**STANDARD OPERATING PROCEDURE**

**Name of procedure: Using Agilent Data Analysis software to visualize, export, organize, and compile data gathered using HS-SPME GC-MS**

Date or update of SOP: 20190612

Supervisor name: Dr. Beck, John After hours contact:

Designated Area: Computer Workstation

Procedure is located in room(s) \_\_\_\_\_\_\_\_\_.

Personal Protection:

* None recognized

Process (in detail):

1. First navigate to the Arwen Data Analysis Program
   * Start menu
   * Agilent folder
   * Data analysis
2. File -
   * Load data file
   * Change path
     + Select the appropriate data folder
     + Select desired data file
   * Open data
   * Chromatogram 🡪 Integrate
3. Open data file
   * Overlay chromatograms
   * Select TIC (total ion chromatogram)
   * Move desired data files over and click process
4. Chromatogram 🡪 integrate
   * Chromatogram 🡪 MS signal integration parameters
     + Initial peak width 0.031
     + Integration profile - event16.e
     + Apply and generate percent report
   * \*want to figure out which data file has highest number of peaks
5. Load data file with largest # of peaks
   * Integrate data
   * Generate percent report
6. Spectrum 🡪 select library
   * Database –
     + NIST14
     + WILEY275
     + Adams2
7. Overlay chromatograms
   * Select TIC
   * Move data files over
   * Integrate
   * Generate percent report
8. Spectrum 🡪 Library search report
   * Select “screen” only
   * Integration profile – event16.e
   * Apex spectrum
9. File 🡪 Export data to CSV file
   * Select current file with data file
   * Generate library search results
   * Do not append results

Navigate to CSV file –

* File explorer
* Local disk
* Mass hunter
* GCMS 🡪 Folder 1
* Data folder
* JTB-E02
* BACandBLUE
* Navigate to desired data folder (the one with the largest number of peaks)
* Click results
* Save as excel workbook and rename as – name of software\_name of microbe\_name of treatment

Organizing the data –

* Create a new data sheet with the name – software\_QUANT FRAGS\_pgs\_#\_#\_#
* For each data set, keep R.T. (retention time) and Area – delete all other columns (i.e. header, peak, Pt max, etc.)
* At the bottom of the workbook see PBM Apex 🡪 highlight, cut & paste the RT and Library/ID columns to the top left corner of the workbook leaving a few blank rows above (you will align the rest of the data to the right of these columns) 🡪 Highlight the above data/information and change the font color to red
* In numerical order of the data files that you downloaded, begin cutting and pasting the R.T. and Area to the right of the red highlighted data. Make sure that all R.T. and Area are aligned
* \*Leave the name of the data file above the R.T. for each file

Organizing

Spill and Accident Procedure:

**Spill** -

**Accident-**

Hazards involved in procedure:

Special Handling Requirements:

Approval Required:

Training Documentation

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| Print Name | Sign | Date |
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