Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

Headspace GC Maintenance Log

Instrument: Headspace 3 **Month/Year:** March 2024

Date	N_2 Tank Pressure	H_2 Pressure / H_2 Water Level	Air Tank Pressure	He Tank Pressure	Air Blank Pass/Fail	SS Pass/Fail	Comments	Initials
3/5/2024	70	70	70	70	Pass	Pass	Agilent Service Engineer, Cash, performed the PM; See Service Report; Verification run.	BAM
	1300	Yes	1550	1325				
3/6/2024	N/A	N/A	N/A	N/A	N/A	N/A	Updated ALC.m calibration table retention times from ALC_20240305_BAM	BAM
	N/A	N/A	N/A	N/A				
3/22/2024	70	70	70	70	Pass	Pass	Changed the air gas cylinder; Competency Exam	JY
	800	Yes	2100	600				
3/27/2024	70	70	70	70	Pass	Pass	DFE test sequence run (Training).	CLR
	700	Yes	1900	400				

Signature: Brooke Ann Mendenhall Digitally signed by Brooke Ann Mendenhall Date: 2024.04.01 10:41:57 -05'00' **Date:** 04/01/2024

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Method Information

Method: C:\CHEM32\1\METHODS\ALC.M
Modified: 3/6/2024 at 1:06:30 PM

VOLATILES.M method approved for analysis of casework on May 17, 2016.
Copied to ALC.M method on July 1, 2021.

Method Audit Trail

Operator : Corissa L. Rodgers, M.S.
Date : 7/1/2021 3:22:32 PM
Change Info: This method was created at 7/1/2021 3:22:32 PM and based on method C:\CHEM32\1\METHODS\VOLATILES.M

Operator : Corissa L. Rodgers, M.S.
Date : 7/1/2021 3:24:12 PM
Change Info: Method saved. User comment: "Copied VOLATILES.M to ALC.M for the sole purpose of renaming method to be consistent with other analysis types. No changes to method parameters were made. -CLR 7/1/2021"

Operator : Corissa L. Rodgers, M.S.
Date : 7/8/2021 10:19:52 AM
Change Info: Method saved. User comment: "Updated method calibration table with average calibrator retention times from ALC_20210706_JR. -CLR 7/8/2021"

Operator : Brooke Mendenhall
Date : 3/25/2022 7:36:54 AM
Change Info: Method saved. User comment: "Updated method calibration table with average calibrator retention times from ALC_20220321_BAM. -BAM 3/25/2022"

Operator : Brooke Mendenhall
Date : 3/3/2023 8:28:13 AM
Change Info: Method saved. User comment: "Updated method calibration table with average calibrator retention times from ALC_20230302_BAM. -BAM 3/"

Operator : Brooke Mendenhall
Date : 3/3/2023 8:31:04 AM
Change Info: Method saved. User comment: "Updating audit trail to fix the inital/date on the change info comment to "-BAM 3/3/2023". No additional edits were made to the method since previous method update. -BAM 3/3/2023"

Operator : Ashley Ann Johnson, M.S.
Date : 6/22/2023 4:00:59 PM
Change Info: Data analysis parameters were copied from the sequence method 'C:\Chem32\1\Data\ALC_20230622_AAJ 2023-06-22 11-00-52\ALC.M'.

Operator : Ashley Ann Johnson, M.S.
Date : 6/22/2023 4:08:07 PM

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM
Change Info: Data analysis parameters were copied from the sequence method
'C:\Chem32\1\Data\ALC_20230622_AAJ 2023-06-22 11-00-52\ALC.M'.

Operator : Ashley Ann Johnson, M.S.
Date : 6/22/2023 4:10:15 PM
Change Info: Method saved. User comment: "Updated master method calibration
table with average calibrator retention times from
ALC_20230622_AAJ. - AAJ 06/22/2023"

Operator : Brooke Mendenhall
Date : 8/29/2023 11:13:20 AM
Change Info: Data analysis parameters were copied from the sequence method
'C:\Chem32\1\Data\ALC_20230828_BAM 2023-08-28 15-50-04\ALC.M'.

Operator : Brooke Mendenhall
Date : 8/29/2023 11:21:54 AM
Change Info: Method saved. User comment: "Updated master method calibration
table with average calibrator retention times from
ALC_20230828_BAM. -BAM 8/29/2023"

Operator : Brooke Mendenhall
Date : 8/29/2023 1:00:26 PM
Change Info: Method saved. User comment: "In the master method's calibration
table the average calibration times on FID2 for Isopropanol and
Acetone were switched. -BAM 8/29/2023"

Operator : Brooke Mendenhall
Date : 8/30/2023 3:59:34 PM
Change Info: Method saved. User comment: "Updated master method calibration
table with average calibrator retention times from
ALC_20230830_BAM. -BAM 8/30/2023"

Operator : Brooke Mendenhall
Date : 8/31/2023 10:21:32 AM
Change Info: Data analysis parameters were copied from the sequence method
'C:\Chem32\1\Data\ALC_20230830_BAM 2023-08-30 12-25-22\ALC.M'.

Operator : Brooke Mendenhall
Date : 8/31/2023 10:30:07 AM
Change Info: Data analysis parameters were copied from the sequence method
'C:\Chem32\1\Data\ALC_20230830_BAM 2023-08-30 12-25-22\ALC.M'.

Operator : Brooke Mendenhall
Date : 8/31/2023 10:33:06 AM
Change Info: Method saved. User comment: "Updated the master method area
responses from ALC_20230830_BAM and checked that the retention
times matched the average retention times from ALC_20230830_BAM.
-BAM 8/31/2023"

Operator : Brooke Mendenhall
Date : 3/6/2024 11:58:00 AM
Change Info: Method saved. User comment: "Updated the master method
calibration table with the average calibrator retention times from
ALC_20240305_BAM. -BAM 3/6/2024"

Operator : Brooke Mendenhall
Date : 3/6/2024 12:09:51 PM
Change Info: Data analysis parameters were copied from the sequence method

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM
'C:\Chem32\1\Data\2024\ALC_20240305_BAM 2024-03-05
14-13-00\ALC.M'.

Operator : Brooke Mendenhall
Date : 3/6/2024 1:06:30 PM
Change Info: Method saved. User comment: "Updated the master method area
responses from ALC_20240305_BAM and checked that the retention
times matched the average retention times from ALC_20240305_BAM.
-BAM 3/6/2024"

Run Time Checklist

Pre-Run Cmd/Macro: off

Data Acquisition: on

Standard Data Analysis: on

Customized Data Analysis: off

Save GLP Data: off

Post-Run Cmd/Macro: off

Save Method with Data: off

Injection Source and Location

Injection Source: HS 10.1.1.102

Injection Location: GC Front

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

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Agilent 7890B

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GC	
GC Summary	
Run Time	4 min
Post Run Time	0 min
Oven	
Equilibration Time	3 min
Max Temperature	260 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled
Temperature	
Setpoint	On
(Initial)	40 °C
Hold Time	4 min
Post Run	50 °C
Front SS Inlet He	
Mode	Split
Heater	On 110 °C
Pressure	On 24.011 psi
Total Flow	On 82.363 mL/min
Septum Purge Flow	On 3 mL/min
Gas Saver	Off
Split Ratio	10 :1
Split Flow	70 mL/min
Liner	Agilent 5190-4047: 65 µL (Straight, Ultra Inert Lin
Column	
Column Outlet Pressure	0 psi
Column #1	
Column Information	Restek
30 m Rtx-BAC Plus 1	
Temperature Range	0 °C—260 °C (260 °C)
Dimensions	30 m x 320 µm x 1.8 µm
Column lock	Unlocked
In	Front SS Inlet He
Out	Front Detector FID
(Initial)	40 °C
Pressure	24.011 psi
Flow	7 mL/min
Average Velocity	80.36 cm/sec
Holdup Time	0.6222 min
Flow	
Setpoint	On
(Initial)	7 mL/min
Post Run	7 mL/min
Column #2	
Column Information	Restek
30 m Rtx-BAC Plus 2	
Temperature Range	0 °C—260 °C (260 °C)

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Dimensions	30 m x 320 µm x 0.6 µm
Column lock	Unlocked
In	Front SS Inlet He
Out	Back Detector FID
(Initial)	40 °C
Pressure	24.011 psi
Flow	7.2148 mL/min
Average Velocity	81.584 cm/sec
Holdup Time	0.61287 min
Pressure	
Setpoint	On
(Initial)	24.011 psi
Post Run	10 psi

Front Detector FID

Makeup	N2
Heater	On 250 °C
H2 Flow	On 30 mL/min
Air Flow	On 400 mL/min
Makeup Flow	On 25 mL/min
Carrier Gas Flow Correction	Does not affect Makeup or Fuel Flow
Flame	On

Back Detector FID

Makeup	N2
Column Compensation	Signal is modified by Column Compensation Curve #2
Heater	On 250 °C
H2 Flow	On 30 mL/min
Air Flow	On 400 mL/min
Makeup Flow	On 25 mL/min
Carrier Gas Flow Correction	Does not affect Makeup or Fuel Flow
Flame	On

Signals

Signal #1: Front Signal

Description	Front Signal
Details	Front Signal (FID)
Save	On
Data Rate	20 Hz

Signal #2: Back Signal

Description	Back Signal
Details	Back Signal (FID)
Save	On
Data Rate	20 Hz

Signal #3: Test Plot

Description	Test Plot
Details	
Save	Off
Data Rate	50 Hz

Signal #4: Test Plot

Description	Test Plot
Details	
Save	Off

Data Rate 50 Hz

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Agilent 7697A

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Agilent 7697A
Instrument Info

Address:	10.1.1.102
Serial Number:	CN16140002
Firmware Revision:	A.01.08.3

Instrument Settings

Vial Pressurization Gas:	Nitrogen
Loop Size (mL):	1
Keyboard Lock:	OFF
Transfer Line Type:	Fused Silica
Transfer Line Diameter (mm):	0.53

System Configuration

Carrier Control:	GC Instrument

Resource Conservation

Vial Standby Flow (mL/min):	20

Temperature Settings:

Oven Temperature (°C):	70
Loop Temperature (°C):	70
Transfer Line Temperature (°C):	90

Timing Settings:

Vial Equilibration (min):	7.00
Injection Duration (min):	0.50
GC Cycle Time (min):	4.50

Vial and Loop Settings:

Vial Size:	20
Vial Shaking:	OFF
Fill Mode:	Default
Fill Pressure (psi):	10
Loop Fill Mode:	Custom
Loop Ramp Rate (psi/min):	30
Loop Final Pressure (psi):	1.5
Loop Equilibration Time:	0.05

Carrier Settings:

Carrier Control Mode:	GC controls Carrier

Advanced Settings:

Extraction Mode:	Single Extraction

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Vent After Extraction:	ON
Post Injection Purge:	Default, 100 mL/min for 1 min
Acceptable Leak Check:	Default, 0.2mL/min

The Data Analysis Parameters of the used Method are :

Integration Events

Non signal specific Integration Events

Event	Value
Tangent Skim Mode	New Exponential
Tail Peak Skim Height Ratio	5.000
Front Peak Skim Height Ratio	5.000
Skim Valley Ratio	20.000
Baseline Correction	Advanced
Peak to Valley Ratio	500.000

Default Integration Event Table "Event"

Event	Value	Time
Initial Slope Sensitivity	1.000	Initial
Initial Peak Width	0.040	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.700	Initial
Initial Shoulders	OFF	Initial

Detector Default Integration Event Table "Event_ADC"

Event	Value	Time
Initial Slope Sensitivity	20.000	Initial
Initial Peak Width	0.040	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.000	Initial
Initial Shoulders	OFF	Initial

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Detector Default Integration Event Table "Event_TCD"

Event	Value	Time
Initial Slope Sensitivity	100.000	Initial
Initial Peak Width	0.040	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.000	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	250000.000	0.000

Detector Default Integration Event Table "Event_ECD"

Event	Value	Time
Initial Slope Sensitivity	100.000	Initial
Initial Peak Width	0.080	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.000	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	0.000	0.000

Detector Default Integration Event Table "Event_NPD"

Event	Value	Time
Initial Slope Sensitivity	500.000	Initial
Initial Peak Width	0.040	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.000	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	0.000	0.000

Detector Default Integration Event Table "Event_FPD"

Event	Value	Time
Initial Slope Sensitivity	50.000	Initial
Initial Peak Width	0.040	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.000	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	0.000	0.000

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Detector Default Integration Event Table "Event_uECD"

Event	Value	Time
Initial Slope Sensitivity	500.000	Initial
Initial Peak Width	0.080	Initial
Initial Area Reject	1.000	Initial
Initial Height Reject	1.000	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	0.000	0.000

Detector Default Integration Event Table "Event_FID"

Event	Value	Time
Initial Slope Sensitivity	20.000	Initial
Initial Peak Width	0.010	Initial
Initial Area Reject	1.500	Initial
Initial Height Reject	1.500	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	250000.000	0.000

Signal Specific Integration Event Table "Event_FID2B"

Event	Value	Time
Initial Slope Sensitivity	20.000	Initial
Initial Peak Width	0.010	Initial
Initial Area Reject	1.500	Initial
Initial Height Reject	1.500	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	250000.000	0.000
Area Reject	3.600	1.100

Signal Specific Integration Event Table "Event_FID1A"

Event	Value	Time
Initial Slope Sensitivity	20.000	Initial
Initial Peak Width	0.010	Initial
Initial Area Reject	1.500	Initial
Initial Height Reject	1.500	Initial
Initial Shoulders	OFF	Initial
Solvent Peak Slope	250000.000	0.000
Area Reject	3.400	1.200

Apply Method's Manual Integration Events: No

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Calibration Table

General Calibration Setting

Calib. Data Modified : 3/6/2024 12:06:47 PM
Signals calculated separately : No

Rel. Reference Window : 2.000 %
Abs. Reference Window : 0.000 min
Rel. Non-ref. Window : 2.000 %
Abs. Non-ref. Window : 0.000 min
Uncalibrated Peaks : not reported
Partial Calibration : Yes, identified peaks are recalibrated
Correct All Ret. Times: No, only for identified peaks

Curve Type : Linear
Origin : Ignored
Weight : Linear (Amnt)

Recalibration Settings:
Average Response : Average all calibrations
Average Retention Time: Floating Average New 75%

Calibration Report Options :
Printout of recalibrations within a sequence:
Calibration Table after Recalibration
Normal Report after Recalibration
If the sequence is done with bracketing:
Results of first cycle (ending previous bracket)

Sample ISTD Information:

ISTD #	ISTD Amount [g/100 mL]	Name
2	1.00000e-2	n-Propanol
1	1.00000e-2	n-Propanol

Signal Details

Signal 1: FID1 A, Front Signal
Signal 2: FID2 B, Back Signal

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

Overview Table

RT	Sig	Lvl	Amount [g/100 mL]	Area	Rsp.Factor	Ref	ISTD	#	Compound
0.872	2	1	1.00000e-2	7.95285	1.25741e-3	No	No	2	Methanol
		2	2.50000e-2	19.25554	1.29833e-3				
		3	5.00000e-2	38.17371	1.30980e-3				
		4	1.00000e-1	78.23712	1.27817e-3				
		5	2.00000e-1	154.01151	1.29860e-3				
		6	4.00000e-1	304.88547	1.31197e-3				
0.934	1	1	1.00000e-2	7.19429	1.38999e-3	No	No	1	Methanol
		2	2.50000e-2	17.44468	1.43310e-3				
		3	5.00000e-2	34.56845	1.44641e-3				
		4	1.00000e-1	70.99758	1.40850e-3				
		5	2.00000e-1	139.40762	1.43464e-3				
		6	4.00000e-1	276.31735	1.44761e-3				
1.032	2	1	1.00000e-2	16.19648	6.17418e-4	No	No	2	Ethanol
		2	2.50000e-2	38.77794	6.44696e-4				
		3	5.00000e-2	76.35773	6.54813e-4				
		4	1.00000e-1	156.66956	6.38286e-4				
		5	2.00000e-1	306.33377	6.52883e-4				
		6	4.00000e-1	611.51740	6.54111e-4				
		7	5.00000e-1	764.36621	6.54137e-4				
1.105	2	1	1.00000e-2	60.90176	1.64199e-4	No	No	2	Acetone
		2	2.50000e-2	148.99429	1.67792e-4				
		3	5.00000e-2	293.29663	1.70476e-4				
		4	1.00000e-1	592.62543	1.68741e-4				
		5	2.00000e-1	1177.73376	1.69818e-4				
		6	4.00000e-1	2327.97778	1.71823e-4				
1.168	1	1	1.00000e-2	14.17835	7.05300e-4	No	No	1	Ethanol
		2	2.50000e-2	34.77093	7.18991e-4				
		3	5.00000e-2	69.10305	7.23557e-4				
		4	1.00000e-1	142.04837	7.03986e-4				
		5	2.00000e-1	278.25089	7.18776e-4				
		6	4.00000e-1	556.13702	7.19247e-4				
		7	5.00000e-1	695.01367	7.19410e-4				
1.168	2	1	1.00000e-2	30.63434	3.26431e-4	No	No	2	Isopropanol
		2	2.50000e-2	74.78753	3.34280e-4				
		3	5.00000e-2	147.59807	3.38758e-4				
		4	1.00000e-1	303.07416	3.29952e-4				
		5	2.00000e-1	590.82703	3.38509e-4				
		6	4.00000e-1	1187.28149	3.36904e-4				
1.420	1	1	1.00000e-2	27.22368	3.67327e-4	No	No	1	Isopropanol
		2	2.50000e-2	67.37306	3.71068e-4				
		3	5.00000e-2	134.56824	3.71559e-4				
		4	1.00000e-1	274.32220	3.64535e-4				
		5	2.00000e-1	535.53180	3.73461e-4				
		6	4.00000e-1	1077.46655	3.71241e-4				
1.540	1	1	1.00000e-2	54.85353	1.82304e-4	No	No	1	Acetone
		2	2.50000e-2	134.89955	1.85323e-4				
		3	5.00000e-2	266.66168	1.87504e-4				
		4	1.00000e-1	537.74280	1.85963e-4				
		5	2.00000e-1	1069.16724	1.87061e-4				
		6	4.00000e-1	2115.46436	1.89084e-4				
1.610	2	1	1.00000e-2	248.21690	4.02873e-5	No	Yes	2	n-Propanol
		2	1.00000e-2	243.08585	4.11377e-5				

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

RT	Sig	Lvl	Amount [g/100 mL]	Area	Rsp.Factor	Ref	ISTD	#	Compound
		3	1.00000e-2	239.37248	4.17759e-5				
		4	1.00000e-2	247.38446	4.04229e-5				
		5	1.00000e-2	239.72580	4.17143e-5				
		6	1.00000e-2	241.05479	4.14843e-5				
		7	1.00000e-2	239.37314	4.17758e-5				
1.944	1	1	1.00000e-2	226.04021	4.42399e-5	No	Yes	1	n-Propanol
		2	1.00000e-2	221.80060	4.50855e-5				
		3	1.00000e-2	218.46500	4.57739e-5				
		4	1.00000e-2	226.06543	4.42350e-5				
		5	1.00000e-2	218.93976	4.56747e-5				
		6	1.00000e-2	220.38487	4.53752e-5				
		7	1.00000e-2	218.29311	4.58100e-5				

Identification Details Table

RT	From	To	Sig	+-	Pk	Usage	Compound
0.872	0.863	0.881	2	0.0000		Main	Methanol
0.934	0.925	0.943	1	0.0000		Main	Methanol
1.032	1.022	1.042	2	0.0000		Main	Ethanol
1.105	1.094	1.116	2	0.0000		Main	Acetone
1.168	1.157	1.180	1	0.0000		Main	Ethanol
1.168	1.157	1.180	2	0.0000		Main	Isopropanol

RT	From	To	Sig	+-	Pk	Usage	Compound

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

1.420	1.405	1.434	1	0.0000	Main	Isopropanol
1.540	1.524	1.555	1	0.0000	Main	Acetone
1.610	1.594	1.626	2	0.0000	Main	n-Propanol
1.944	1.925	1.964	1	0.0000	Main	n-Propanol

Peak Sum Table

No Entries in table

1 Warnings or Errors :

Warning : Curve requires more calibration points., (n-Propanol)

Component Details Table

RT	Sig	Grp	Lvl	Amount [g/100 mL]	Low Limit	High Limit	Compound
0.872	2		1	1.00000e-2	0.00000	0.00000	Methanol
			2	2.50000e-2			
			3	5.00000e-2			
			4	1.00000e-1			
			5	2.00000e-1			

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

RT	Sig Grp	Lvl	Amount [g/100 mL]	Low Limit	High Limit	Compound
		6	4.00000e-1			
0.934	1	1	1.00000e-2	0.00000	0.00000	Methanol
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
1.032	2	1	1.00000e-2	0.00000	0.00000	Ethanol
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
		7	5.00000e-1			
1.105	2	1	1.00000e-2	0.00000	0.00000	Acetone
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
1.168	1	1	1.00000e-2	0.00000	0.00000	Ethanol
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
		7	5.00000e-1			
1.168	2	1	1.00000e-2	0.00000	0.00000	Isopropanol
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
1.420	1	1	1.00000e-2	0.00000	0.00000	Isopropanol
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
1.540	1	1	1.00000e-2	0.00000	0.00000	Acetone
		2	2.50000e-2			
		3	5.00000e-2			
		4	1.00000e-1			
		5	2.00000e-1			
		6	4.00000e-1			
1.610	2	1	1.00000e-2	0.00000	0.00000	n-Propanol
		2	1.00000e-2			
		3	1.00000e-2			
		4	1.00000e-2			
		5	1.00000e-2			
		6	1.00000e-2			
		7	1.00000e-2			
1.944	1	1	1.00000e-2	0.00000	0.00000	n-Propanol
		2	1.00000e-2			
		3	1.00000e-2			

method: C:\CHEM32\1\METHODS\ALC.M
Modified on: 3/6/2024 at 1:06:30 PM

RT	Sig	Grp	Lvl	Amount [g/100 mL]	Low Limit	High Limit	Compound
			4	1.00000e-2			
			5	1.00000e-2			
			6	1.00000e-2			
			7	1.00000e-2			

Sample related custom fields

Custom Field	Type	Mand.	Default Value
None defined			

Compound related custom fields

Custom Field	Type	Mand.	Default Value
None defined			