Body Fluid Identification by Proteomic Mass Spectrometry - Analysis			
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Body Fluid Identification by Proteomic Mass Spectrometry -Analysis

Purpose 1

Process data accumulated through the use of the liquid chromatographer and mass spectrometer 1.1 in order to identify presence of specific body fluids on evidence samples using Skyline and R Script. Skyline is an open-source software for targeted proteomics data analysis.

2 **Skyline Analysis Procedure**

- Double-click on Skyline (version 22.2.0.255) software on desktop. 2.1
- 2.2 On the Start Page click on Blank Document



2.3 Click Settings \rightarrow Peptide Settings \rightarrow Modifications and ensure "Internal standard type" to "None". If not, set to "None". Click OK.

Pe	ptide Settings
1	Digestion Prediction Filter Library Modifications Quantification
l	Structural modifications: Carbanicomethyl (C) Oxidation (M) Edit list
l	Max variable mods: Max losses: 3 1
	heavy ~
	Isotope modifications: Label: 13C(6)15N(4) (C-term R) Label: 13C(6)15N(2) (C-term K)
	internal standard type : none
	OK Cancel

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- 2.4 Open the file labeled "Final B SE and SA transitions with Cyto C and DI 2021Feb" .sky file FOUND IN M DRIVE: Molecular Serology Data folder
- 2.5 Click File \rightarrow Save As \rightarrow Rename File as DATE (YYYYMMDD) Batch A
- 2.6 Select File \rightarrow Import \rightarrow Results



- 2.8 Select all samples within the batch found in Gertrude folder and click open.
- 2.9 Save file once all sample injections are imported and close software.

MSDA (Molecular Serology Data Analysis)-Script Procedure 3



3.1 Find the bfassay cmd ps Shortcut icon on the processing computer desktop.

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Right click on the bfassay_cmd_ps Shortcut icon and select Run with PowerShell. 3.2



3.3 Right click on the skyline file and select Properties.

Ν.

Name		Date modified	Туре	Size
20210325A_Peptide_D	etails_pdf_2022-10	10/7/2022 3:48 PM	File folder	
20210325A.midas		10/7/2022 3:43 PM	MIDAS File	609 KB
20210325A		10/7/2022 3:43 PM	Skyline Document	957 KB
🗋 20210325A.sky.v 🔅	AMD Radeon Pro and	AMD FirePro Settings		12 KB
20210325A	AMD Radeon Pro and AMD FirePro Advanced Settings			3,862 KB
20210325A.skyl —				29 KB
20210325A_Bod	View		> .	2 KB
20210325A_Cas	Sort by		> .	627 KB
	Group by		>	
	Refresh			
	Customize this folder			
	Paste			
	Paste shortcut			
	Undo Rename		Ctrl+Z	
	New		>	
C	Properties			

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3.4 Copy the location of the file and paste into bfassay cmd ps command window.



3.8 The script will run. The .csv export will be saved in the same folder as the Skyline documents, with the same name and the addition of 'CaseReport.csv' at the end.

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