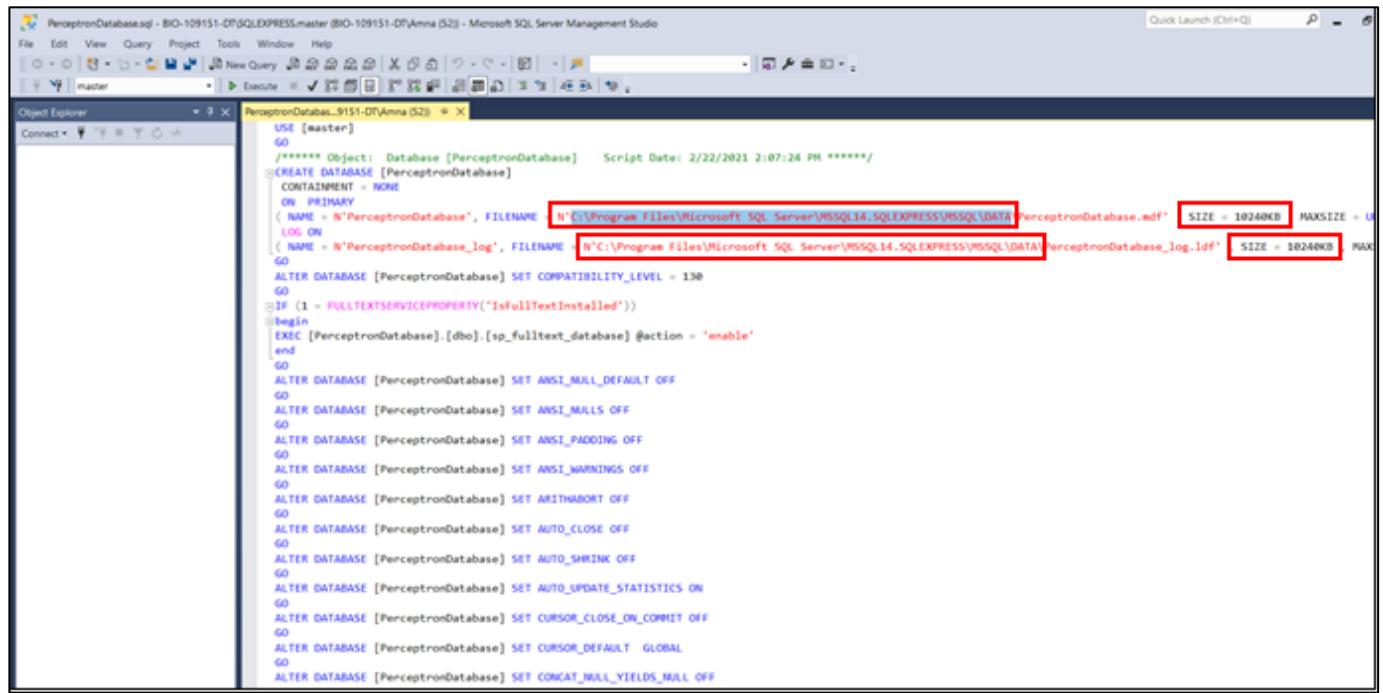


Figure 33. Steps to add SQL file downloaded from GitHub

Change file paths and size information, as required e.g., file path for MSSQL14.SQLEXPRESS: “C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA...” and file size: 10240 KB (Figure 34) and click “Execute” in toolbar.

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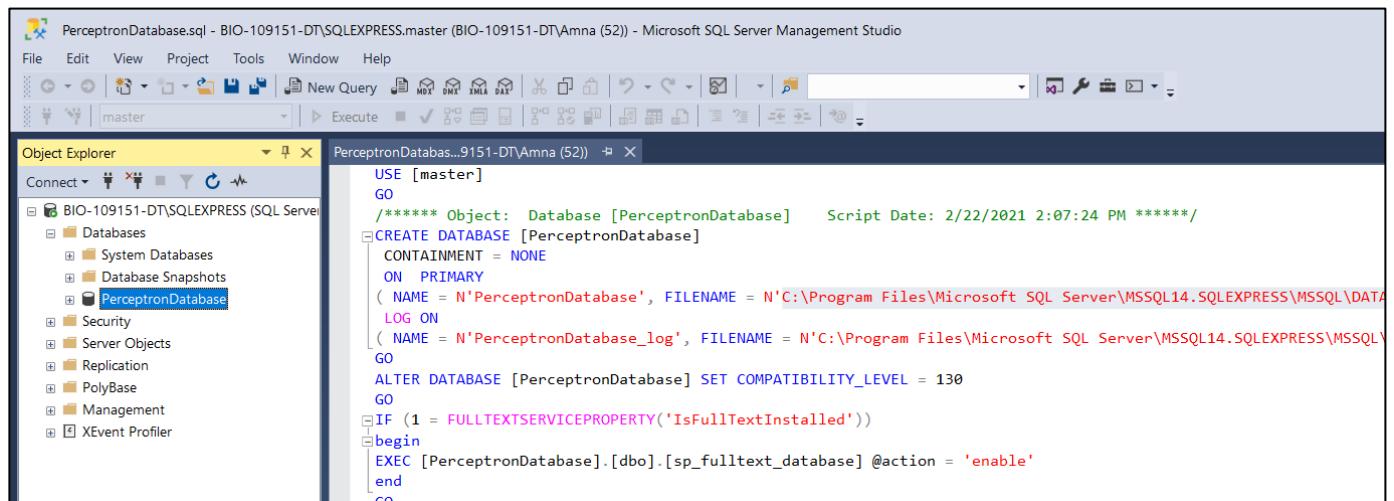


The screenshot shows the Microsoft SQL Server Management Studio interface. In the Object Explorer, a new database named 'PerceptronDatabase' is being created under the 'master' database. The script window displays the SQL code for creating the database, specifying the data file path as 'N'C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA\PerceptronDatabase.mdf', size as 10240KB, and max size as 10240KB. It also specifies the log file path as 'N'C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA\PerceptronDatabase_log.ldf', size as 10240KB, and max size as 10240KB.

```
USE [master]
GO
***** Object: Database [PerceptronDatabase] Script Date: 2/22/2021 2:07:24 PM *****/
CREATE DATABASE [PerceptronDatabase]
CONTAINMENT = NONE
ON PRIMARY
( NAME = N'PerceptronDatabase', FILENAME = N'C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA\PerceptronDatabase.mdf' , SIZE = 10240KB , MAXSIZE = 102400KB , FILEGROWTH = 10240KB )
LOG ON
( NAME = N'PerceptronDatabase_log', FILENAME = N'C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA\PerceptronDatabase_log.ldf' , SIZE = 10240KB , MAXSIZE = 102400KB , FILEGROWTH = 10240KB )
GO
ALTER DATABASE [PerceptronDatabase] SET COMPATIBILITY_LEVEL = 130
GO
IF (1 = FULLTEXTSERVICEPROPERTY('IsFullTextInstalled'))
BEGIN
EXEC [PerceptronDatabase].[dbo].[sp_fulltext_database] @action = 'enable'
END
GO
ALTER DATABASE [PerceptronDatabase] SET ANSI_NULL_DEFAULT OFF
GO
ALTER DATABASE [PerceptronDatabase] SET ANSI_NULLS OFF
GO
ALTER DATABASE [PerceptronDatabase] SET ANSI_PADDING OFF
GO
ALTER DATABASE [PerceptronDatabase] SET ANSI_WARNINGS OFF
GO
ALTER DATABASE [PerceptronDatabase] SET ARITHABORT OFF
GO
ALTER DATABASE [PerceptronDatabase] SET AUTO_CLOSE OFF
GO
ALTER DATABASE [PerceptronDatabase] SET AUTO_SHRINK OFF
GO
ALTER DATABASE [PerceptronDatabase] SET AUTO_UPDATE_STATISTICS ON
GO
ALTER DATABASE [PerceptronDatabase] SET CURSOR_CLOSE_ON_COMMIT OFF
GO
ALTER DATABASE [PerceptronDatabase] SET CURSOR_DEFAULT GLOBAL
GO
ALTER DATABASE [PerceptronDatabase] SET CONCAT_NULL_YIELDS_NULL OFF
GO
```

Figure 34. Steps to execute SQLfile

Upon successful execution, “PerceptronDatabase” will appear in Databases panel on left (Figure 35).



The screenshot shows the Microsoft SQL Server Management Studio interface. The 'Object Explorer' pane on the left lists the databases available on the server, including the newly created 'PerceptronDatabase'. The script window shows the same SQL code as in Figure 34, confirming the database creation.

```
USE [master]
GO
***** Object: Database [PerceptronDatabase] Script Date: 2/22/2021 2:07:24 PM *****/
CREATE DATABASE [PerceptronDatabase]
CONTAINMENT = NONE
ON PRIMARY
( NAME = N'PerceptronDatabase', FILENAME = N'C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA\PerceptronDatabase.mdf' , SIZE = 10240KB , MAXSIZE = 102400KB , FILEGROWTH = 10240KB )
LOG ON
( NAME = N'PerceptronDatabase_log', FILENAME = N'C:\Program Files\Microsoft SQL Server\MSSQL14.SQLEXPRESS\MSSQL\DATA\PerceptronDatabase_log.ldf' , SIZE = 10240KB , MAXSIZE = 102400KB , FILEGROWTH = 10240KB )
GO
ALTER DATABASE [PerceptronDatabase] SET COMPATIBILITY_LEVEL = 130
GO
IF (1 = FULLTEXTSERVICEPROPERTY('IsFullTextInstalled'))
BEGIN
EXEC [PerceptronDatabase].[dbo].[sp_fulltext_database] @action = 'enable'
END
GO
```

Figure 35. Importing PERCEPTRON Database using SQL File

10.7 Installing NVIDIA GeForce Graphics Driver 456.71 (for PERCEPTRON GPU)

User can download the NVIDIA GeForce graphics driver 456.71 using the following link:
<https://www.nvidia.com/en-us/drivers/results/165686/>

Click on ‘Download Now’ to download the setup (Figure 36). Run the .exe file.

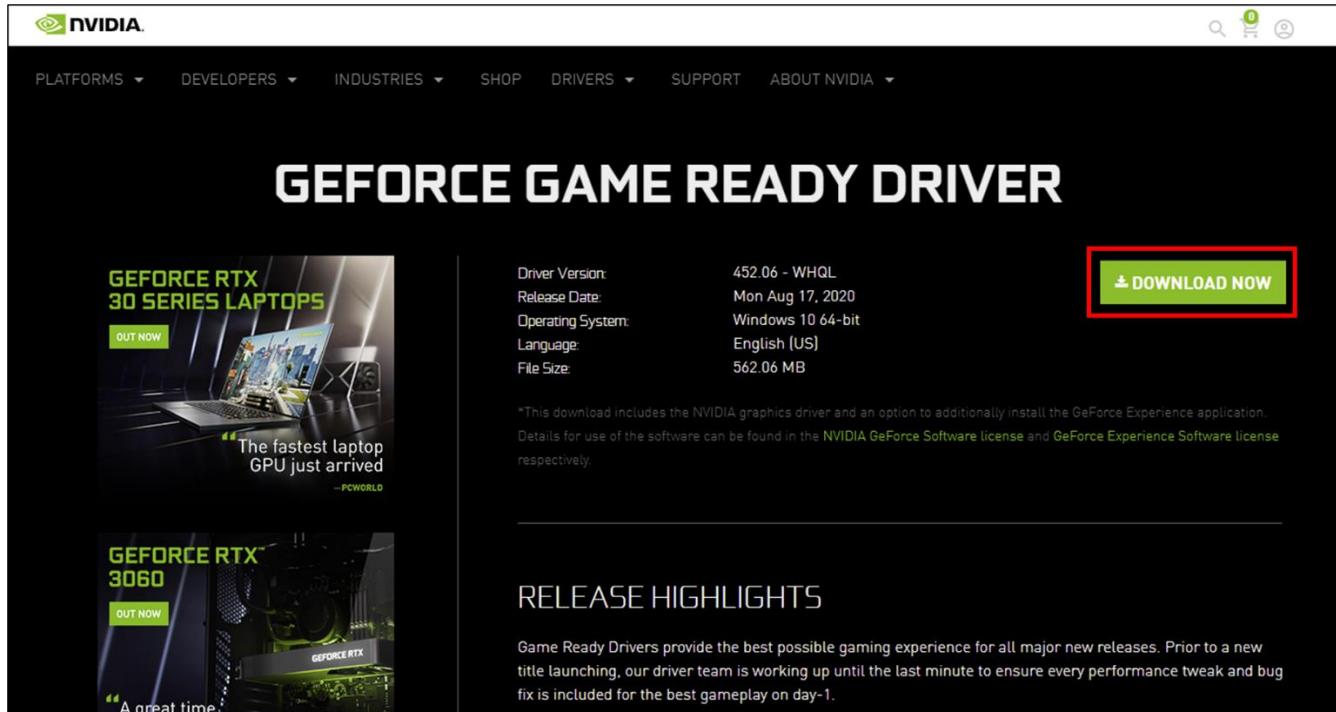
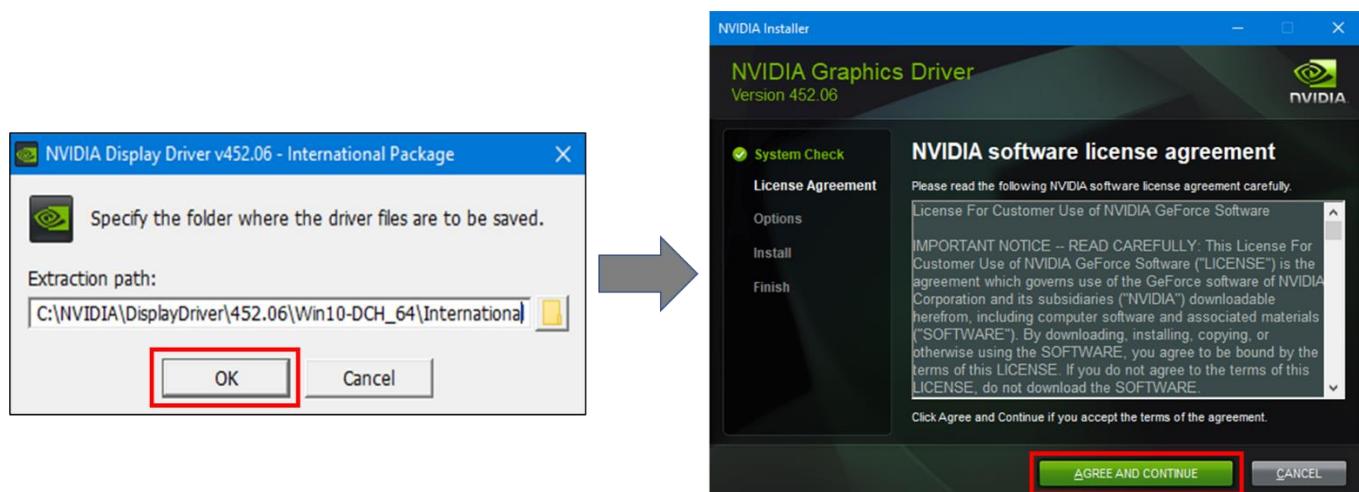


Figure 36. Downloading NVIDIA GeForce graphics driver

Choose a destination for the installation and click ‘Ok’. Accept the license terms and continue (Figure 37).



Select ‘Express’ under Installation options. Close once installation has been finished.

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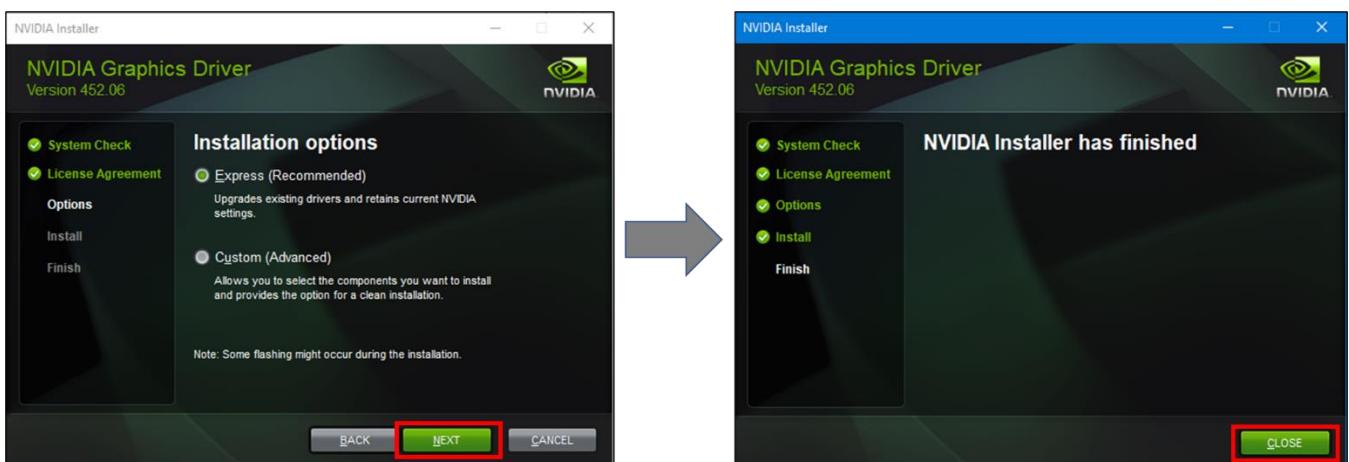


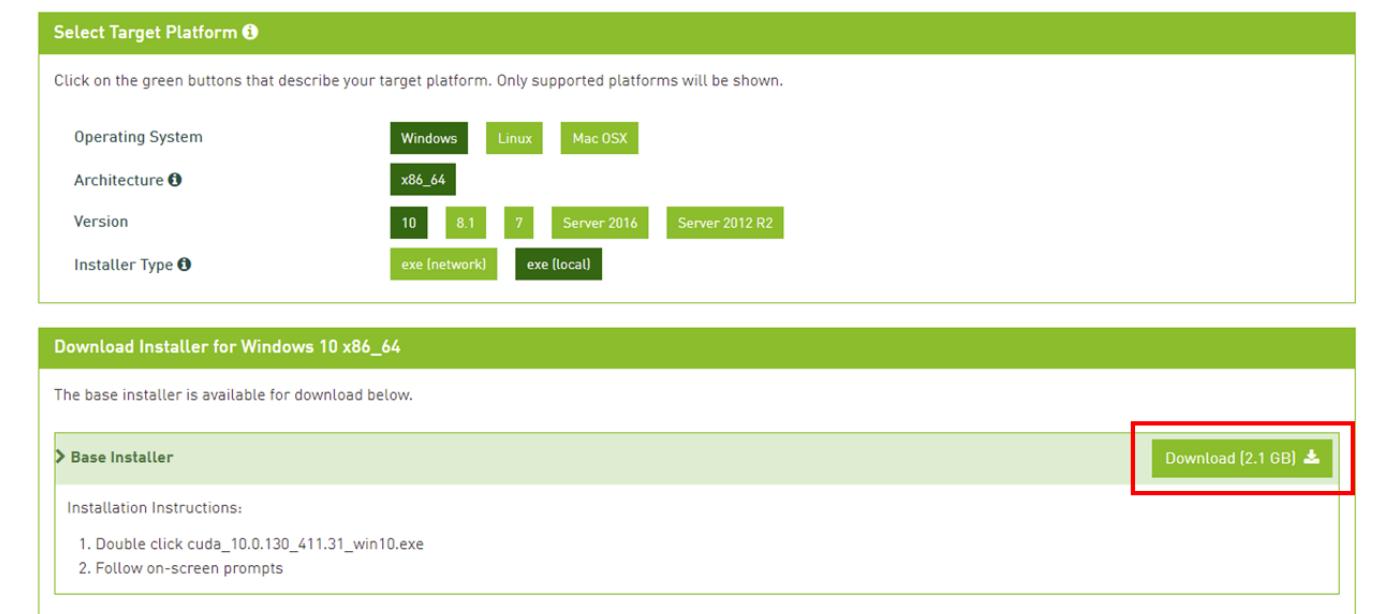
Figure 37. Steps to install NVIDIA GeForce graphics driver

To confirm if all driver components have been installed properly, run a sample code downloaded at the path “C:\ProgramData\NVIDIA Corporation\CUDA Samples\v10.0\0_Simple”

10.8 Installing CUDA Toolkit 10.0 (for PERCEPTRON GPU)

Users can download CUDA Toolkit 10.0 (Figure 38), by following the link:
https://developer.nvidia.com/cuda-10.0-download-archive?target_os=Windows&target_arch=x86_64&target_version=10&target_type=exelocal

CUDA Toolkit 10.0 Archive



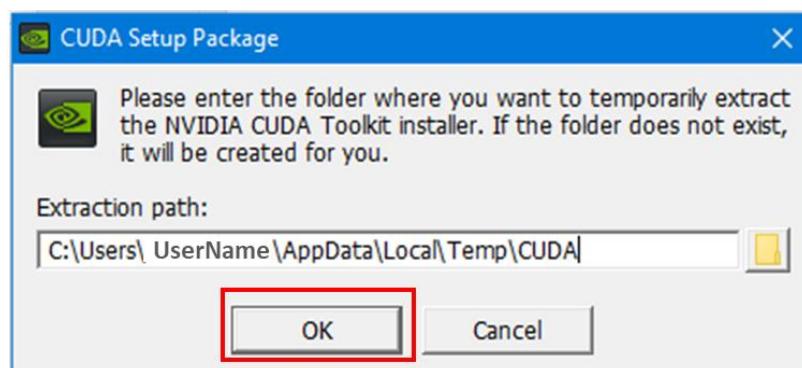
The screenshot shows the 'Select Target Platform' section with the following configuration:

- Operating System:** Windows (selected)
- Architecture:** x86_64 (selected)
- Version:** 10 (selected)
- Installer Type:** exe [network] (selected)

Below this, the 'Download Installer for Windows 10 x86_64' section shows the 'Base Installer' available for download. A red box highlights the 'Download [2.1 GB]' button.

Figure 38. Downloading CUDA Toolkit 10.0 for deploying PERCEPTRON Local Service (GPU)

Next, install the setup downloaded (Figure 39).



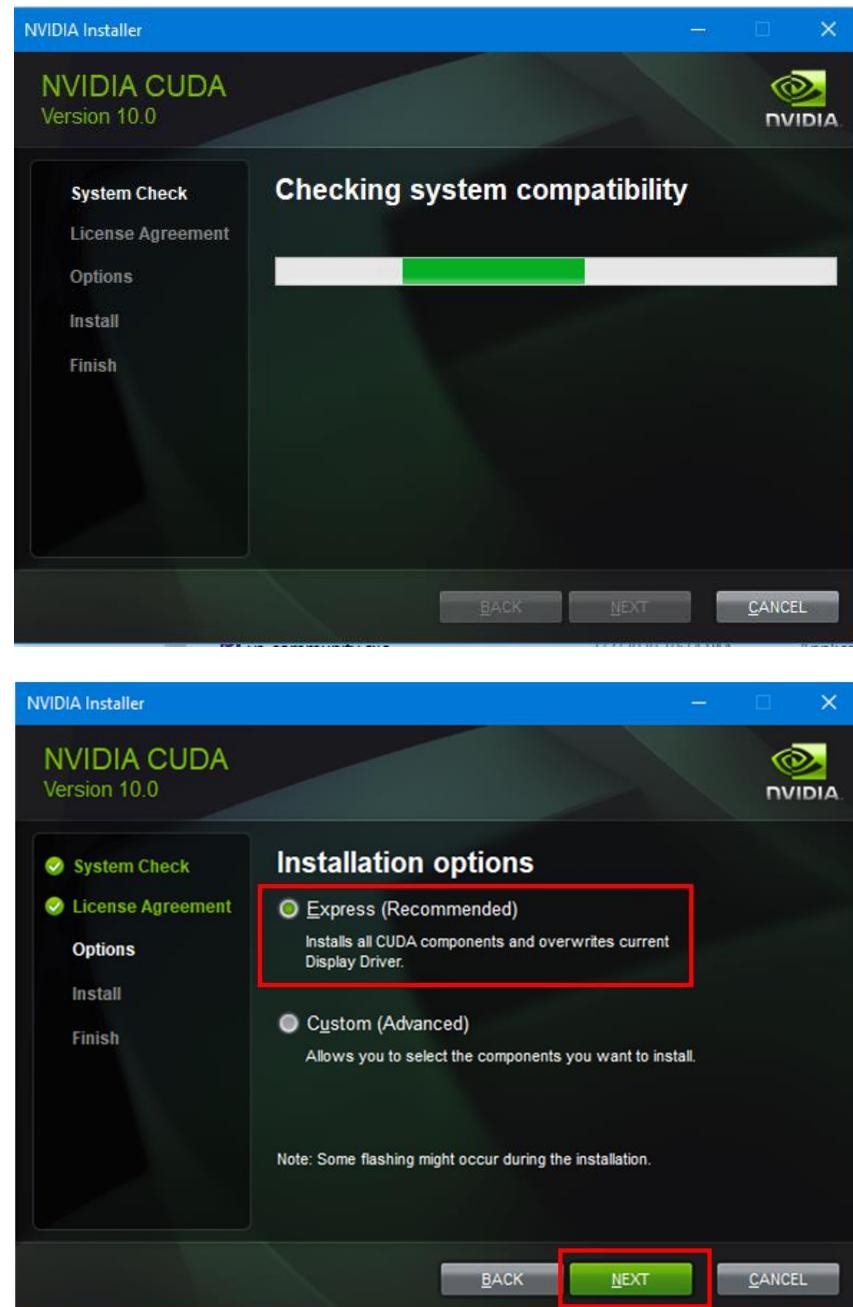


Figure 39. Steps to install CUDA Toolkit 10.0

Note: Visual Studio installation is required for Nsight Visual Studio feature installation (Figure 40).

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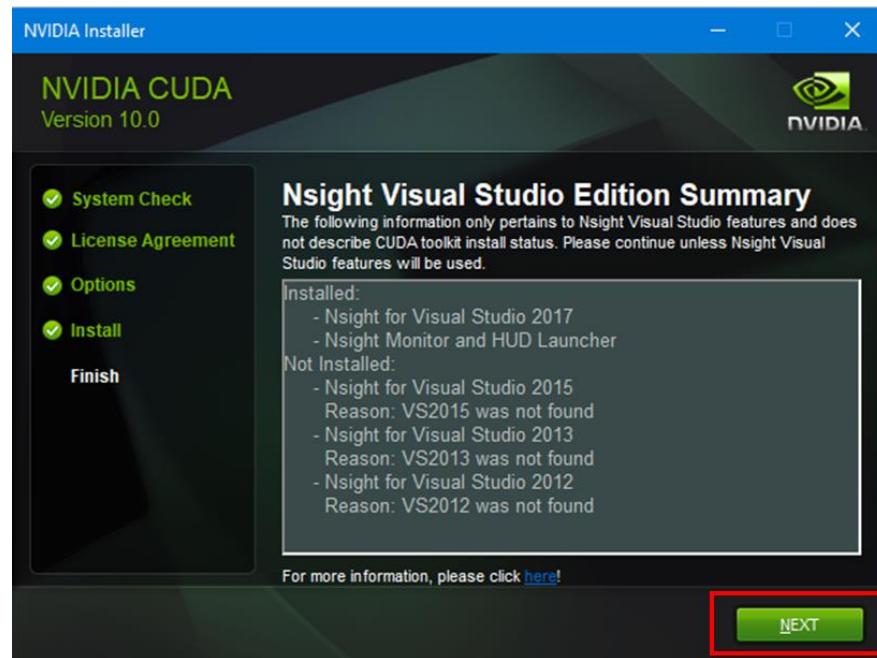


Figure 40. Installing Nsight Visual Studio feature

Click “CLOSE” to finish installation (Figure 41).

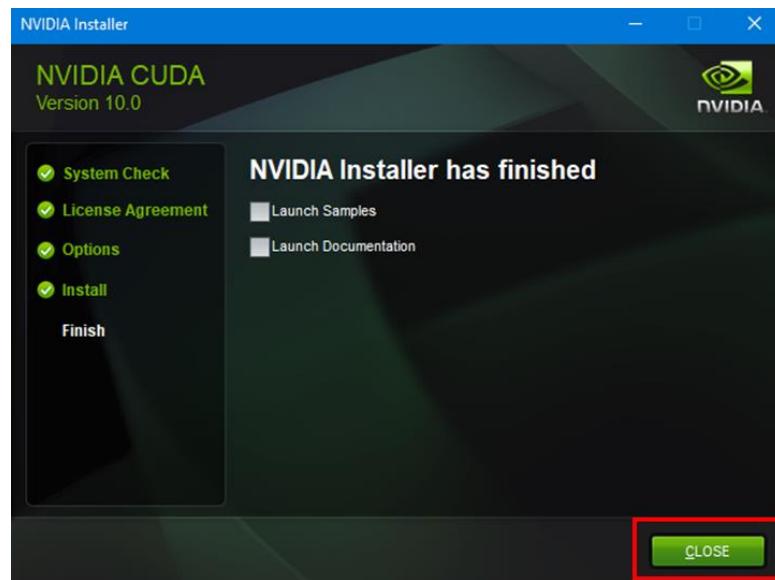


Figure 41. Confirmation of NVIDIA CUDA Toolkit Installation

To install Visual Studio (VS) 2017 with the specific Workloads and Individual Components, open VS installer, next go to “Modify” and select the following options (Figure 42).

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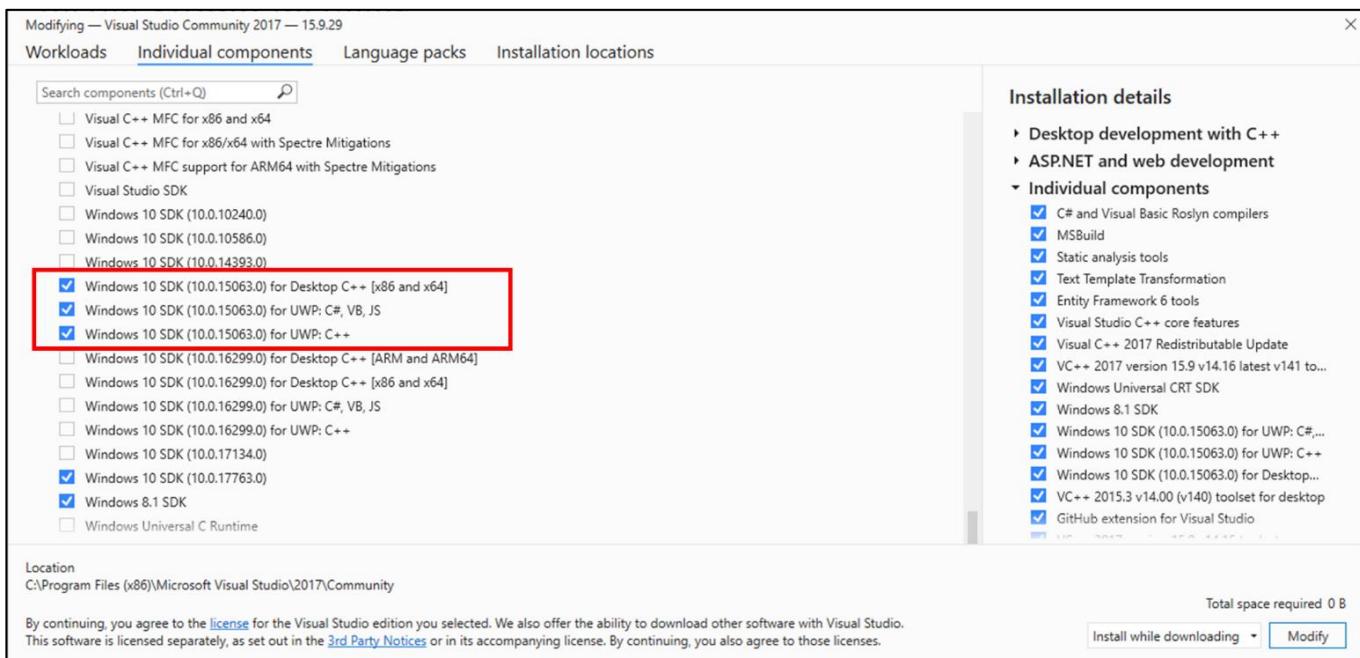
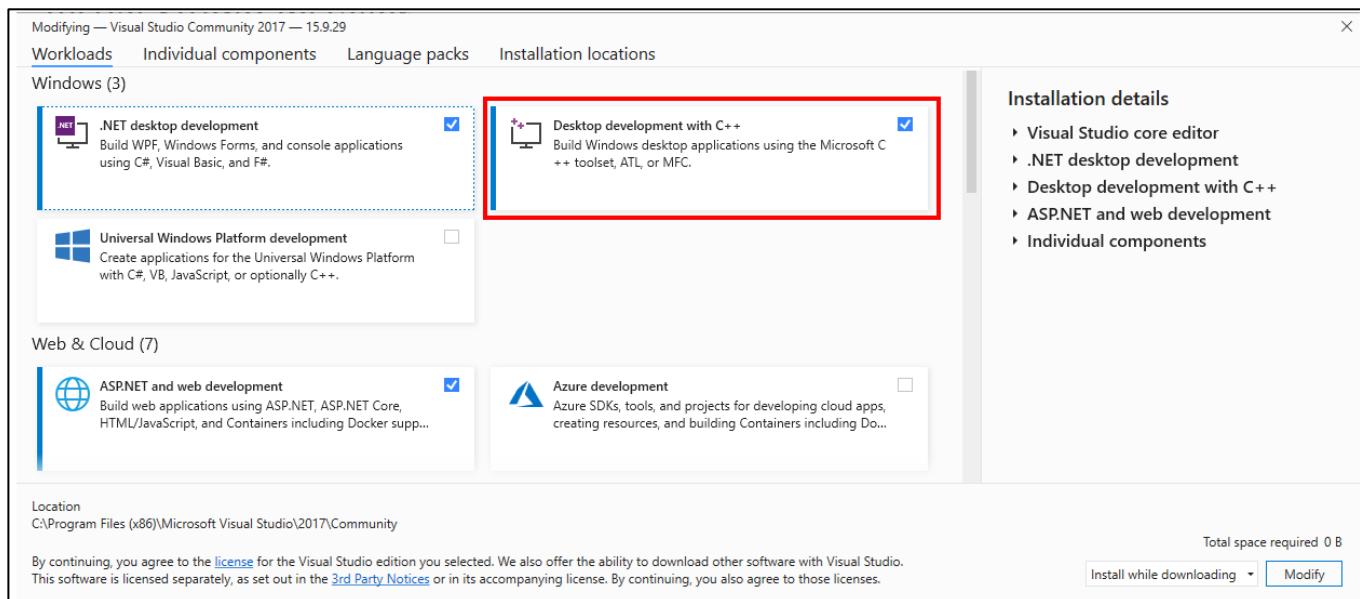


Figure 42. Installing specific Workloads and Individual Components in Visual Studio 2017

10.9 Installing Windows Software Development Kit (SDK)

Users can access PERCEPTRON application programming interface (API) using the Windows Software Development Kit (SDK). Users can download SDK using the following link:
<https://developer.microsoft.com/en-us/windows/downloads/sdk-archive/>

Click on ‘Install SDK’ corresponding to version 10.0.19041.0 to download the setup (Figure 43). Run the .exe file.

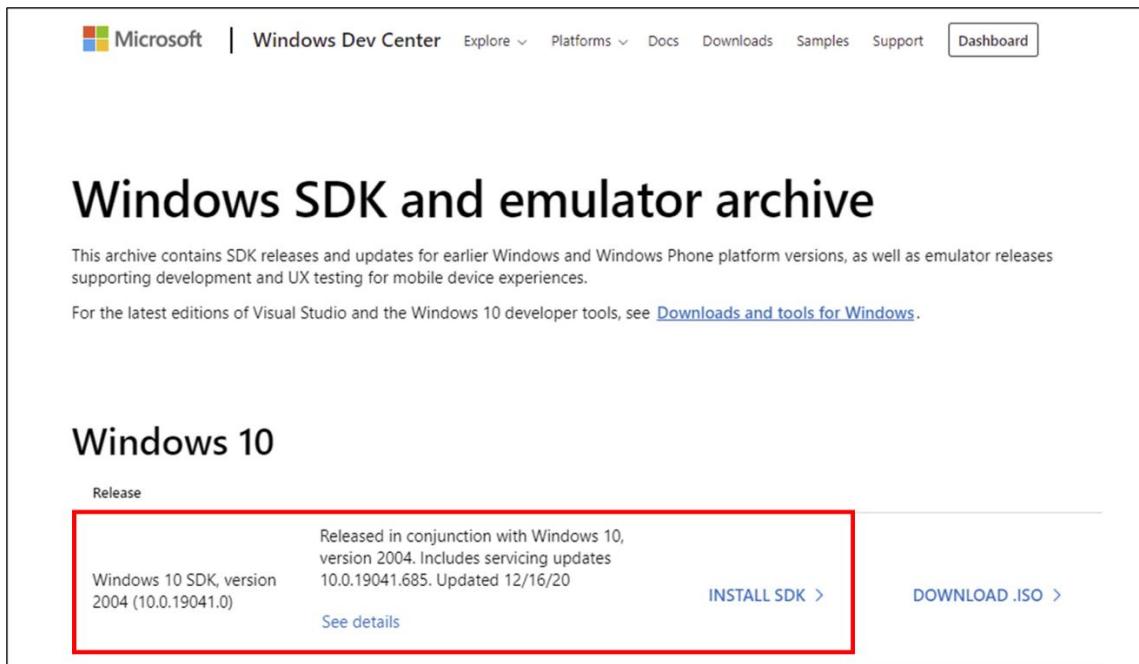
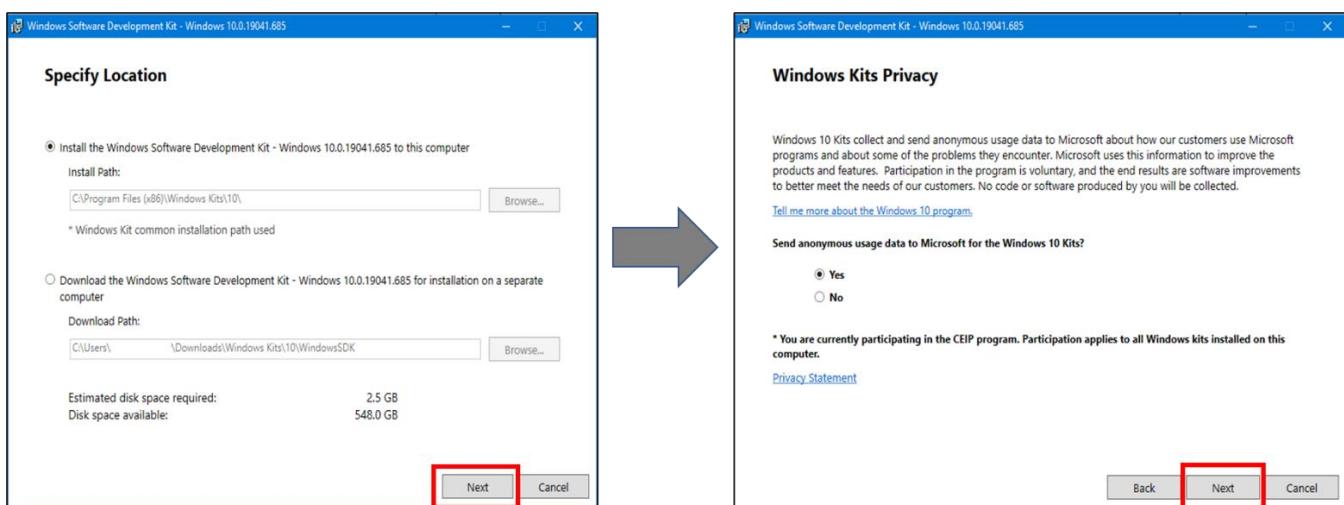


Figure 43. Downloading Windows Software Development Kit (SDK)

Choose a destination for the installation and click ‘Next’ (Figure 44).



Accept the license terms, select the features shown below and click ‘Install’.

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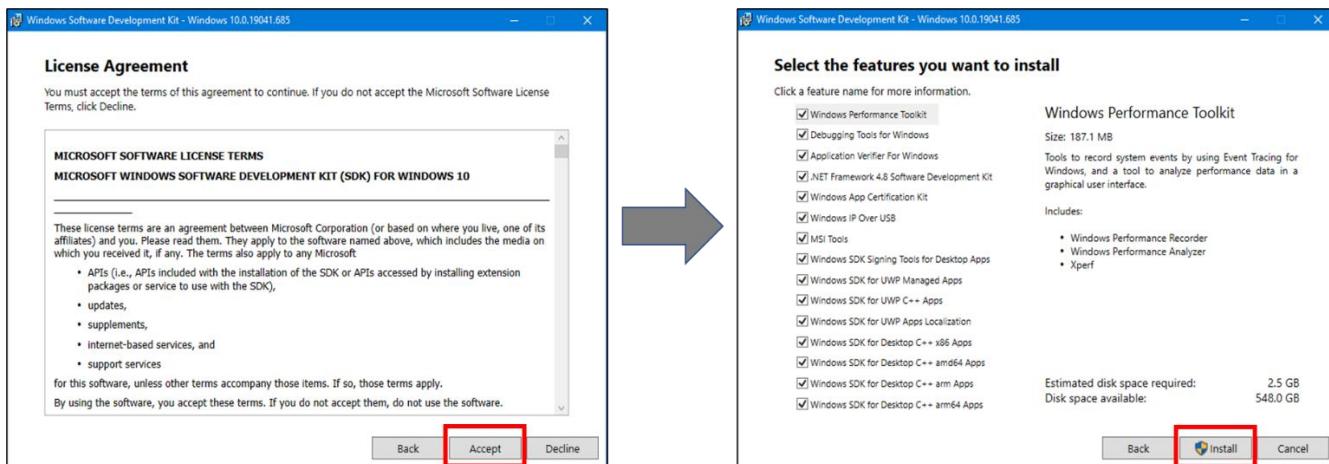


Figure 44. Steps to Install Windows Software Development Kit (SDK)

11. Building PERCEPTRON for in-house Deployment

11.1 Downloading PERCEPTRON

Users can download PERCEPTRON from GitHub for in-house deployment by following the link:

<https://github.com/BIRL/PERCEPTRON>

Click ‘Code’, then ‘Download ZIP’ (Figure 45).

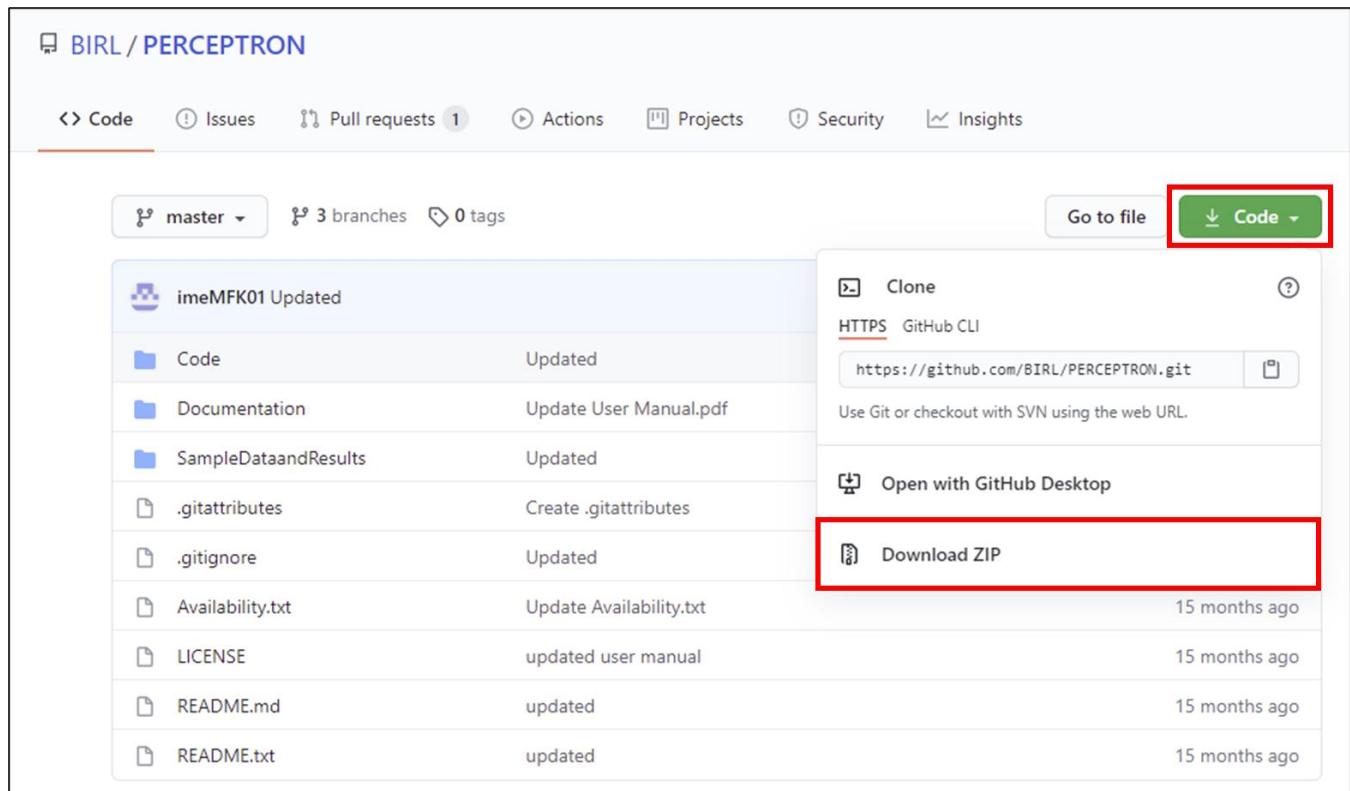


Figure 45. Downloading PERCEPTRON for in-house deployment

Unzip the downloaded file to use the code.

11.2 PERCEPTRON Application Programming Interface (API)

Open ‘PerceptronAPI.sln’ from the folder PERCEPTRON-master\Code\PerceptronAPI in visual studio (Figure 46). In “Solution Explorer,” click on ‘**PerceptronAPI**’. Go to ‘**App_Start**’ and open ‘**WebApiConfig.cs**’

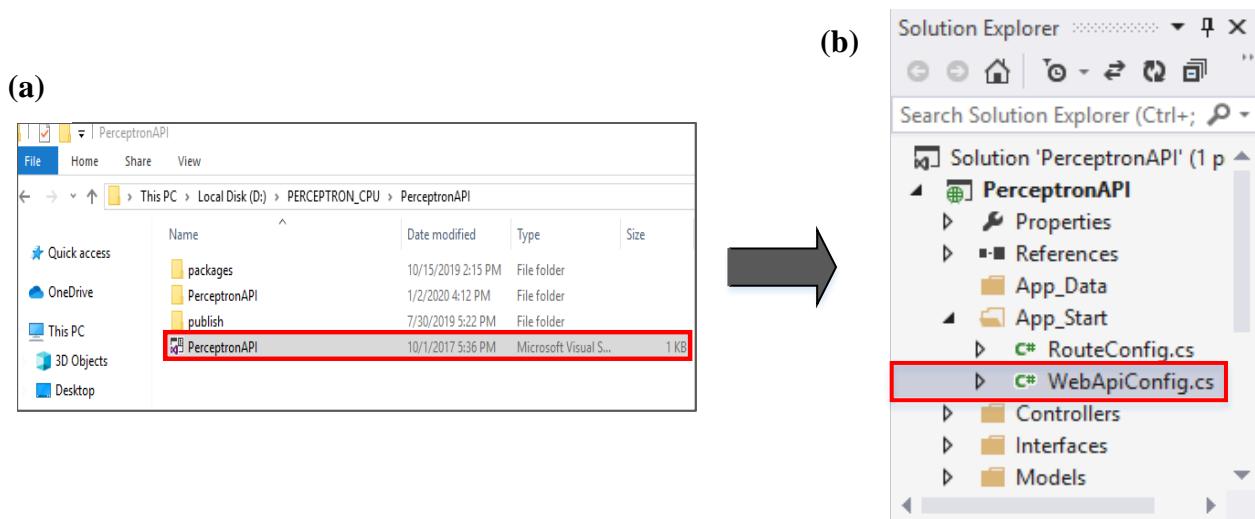


Figure 46. Building PERCEPTRON API. (a) Opening solution PerceptronAPI.sln; (b) Opening WebApiConfig.cs from Solution Explorer of Visual Studio

Open SQL Server Management Studio. Copy the given server name from SQL Server Pop Up (Figure 47).

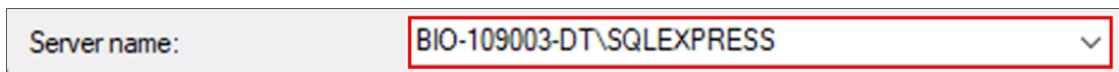
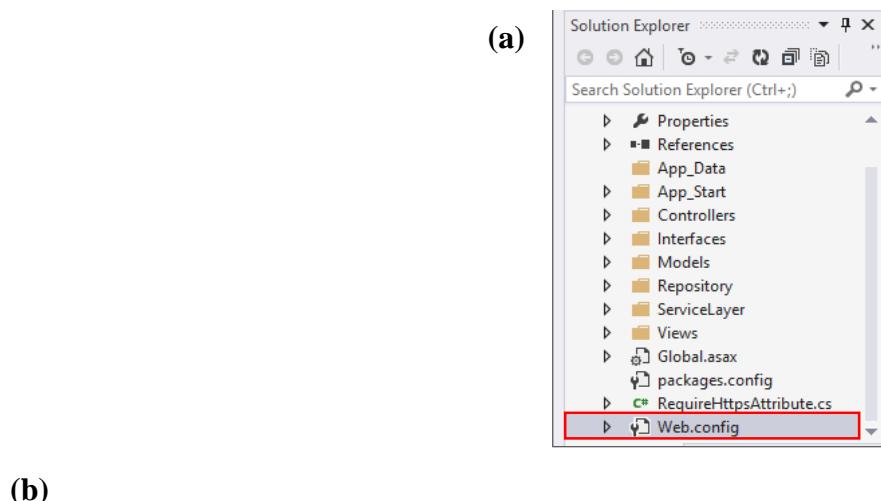


Figure 47. Copying Server Name from SQL Server Management Studio

In Visual Studio, open ‘**Web.config**’ from the Solution Explorer (Figure 48). Press **CTRL+F** to search item. Type server name, e.g. ‘**CHIRAGH-I**’ and press **ENTER**. Replace this server name with the name copied in Figure 47. Copying Server Name from SQL Server Management Studio, e.g., **BIO-109003-DT\SQLEXPRESS**.



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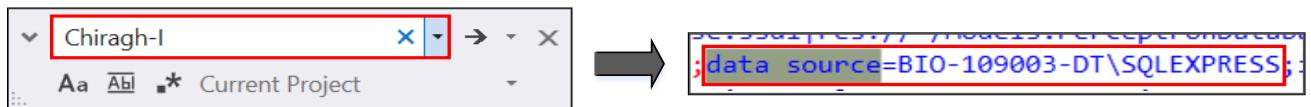


Figure 48. (a) Opening Web.config from Solution Explorer of Visual Studio (b) Changing data source (Server Name) in Web.config

Similarly, change the server name in Sqldatabase.cs (in Repository folder) as well. (Figure 49). Replace the given name for all occurrences of ‘Server’ and ‘Data Source’ in Sqldatabase.cs with the server name from SQL Pop Up. In each case, add ‘@’ right before the inverted commas start for ‘Server’ and ‘Data Source’.

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

Figure 49. Changing server name in Sqldatabase.cs

Run on ‘Google Chrome’ and save the URL obtained.

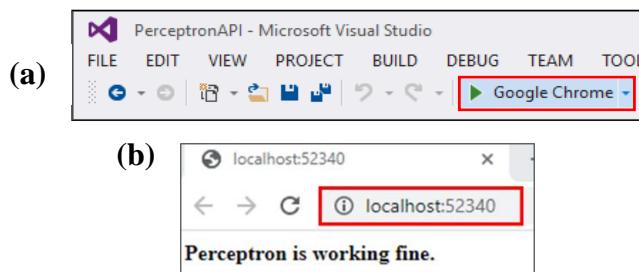


Figure 50. Steps to build PERCEPTRON API. (a) Building PERCEPTRON API solution file (PerceptronAPI.sln); (b) Run PerceptronAPI; (c) Google chrome page with URL localhost:52340 displaying the message “PERCEPTRON is working fine”

Message in Figure 50 i.e., “PERCEPTRON API is working fine” ensures that PERCEPTRON API has been successfully built and is running fine.

11.3 PERCEPTRON Front-End

Open Visual Studio Code. From 'File' dropdown menu, select 'Open Folder' (Figure 55). Select the folder 'PerceptronFrontEnd' from the path \PERCEPTRON-master\Code\.

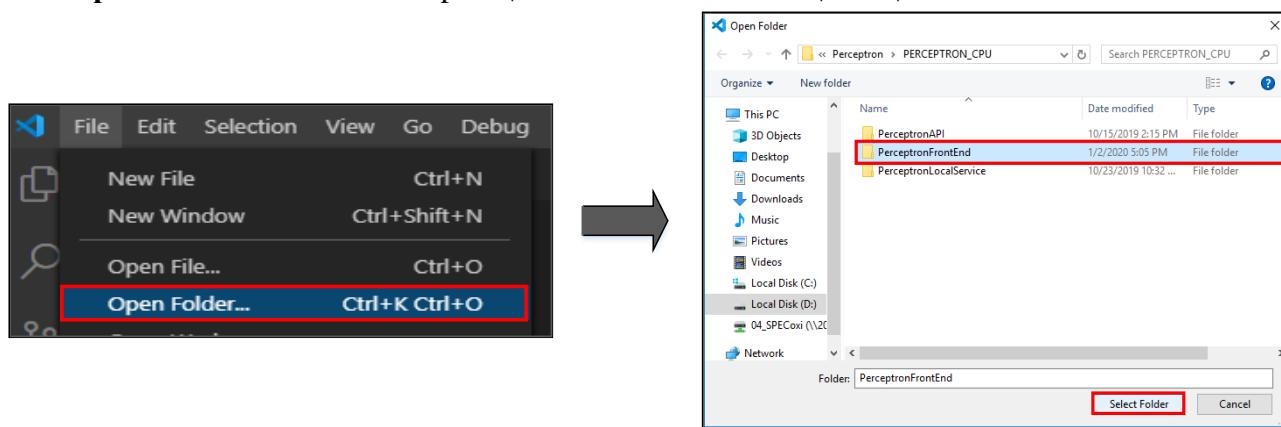


Figure 51. Opening PerceptronFrontEnd folder in Visual studio code

11.4 Connecting PERCEPTRON API to PERCEPTRON Front-End

In Visual Studio Code, type ‘**baseAPI**’ in the search bar and select the one shown below (Figure 52). Replace the given URL with the one saved before in Figure 50. 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”



Open terminal, type 'ng serve' and press **ENTER**. Open the link (<http://localhost:52340/>) provided in Figure 50 by pressing CTRL button + left mouse button.

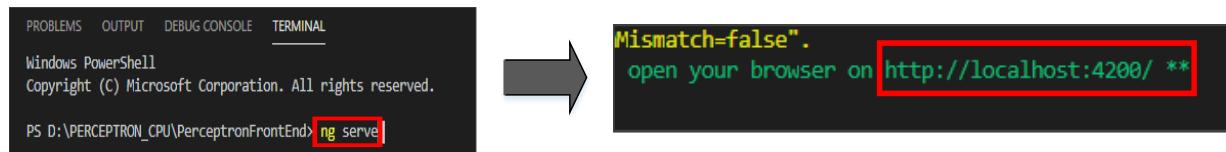


Figure 52. Hosting Perceptron Front-End on system with default URL

11.5 PERCEPTRON Local Service

Open SQL Server Management Studio. Copy the given server name from SQL Server Pop Up (Figure 53).

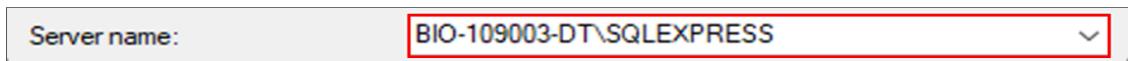
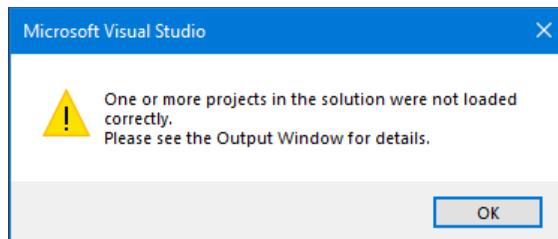


Figure 53. Copying Server Name from SQL Server Management Studio

Open ‘PerceptronLocalService.sln’ from the folder PERCEPTRON-master\Code\PercpetronLocalService\ in visual studio (Figure 54).

If user’s computer is not GPU-enabled (i.e. does not have GPU along with installations required for GPU), they will receive the following error.



To resolve this error, right click on PerceptronCuda project, remove it from the solution and continue with the below mentioned steps.

If user’s computer is GPU-enabled, follow all the steps in section 11.6 in addition to the below steps.
In the Solution Explorer, select ‘App.config’.

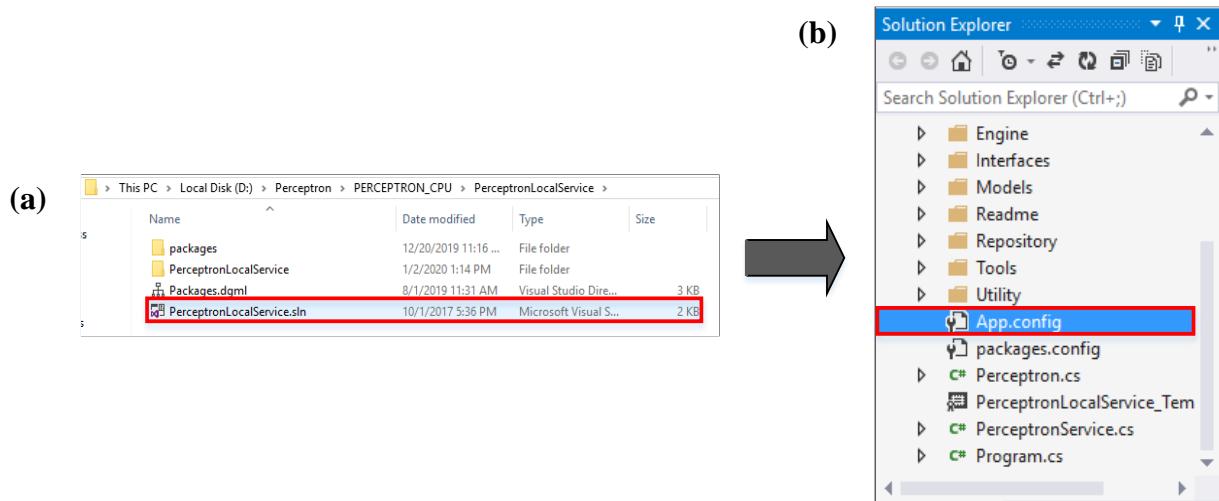


Figure 54. Building Perceptron Local Service. (a) Opening PerceptronLocalService.sln; (b) Opening App.config from Solution Explorer of Visual Studio

Press **CTRL+F** to search server name (Figure 55). Type ‘CHIRAGH-I’ and press **ENTER**. Replace this server name with the name copied in Figure 53. 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.

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Figure 55. Changing data source value (Server Name) in App.config

Go to “Repository” under PerceptronLocalService to open “SQLDatabase.cs”. Search for ‘CHIRAGH-I’ and replace it with the Server name same as it was done for App.config. Also, add an ‘@’ before the inverted commas for Server start as shown in the figure below.

```
public List<PerceptronSdkResults> PreparePerceptronSdkResults(DateTime JobSubmissionTime)
{
    List<PerceptronSdkResults> ListPerceptronSdkResults = new List<PerceptronSdkResults>();
    using (var db = new PerceptronDatabaseEntities())
    {
        var sqlConnection1 =
            new SqlConnection(
                @"Server= BIO-109003-DT\SQLEXPRESS Database= PerceptronDatabase; Integrated Security=SSPI");
        var cmd = new SqlCommand
        {
            CommandText =
                "SELECT * FROM PerceptronSdk WHERE JobSubmission= '" + JobSubmissionTime + "' AND ResultsAvailable = 'False' ORDER BY JobSubmission Desc ", //Updated
            CommandType = CommandType.Text,
            Connection = sqlConnection1
        };
        sqlConnection1.Open();

        var dataReader = cmd.ExecuteReader();
        while (dataReader.Read())
        {
            var temp = new PerceptronSdkResults
            {
                QueryId = dataReader["QueryId"].ToString(),
                Title = dataReader["Title"].ToString(),
                UserName = dataReader["UserName"].ToString(),
                ResultsAvailable = dataReader["ResultsAvailable"].ToString()
            };
            ListPerceptronSdkResults.Add(temp);
        }
        dataReader.Close();
        cmd.Dispose();
        sqlConnection1.Close();
    }
    return ListPerceptronSdkResults;
}
```

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

Open SQL Server Management Studio and click on ‘Connect’ (Figure 56).

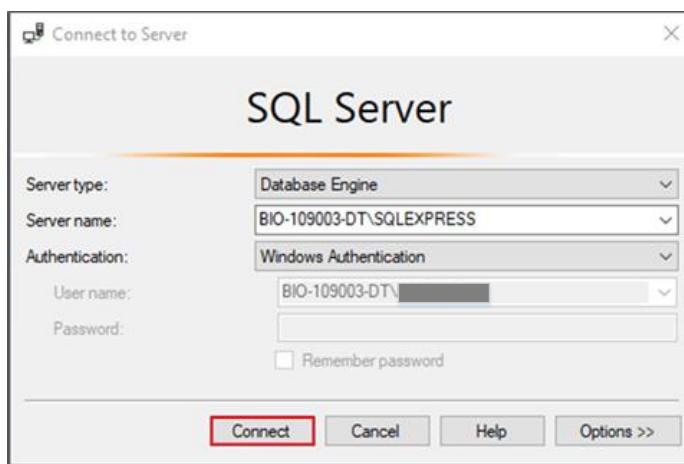
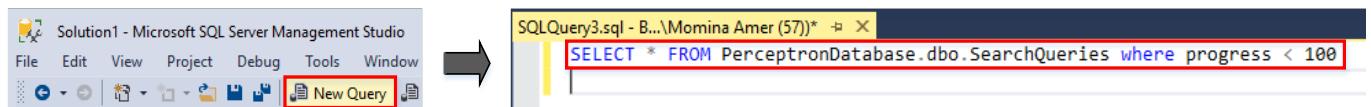


Figure 56. Connecting Server Management Studio to SQL server

Select ‘New Query’ and type ‘SELECT * FROM PerceptronDatabase.dbo.SearchQueries where progress < 100’ in the window that appears (Figure 57).

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In SQL, click on ‘Execute’.

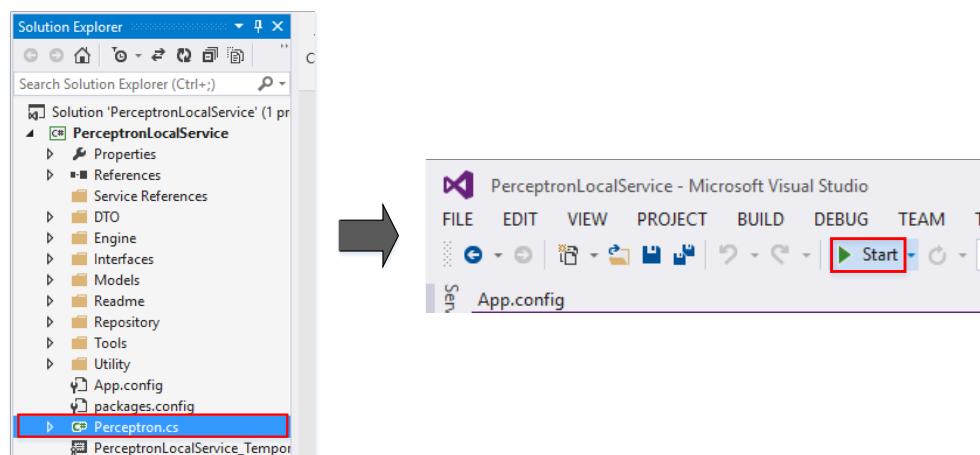


The query will show up in the Results Window.

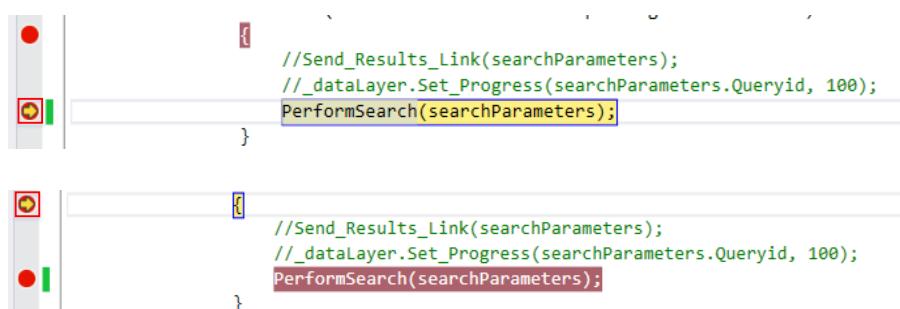
QueryId	UserId	Progress	CreationTime	Email
1	1ec2fba3-d044-43fc-ba87-15edc62fd6d	0	01/21/2020 18:55:20	NULL

Figure 57. Steps to execute Protein Search Query

In Visual Studio, open ‘PerceptronLocalService.sln’. Go to Solution Explorer and open ‘Perceptron.cs’. Click ‘Start’ to run it (Figure 58).



If breakpoints have been set, click ‘Continue’ to step over the breakpoints.



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

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The screenshot shows the PERCEPTRON User Manual interface. On the left, there is a sidebar with three items: 'Protein Search Query' (with a magnifying glass icon), 'Search Results & History' (with a clock icon, highlighted with a red box), and 'Sample Data' (with a document icon). A large grey arrow points from the sidebar to the main content area. The main content area displays search results for a query named 'TEST1'. The results table has the following columns: Sr. #, File Name, Protein ID, Protein Score, Molecular Weight, Truncation, Spectral Matches, No. of Modifications, and Total Search Time. One result is shown:

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_Q4VC39 6sc_mono.txt	Q4VC39	0.2316	11397.7953	No	1	1	

Figure 58. Testing Perceptron Local Service

11.6 PERCEPTRON Local Service (GPU)

Open **PerceptronLocalService.sln** from the folder PERCEPTRON-master\Code\PerceptronLocalService in Visual Studio 2017 and check if all the below configurations have been set properly. Right click on “PerceptronLocalService” in Microsoft Visual Studio’s Solution Explorer, then go to “Properties” and then “Build”. Next, set the “Platform target” to “x64” (Figure 59).

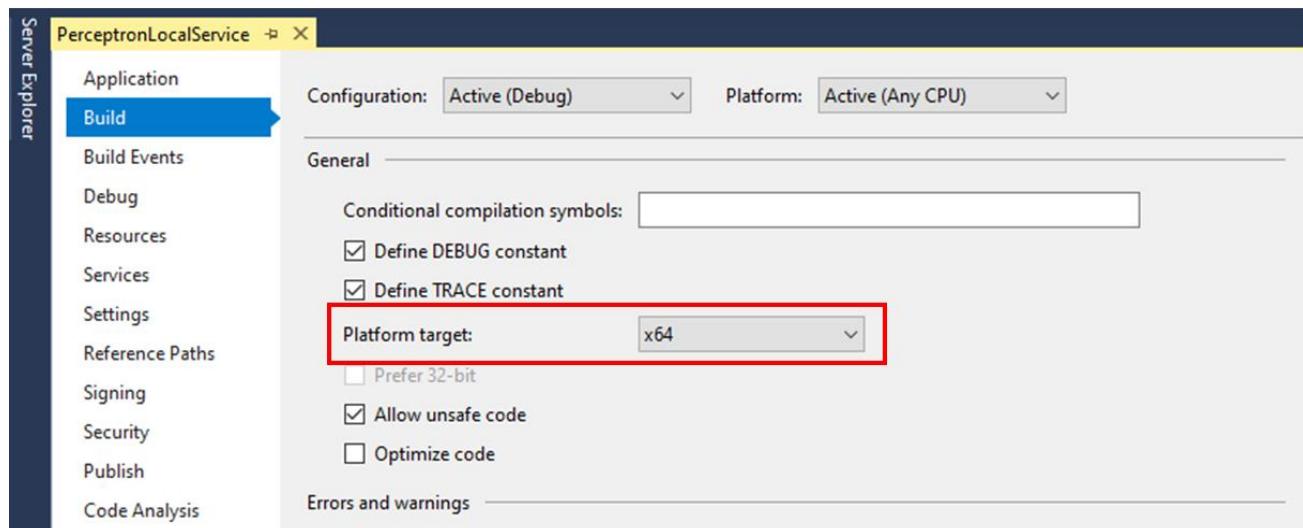


Figure 59. Selecting Platform target to build PERCEPTRON Local Service (GPU)

In Microsoft Visual Studio’s Solution Explorer, right click on “PerceptronLocalService.” Next go to “Properties” and then “Debug.” Check the option “Enable native code debugging” (Figure 60).

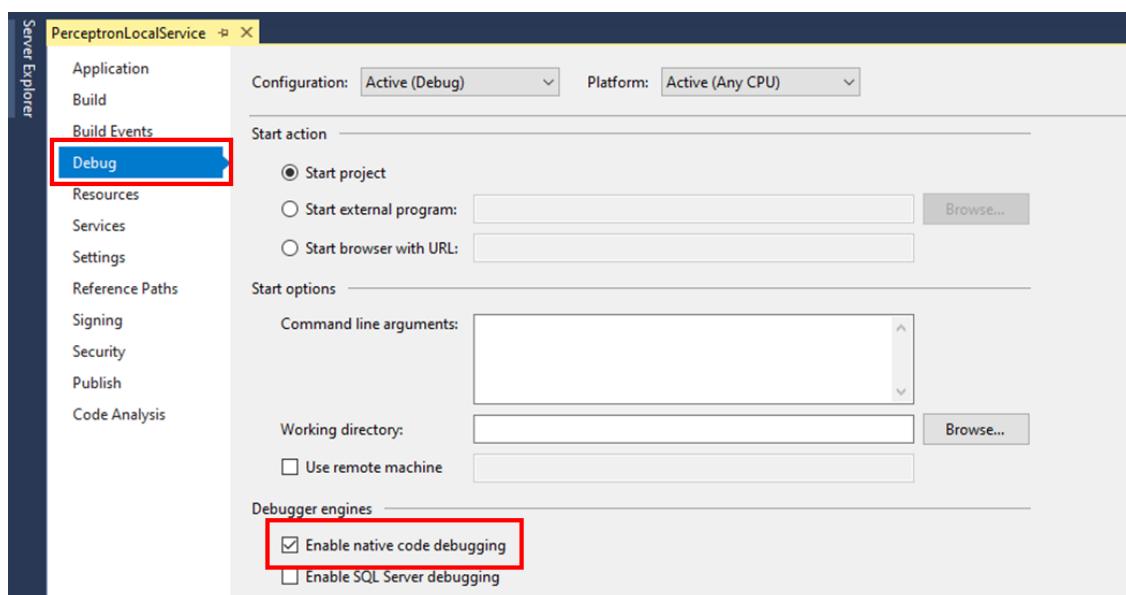


Figure 60. Enabling “Debug” option for PERCEPTRON Local Service (GPU)

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Next, in the Menu bar, go to “Build” and then “Configuration Manager.” Click to change ‘PerceptronCuda platform” to “x64” and check the option “Build” (Figure 61).

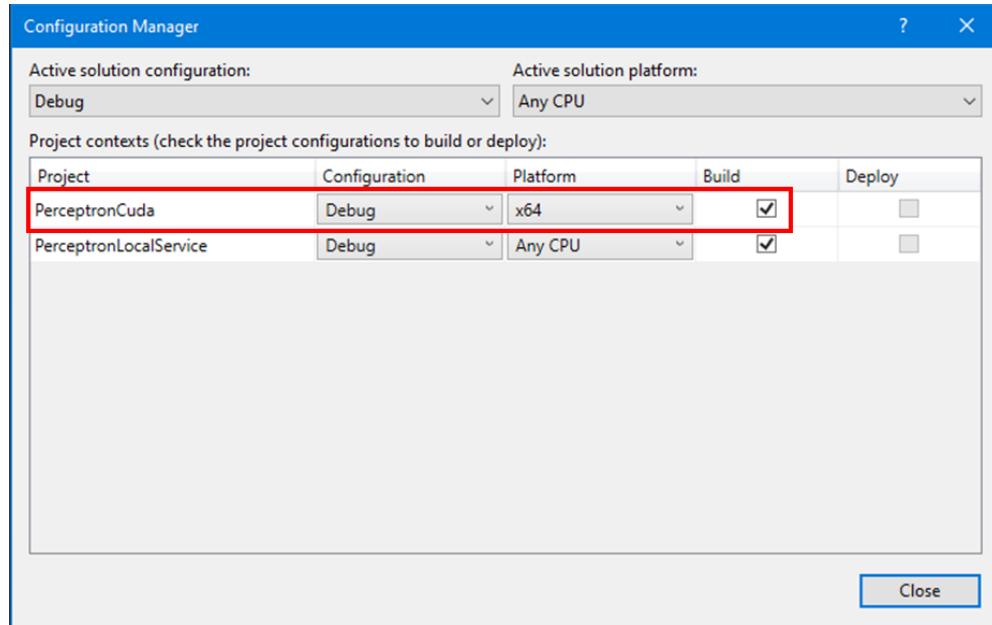


Figure 61. Enabling features in “Configuration Manager” to build PERCEPTRON Local Service (GPU)

In Solution Explorer, right click on “PerceptronCuda” project; go to “Build Dependencies” and then “Build Customizations”. Check “CUDA 10.0 (.targets, .props)” (Figure 62).

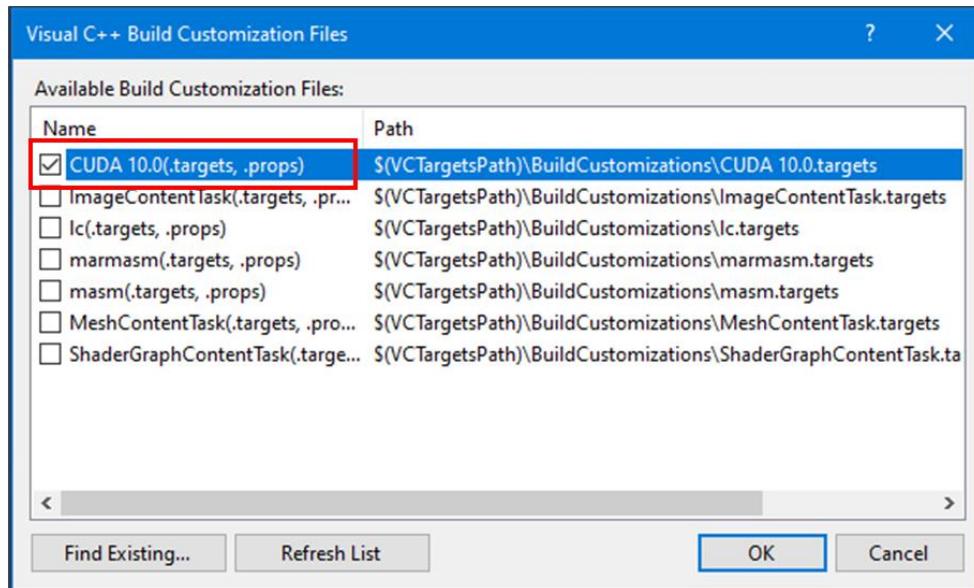


Figure 62. Customizing features in Solution Explorer to build PERCEPTRON Local Service (GPU)

Next, in Solution Explorer, right click on “PerceptronCuda” project; go to “Build Dependencies” and then “Project Dependencies”. Check “PerceptronLocalService” as shown in Figure 63.

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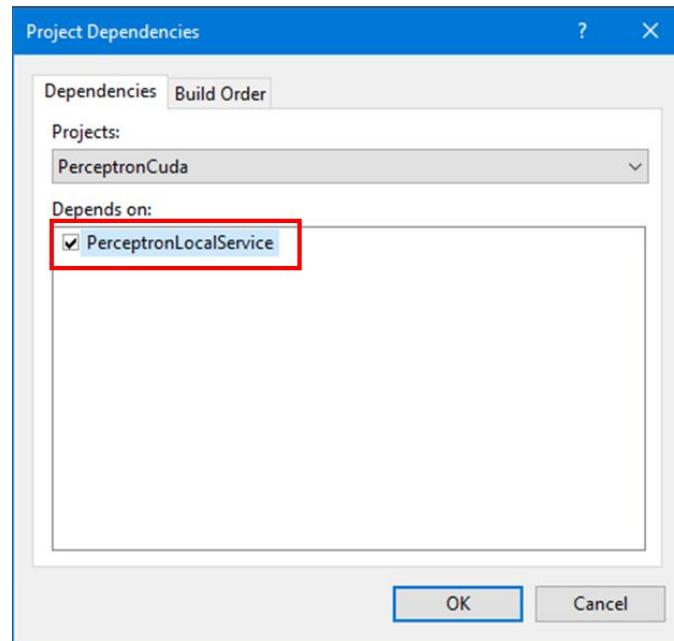


Figure 63. Customizing Project Dependencies to build PERCEPTRON Local Service (GPU)

In Solution Explorer, right click on “PerceptronCuda” project; go to “Properties” and then “VC++ Directories”. Add path to “Executable Directories” for example: “C:\Program Files\NVIDIA GPU Computing Toolkit\CUDA\v10.0\include”. Add the same path to “Include Directories”. Next, in “Library Directories”, add path i.e. “C:\Program Files\NVIDIA GPU Computing Toolkit\CUDA\v10.0\lib\x64” as shown in Figure 64.

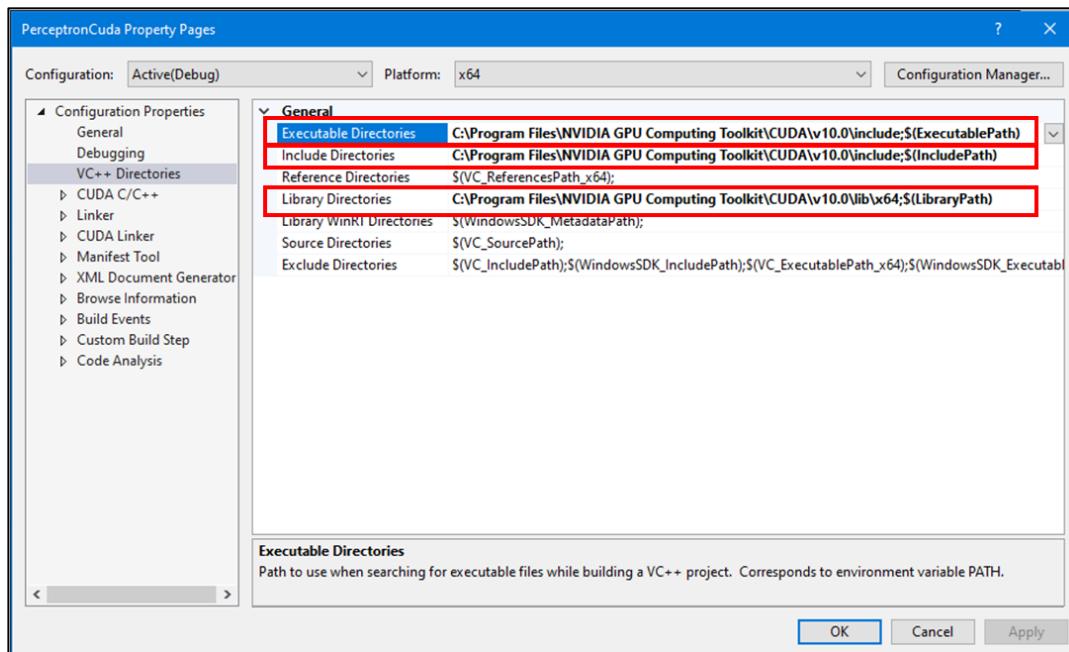


Figure 64. Adding paths to VC++ directories

Lastly, in Solution Explorer, right click on “PerceptronCuda” project, go to “Properties”, then “Linker” and then “Input”. In “Additional Dependencies”, add “cudart.lib” and “cudadevrt.lib” (Figure 65).

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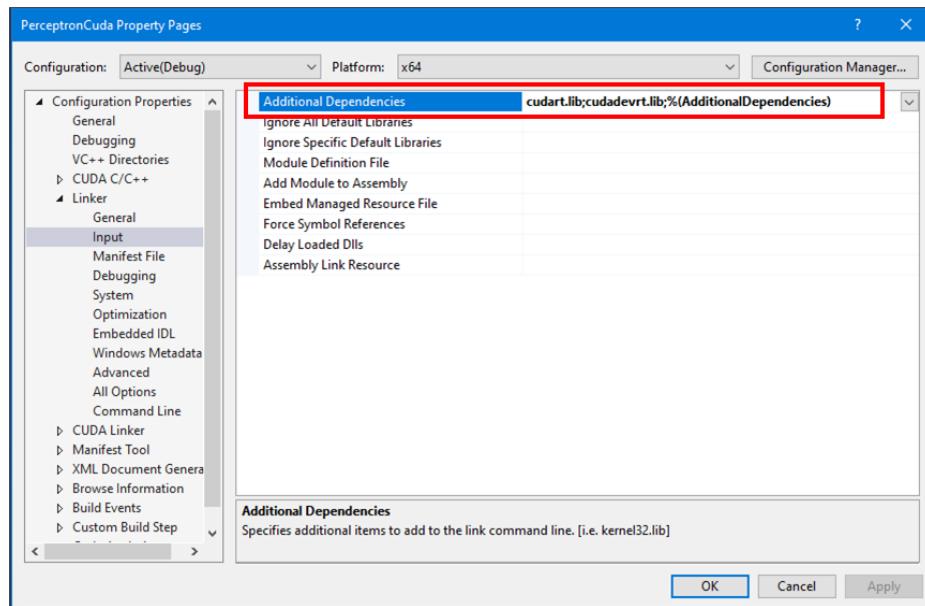


Figure 65. Adding additional directories to the project

Right click on ‘PerceptronCuda’ project and rebuild it to generate the .dll file.

In Perceptron.cs, search for ‘DllFilePath’ and give the path to ‘...\\PERCEPTRON-master\\Code\\PerceptronLocalService \\x64\\Debug\\PerceptronCuda.dll’.

```
// --- GPU Code Below --- Updated: 20210223
public static class NativeCudaCalls
{
    private const string DllFilePath = @"D:\\01_GitHub\\PERCEPTRON-master\\Code\\PerceptronLocalService\\x64\\Debug\\PerceptronCuda.dll";
    [DllImport(DllFilePath, CallingConvention = CallingConvention.Cdecl)]
    private extern static void MainInitializer();
    public static void InitializingGpu()
    {
        MainInitializer();
    }
}
```

Next, uncomment the following lines of code in Perceptron.cs:

```
foreach (ManagementObject mo in searcher.Get())
{
    foreach (PropertyData property in mo.Properties)
    {
        if (property.Name == "Description")
        {
            graphicsCard = property.Value.ToString();
            if (graphicsCard.Contains("NVIDIA"))
            {
                //NativeCudaCalls.InitializingGpu();
                //IsGpu = true;
            }
            break;
        }
    }
    return IsGpu;
}
```

12. Using PERCEPTRON API through software development kit (SDK)

PERCEPTRON application programming interface (API) has been made accessible for use without the need for graphical user interface (GUI) using a software development kit (SDK). Users can download the MATLAB scripts from GitHub by following the link: <https://github.com/BIRL/PERCEPTRON/tree/master/Code/PerceptronSdk>

Open “PerceptronSdkMainFunction.m” in new tab and click on “Raw” to save the script file by selecting the destination folder (Figure 66).

Code Issues Pull requests Actions Projects Security Insights

BIRL Create ReadMe.txt 376cad yesterday History

ResultFiles/Create ReadMe.txt yesterday

PerceptronSdkMainFunction.m Updated PerceptronSdk 3 days ago

RegisterUser.m Updated PerceptronSdk 6 days ago

ResultsDownload.m Updated PerceptronSdk 6 days ago

SearchQuery.m Updated 6 days ago

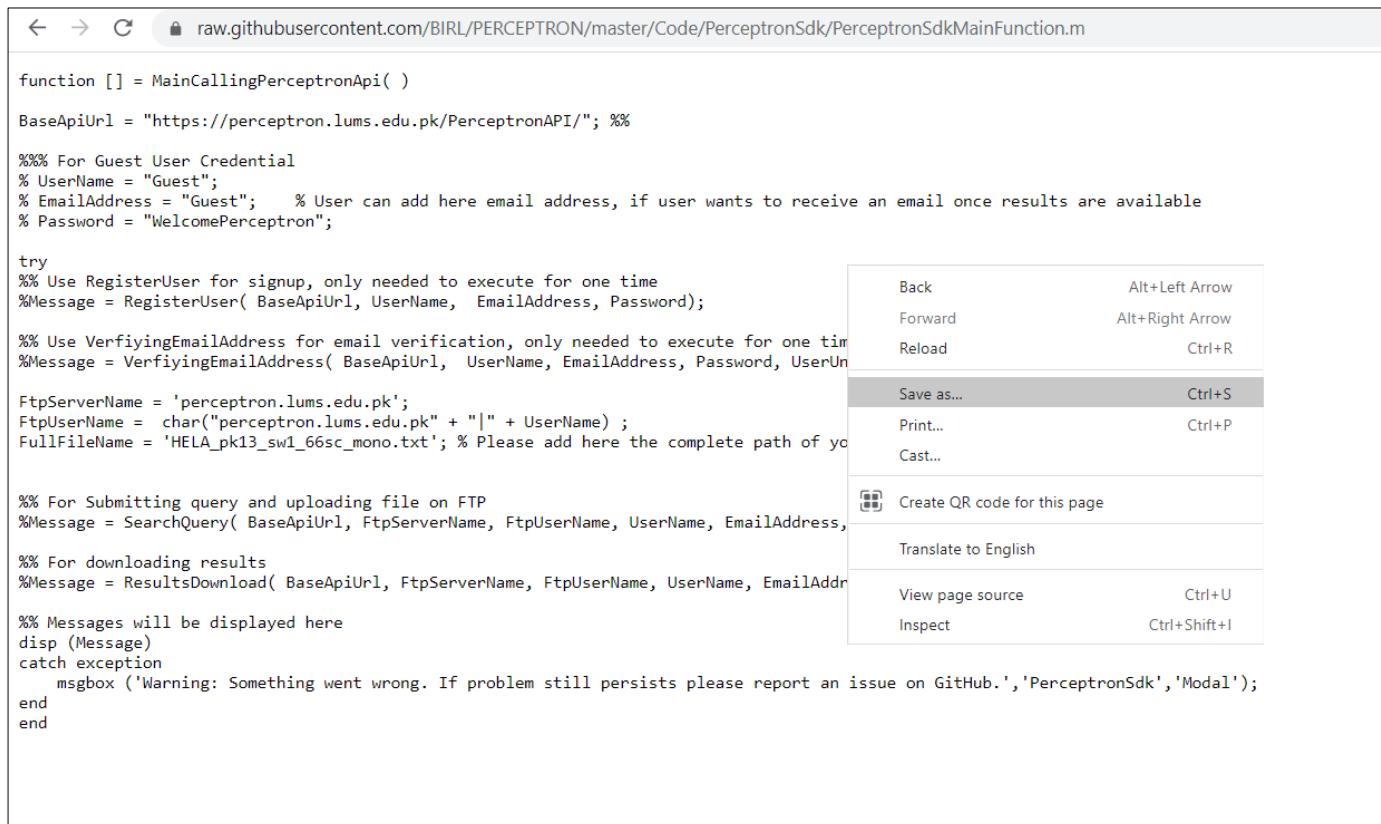
VerifyingEmailAddress.m Updated PerceptronSdk 3 days ago

```

33 lines (24 sloc) | 1.33 KB
1 function [] = MainCallingPerceptronApi()
2
3 BaseApiUrl = "https://perceptron.lums.edu.pk/PerceptronAPI/";
4
5 %% For Guest User Credential
6 % UserName = "Guest";
7 % EmailAddress = "Guest"; % User can add here email address, if user wants to receive an email once results are available
8 % Password = "WelcomePerceptron";
9
10 try
11 %% Use RegisterUser for signup, only needed to execute for one time
12 %Message = RegisterUser( BaseApiUrl, UserName, EmailAddress, Password);
13
14 %% Use VerifyingEmailAddress for email verification, only needed to execute for one time
15 %Message = VerifyingEmailAddress( BaseApiUrl, UserName, EmailAddress, Password, UserUniqueId);
16
17 FtpServerName = 'perceptron.lums.edu.pk';

```

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The screenshot shows a web browser displaying a MATLAB script titled 'PerceptronSdkMainFunction.m'. The script performs various operations such as calling APIs, handling user credentials, and interacting with an FTP server. A context menu is open on the right side of the page, listing options like Back, Forward, Reload, Save as..., Print..., Cast..., Create QR code for this page, Translate to English, View page source, and Inspect.

```
function [] = MainCallingPerceptronApi( )
BaseApiUrl = "https://perceptron.lums.edu.pk/PerceptronAPI/"; %

%%% For Guest User Credential
% UserName = "Guest";
% EmailAddress = "Guest"; % User can add here email address, if user wants to receive an email once results are available
% Password = "WelcomePerceptron";

try
%% Use RegisterUser for signup, only needed to execute for one time
%Message = RegisterUser( BaseApiUrl, UserName, EmailAddress, Password);

%% Use VerfiyingEmailAddress for email verification, only needed to execute for one time
%Message = VerfiyingEmailAddress( BaseApiUrl, UserName, EmailAddress, Password, UserUn

FtpServerName = 'perceptron.lums.edu.pk';
FtpUserName = char("perceptron.lums.edu.pk" + "|" + UserName) ;
FullFileName = 'HELA_pk13_sw1_66sc_mono.txt'; % Please add here the complete path of yo

%% For Submitting query and uploading file on FTP
%Message = SearchQuery( BaseApiUrl, FtpServerName, FtpUserName, UserName, EmailAddress, EmailAddres

%% For downloading results
%Message = ResultsDownload( BaseApiUrl, FtpServerName, FtpUserName, UserName, EmailAddress, EmailAddres

%% Messages will be displayed here
disp (Message)
catch exception
    msgbox ('Warning: Something went wrong. If problem still persists please report an issue on GitHub.', 'PerceptronSdk', 'Modal');
end
end
```

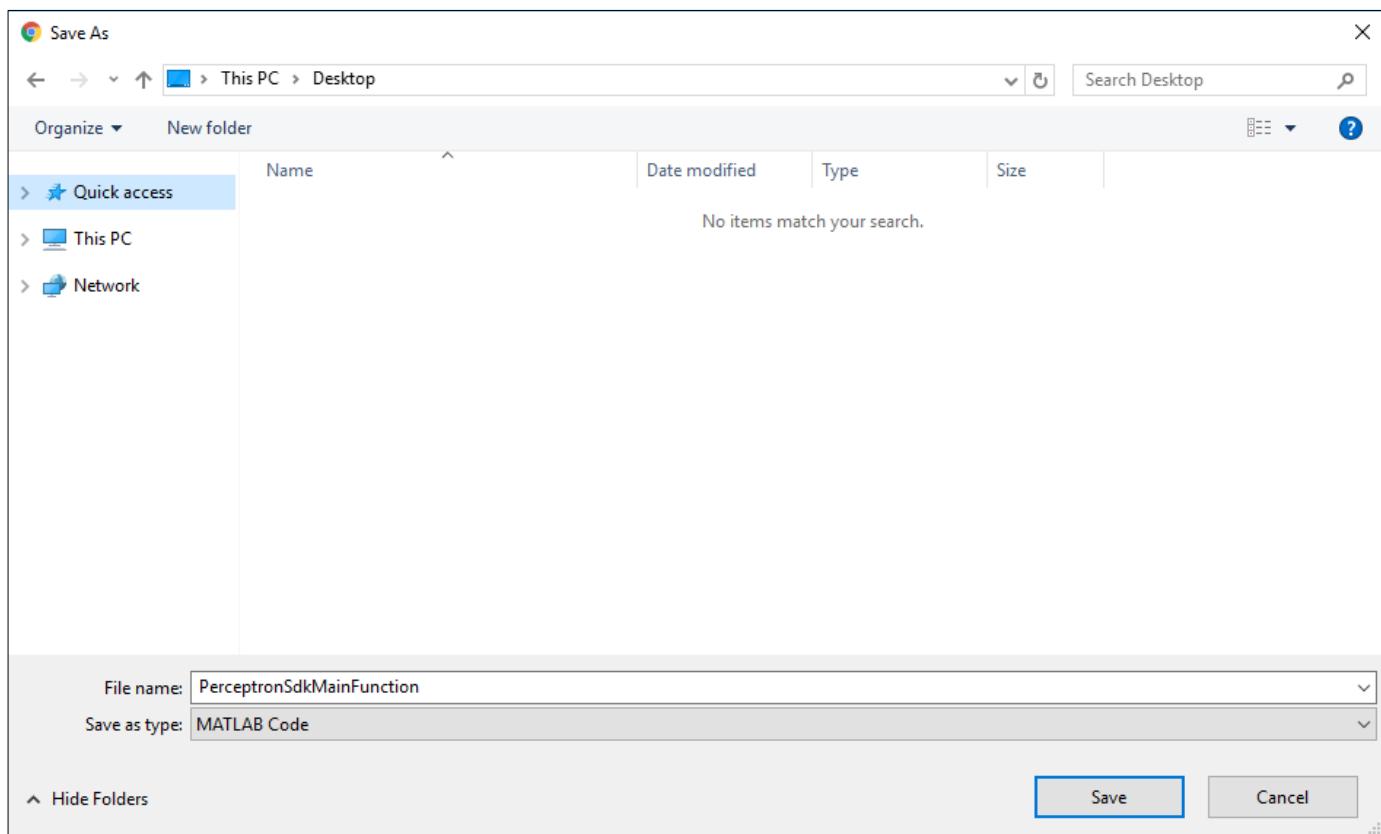
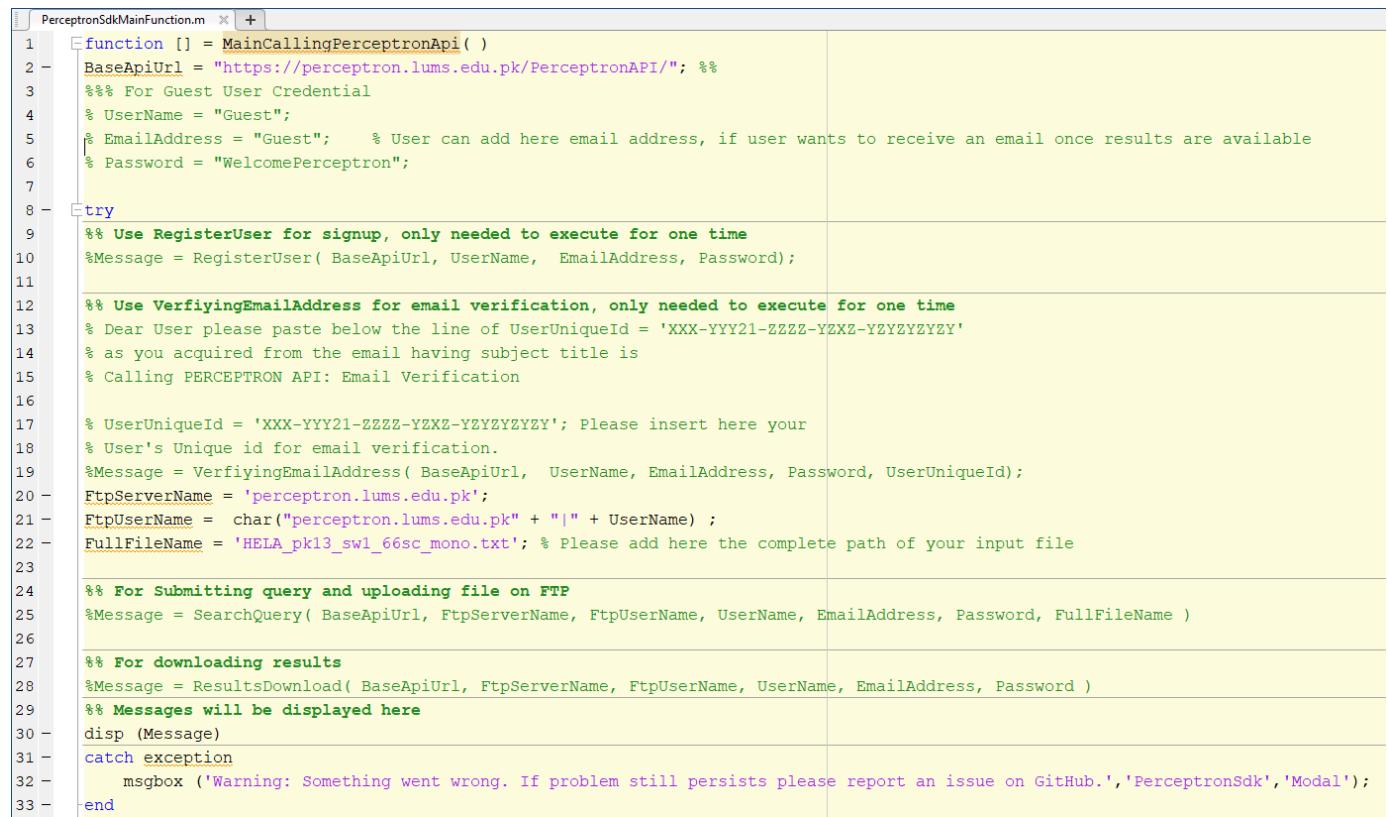


Figure 66. Steps to download PERCEPTRON SDK MATLAB scripts from GitHub

Note: MATLAB download is required to run these scripts. Keep all MATLAB scripts in the same destination folder.

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After successfully downloading all MATLAB scripts in “PerceptronSdk” folder, open MATLAB and click “Run” button in the toolbar at the top. Select “Change folder” option to make the destination folder containing downloaded script files as the current working folder in MATLAB (Figure 67).



The screenshot shows a MATLAB code editor window with the file 'PerceptronSdkMainFunction.m' open. The code is a MATLAB script with the following content:

```
1 function [] = MainCallingPerceptronApi()
2 - BaseApiUrl = "https://perceptron.lums.edu.pk/PerceptronAPI/"; %%
3 %% For Guest User Credential
4 % UserName = "Guest";
5 % EmailAddress = "Guest"; % User can add here email address, if user wants to receive an email once results are available
6 % Password = "WelcomePerceptron";
7
8 - try
9 %% Use RegisterUser for signup, only needed to execute for one time
10 %Message = RegisterUser( BaseApiUrl, UserName, EmailAddress, Password);
11
12 %% Use VerifiyingEmailAddress for email verification, only needed to execute for one time
13 % Dear User please paste below the line of UserUniqueId = 'XXX-YYY21-ZZZZ-YZXZ-YZYXYZZY'
14 % as you acquired from the email having subject title is
15 % Calling PERCEPTRON API: Email Verification
16
17 % UserUniqueId = 'XXX-YYY21-ZZZZ-YZXZ-YZYXYZZY'; Please insert here your
18 % User's Unique id for email verification.
19 %Message = VerifiyingEmailAddress( BaseApiUrl, UserName, EmailAddress, Password, UserUniqueId);
20 - FtpServerName = 'perceptron.lums.edu.pk';
21 - FtpUserName = char("perceptron.lums.edu.pk" + "|" + UserName) ;
22 - FullFileName = 'HELA_pk13_sw1_66sc_mono.txt'; % Please add here the complete path of your input file
23
24 %% For Submitting query and uploading file on FTP
25 %Message = SearchQuery( BaseApiUrl, FtpServerName, FtpUserName, UserName, EmailAddress, Password, FullFileName )
26
27 %% For downloading results
28 %Message = ResultsDownload( BaseApiUrl, FtpServerName, FtpUserName, UserName, EmailAddress, Password )
29 %% Messages will be displayed here
30 - disp (Message)
31 - catch exception
32 - msgbox ("Warning: Something went wrong. If problem still persists please report an issue on GitHub.", 'PerceptronSdk', 'Modal');
33 - end
```

Figure 67. Running PerceptronSdkMainFunction.m MATLAB script

Users can access PERCEPTRON web services through PERCEPTRON SDK using available MATLAB script or by writing their own code for submitting batch queries. The MATLAB script has instructions to use this utility. Step-by-step instructions have also been provided below.

To register as a user, users are required to add: (i) a username, (ii) a valid email address, and (iii) a password under “Guest User Credentials”. Next, uncomment the line with function call to “RegisterUser” and run the program.

To complete registration, verify the email address by uncommenting the line with “UserUniqueId,” and inserting the unique code sent to the email ID.

Next, enter the path to input file to be run as protein search query in “FullFileName” variable.

To submit the query, uncomment the line containing function call to “SearchQuery.”

To download results, uncomment the line with function call to “ResultsDownload”. Your results will be saved as a subfolder in PERCEPTRONSdk folder: “...\\ PerceptronSdk\\ResultFiles\\folder.”

13. References

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