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#### 1. **Principle**

1.1. This procedure is designed to aid the user in setting up an instrument sequence used to analyze Organic Base Screen, Acid and Neutral Screen and Quantification methods with an Agilent GC (NPD, FID) and/or an Agilent GC/MS.

2. Specimens

2.1. N/A

#### 3. **Reagents and Materials**

3.1. N/A

#### 4. Instrumentation and Equipment

- 4.1. Agilent GC (NPD, FID) or Agilent GCMS
- 4.2. Agilent Chemstation Software
- 4.3. Data reporting system (PC)

#### 5. **Procedure**

- 5.1. Sequence Setup (Agilent GC/MS)
  - 5.1.1. On an instrument PC with Agilent Chemstation Software installed, open the Chemstation software by double-clicking the Shortcut.



- 5.1.2. From the menu bar, select "View Top" (Skip this step if using version E.02.02.1431 or above).
- 5.1.3. Load a previous sequence to use as a template.
  - 5.1.3.1.Select "Sequence Load ..." In the Load Sequence Window, navigate to C:\HPCHEM\1\Sequence and select a sequence to load.
  - 5.1.3.2.From the menu bar, select "Sequence Edit Sample Log Table" to open the Sequence for editing.



- versions).
- 5.1.3.4.In the file name field, enter the load number minus the 1<sup>st</sup> two digits (2013010705 becomes 13010705).

- 5.1.3.5.Enter the following information for each specimen in the order they are to be injected starting at the top of the sequence table. Click on the Repeat Button to add a new line (or arrow down in newer software versions).
  - 5.1.3.5.1. <u>Type</u> = Sample
  - 5.1.3.5.2. <u>Vial</u> = The position the specimen is to be placed on the autosampler
  - 5.1.3.5.3. <u>Data File</u> = Unique identifier for each Specimen Typically the Standard Level, QC level, or Blank (all differentiated by matrix type) or the last 4 or 5 digits of the S#. If a specimen is to be injected in duplicate, the letter "d" is entered at the end of the data File name).
  - 5.1.3.5.4. <u>Method</u> = instrument Method to be used to collect data
  - 5.1.3.5.5. <u>Sample Name</u> = Description of Control or Complete S# and T# followed by aliquot volume and matrix type (see 5.1.3.2.1)
  - 5.1.3.5.6. <u>Miscellaneous Information</u> = Contains the SOP description, extraction date, and analyst initials.
  - 5.1.3.5.7. <u>Multiplier</u> = Dilution factor of Specimen. (Click the "More>>" button to view this field in earlier software versions).
- 5.1.3.6.Once sequence information is entered, Save (overwrite) the Sequence.
- 5.1.3.7.To print the sequence table for verification, select "Sequence Simulate Sequence" – the software will run through the sequence to check for errors and check hard drive space.

5.1.3.8.Select "File – Print" to print the sequence.

- 5.1.3.8.1. Have another analyst verify the printed sequence table against the vial positions in the autosampler tray.
- 5.1.3.9.To start the run, select "Sequence Run" (see below).

✓ Method Sections to Run I Full Method C Reprocessing Only	Sequence Barcode Options     Oisable Barcode for This Sequence     On Mismatch – Inject Anyway, Continue Sequence     On Mismatch – Don't Inject. Continue Sequence
Overwrite Existing Data Files	i i
Sequence Comment: OB scree	n
Operator Name: dls	
Data File Directory: C:\MSDC	HEM(1\DATA)2013120303 Browse
Pre-Seq Macros/Commands	
Instrument Control: Data Analysis:	
- Post-Seq Macros/Commands	c v
Instrument Control: Data Analysis:	
Run Sequence	OK Cancel Help

- 5.1.3.10. Enter assay name in the "Sequence Comment" Field
- 5.1.3.11. Enter Analyst initials in the "Operator Name" Field
- 5.1.3.12. Enter the correct Path for the data files (C:\HPCHEM\1\DATA\"Truncated Load Number") in the "Data File Directory" field.
- 5.1.3.13. Select "Run Sequence" and wait until the first autosampler vial in injected into the instrument.

5.2. Sequence Setup (Agilent GC)

5.2.1. On an instrument PC with Agilent Chemstation Software installed, open the Chemstation software by double-clicking the Shortcut.



5.2.2. Load a previous sequence to use as a template.

- 5.2.2.1.Select "Sequence Load Sequence …" In the Load Sequence Window, navigate to C:\HPCHEM\1\Sequence and select a sequence to load.
- 5.2.2.From the menu bar, select "Sequence Sequence Table" to open the Sequence for editing.



- 5.2.2.3.Enter the following information for each specimen in the order they are to be injected starting at the top of the sequence table. Click on the "Append Line" button to add a new line.
  - 5.2.2.3.1. <u>Location</u> = The position the specimen vial is to be placed on the autosampler tray
  - 5.2.2.3.2. <u>Sample Name</u> = Description of Control or Complete S# and Partial T# (to be completed during data reduction
  - 5.2.2.3.3. <u>Method Name</u> = instrument Method to be used to collect data
  - 5.2.2.3.4. <u>Inj/Location</u> = Number of injections for each vial (typically =1)
  - 5.2.2.3.5. <u>SampleType</u> = Sample
  - 5.2.2.3.6. <u>Data File</u> = Unique identifier for each Specimen Typically the Standard Level, QC level, or Blank (all differentiated by matrix type) or the last 4 or 5 digits of the S#. If a specimen is to be injected in duplicate, the letter "d" is entered at the end of the data File name).
- 5.2.2.4.Once sequence information is entered, Save the Sequence:
  - 5.2.2.4.1. Select "Sequence Save Sequence As...". In the file name field, enter the load number minus the 1<sup>st</sup> two digits (2013010705 becomes 13010705).

5.2.2.5.Select "Sequence – Sequence Parameters..."

Auto       Prefix/Counter       Prefix:         Signal 1:       SiG1         Subdirectory:       13121901       Signal 2:         Path:       C:\HPCHEM\1\DATA\         Part of methods to run       Bar Code Reader         According to Runtime Checklist       Use In Sequence         Use Seguence Table Information       On a bar code methods	Counte 0001 0001
Signal 1: SIG1 Subdirectory: 13121901 Signal 2: SIG2 Path: C:\HPCHEM\1\DATA\ Part of methods to run According to Runtime Checklist I Use Seguence Table Information On a bar code methods to run	0001
Path: C:\HPCHEM\1\DATA\ Part of methods to run According to Runtime Checklist Use Seguence Table Information On a bar code m	
Part of methods to run       Bar Code Reader         According to Runtime Checklist       Use In Sequence         Use Seguence Table Information       On a bar code methods	
According to Runtime Checklist Use Seguence Table Information On a bar code n	
Use Seguence Table Information On a bar code m	e
	nismatcl
Shutdown O Inject anyw	ray
Post-Sequence Cmd / Macro	t
equence Commen <u>t</u> :	
b quant	

- 5.2.2.5.2. Enter Analyst initials in the "Operator Name" Field
- 5.2.2.5.3. Enter the Truncated Load Number in the "Subdirectory:" field

5.2.2.5.4. Click "OK".

- 5.2.2.6.Save the Sequence: Select "Sequence Save Sequence ..."
- 5.2.2.7.To print the sequence table for verification, select "Sequence Print Sequence"

	Print Sequence: NPD#3	<u>×</u>
	Select Parts of the Sequence to be printed	d:
	Sequence <u>Parameters</u>	
	Sequence l'able	Select Destination for Printout
	Sample Information Part	Printer
	✓ Method and Injection Info Part	<u>O File:</u>
		Path: C:\HPCHEM\1\SEQUENCE\
		Tutt. 0. III OILIAT IOLQULIOLI
	Lalibration Part	
	D Duran King King David	
	Uuantification Part	
	Sequence Output	
	Sequence Summary	<u>All Print Cancel H</u> elp
5.2.2.7.1.		

5.2.2.7.2. Check the box next to "Method and Injection Info Part" and select "Printer" as the Destination for Printout and click "Print All".

- 5.2.2.8.Have another analyst verify the printed sequence table against the vial positions in the autosampler tray.
- 5.2.2.9.To start the run, select "Sequence Table... Run Sequence" and wait until the first autosampler vial in injected into the instrument.

#### 6. **References**

6.1. Understanding Your Chemstation. Waldbronn, Gemany: Agilent Technologies, July 2009. PDF.