LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110122\
Data File : VU051664.D
Acq On : 01 Nov 2022 19:20
Operator : JC/MD
Sample : N5353-20
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU051664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	30	rVB	290143	281322	4.29%	1.728%
2	1.465	30	39	54	rBV2	230385	467044	7.12%	2.869%
3	1.600	72	81	94	rBV	355737	443399	6.76%	2.724%
4	1.909	169	177	193	rVV	90982	134299	2.05%	0.825%
5	1.993	195	203	214	rVB	68150	95569	1.46%	0.587%
6	2.199	260	267	279	rVB	90010	129624	1.97%	0.796%
7	2.565	368	381	394	rBV2	175478	305708	4.66%	1.878%
8	4.665	1009	1034	1097	rBV	2797006	6563928	100.00%	40.325%
9	5.060	1140	1157	1184	rBV2	160630	379163	5.78%	2.329%
10	5.722	1342	1363	1369	rBV2	315003	774810	11.80%	4.760%
11	5.771	1369	1378	1410	rVB	1042593	2149507	32.75%	13.205%
12	6.247	1512	1526	1556	rBV	244758	477046	7.27%	2.931%
13	6.690	1649	1664	1682	rBV	196539	391087	5.96%	2.403%
14	7.565	1922	1936	1952	rBV	87921	157562	2.40%	0.968%
15	7.896	2023	2039	2053	rBV	353366	609278	9.28%	3.743%
16	8.179	2115	2127	2144	rBV	55269	93295	1.42%	0.573%
17	8.629	2255	2267	2305	rBV	430595	804851	12.26%	4.944%
18	9.417	2499	2512	2536	rBV	350856	602630	9.18%	3.702%
19	10.754	2916	2928	2941	rBV	163570	261360	3.98%	1.606%
20	11.809	3242	3256	3275	rBV	316997	527840	8.04%	3.243%
21	12.060	3323	3334	3358	rBV4	32405	82677	1.26%	0.508%
22	12.192	3362	3375	3393	rBV	327632	545744	8.31%	3.353%

Sum of corrected areas: 16277743

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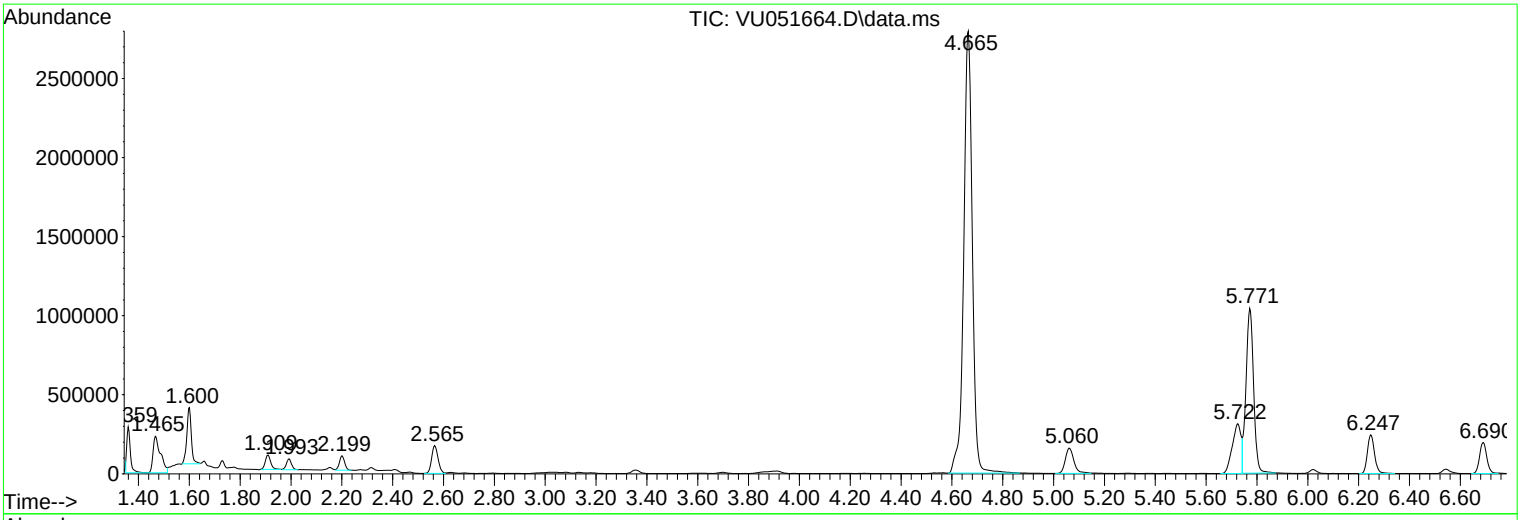
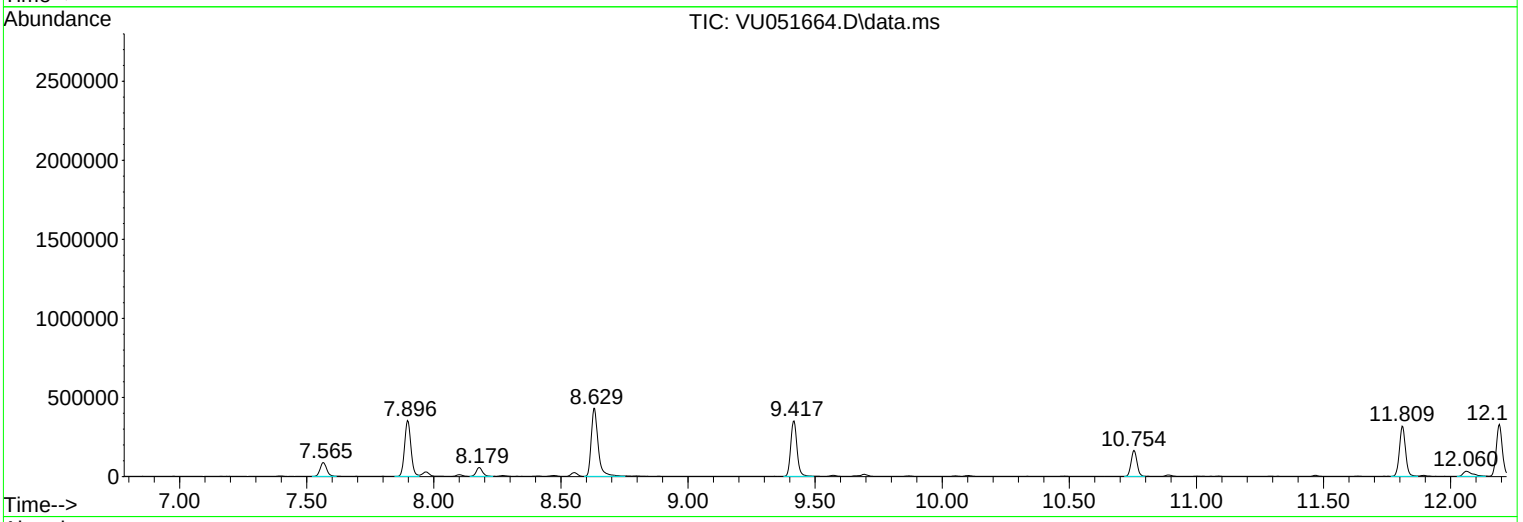
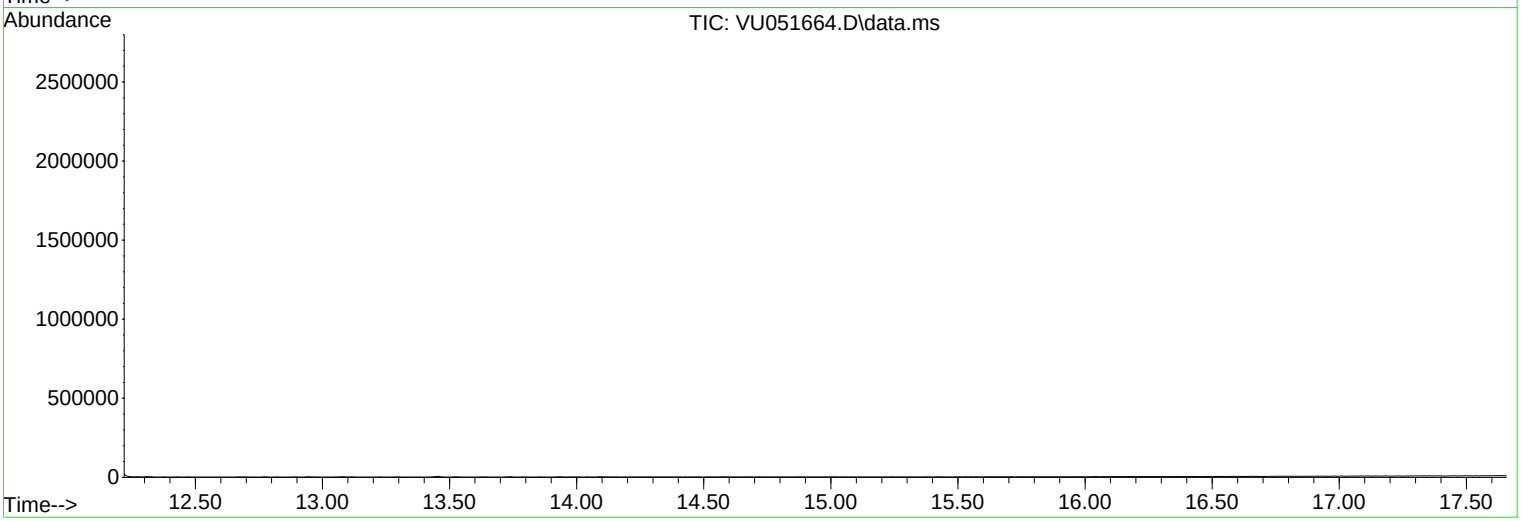
MSVOA_U
ClientSampleId :
DBXB3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Instrument :
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ClientSampleId :
DBXB3

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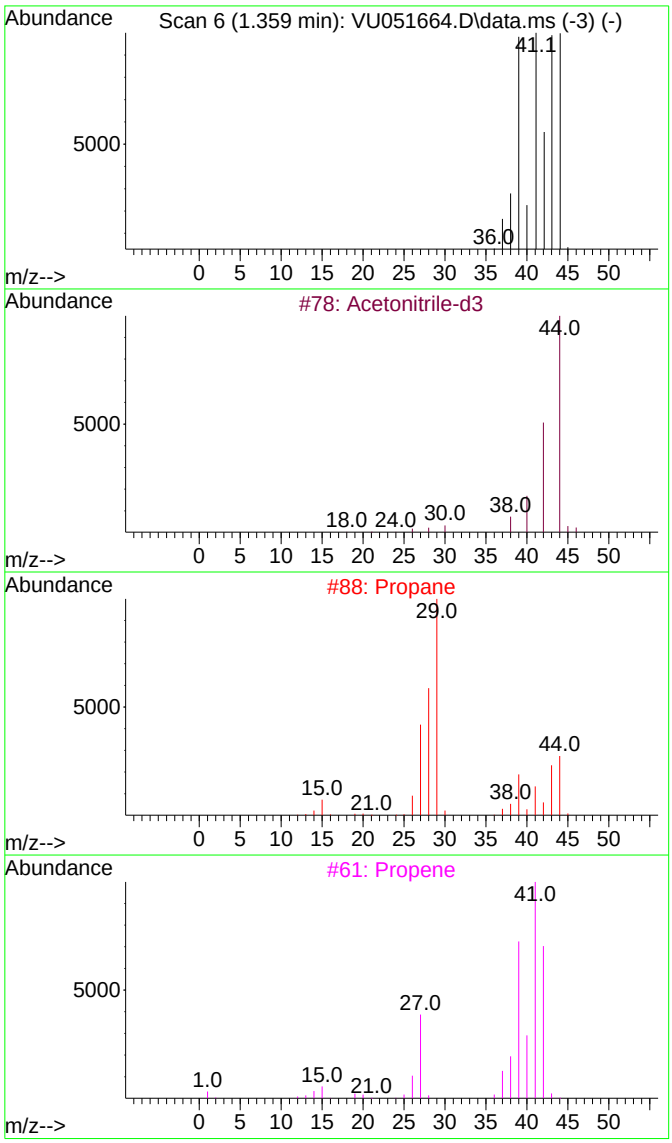
Quant Title : TRACE VOA SFAM1.0

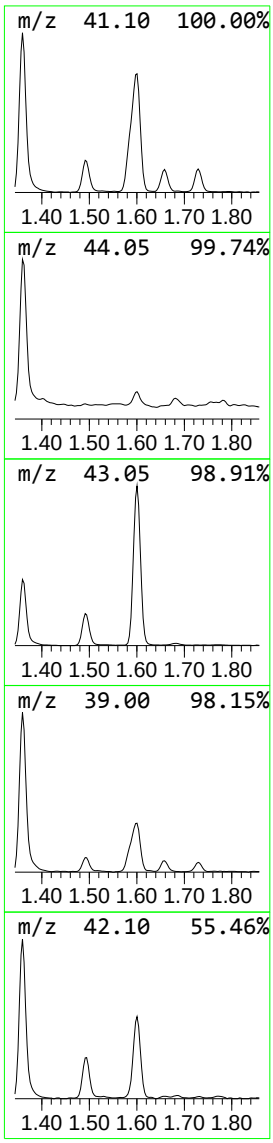
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	2.95 ug/L	281322	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile-d3	44	C2D3N	002206-26-0	9
2	Propane	44	C3H8	000074-98-6	9
3	Propene	42	C3H6	000115-07-1	7
4	Acetonitrile-d3	44	C2D3N	002206-26-0	4
5	Propane	44	C3H8	000074-98-6	4





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Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB3

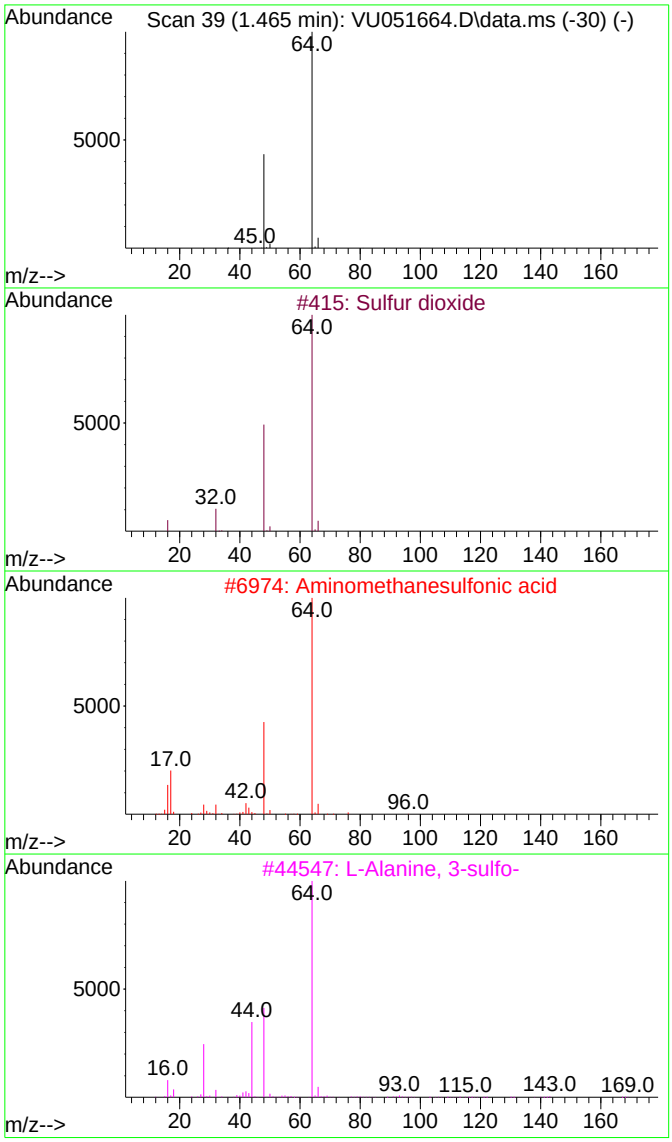
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

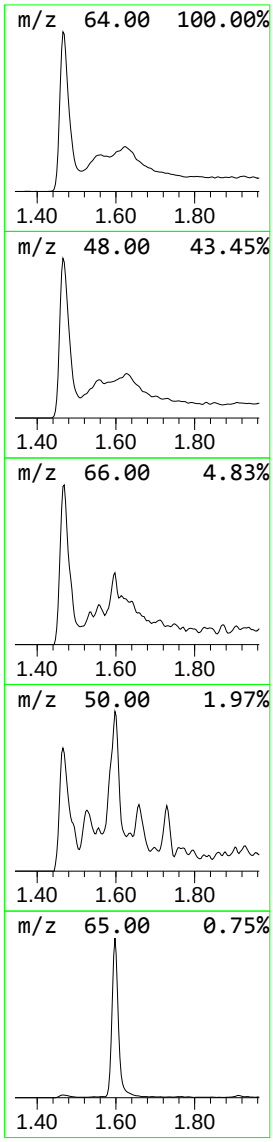
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	4.90 ug/L	467044	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Sulfur dioxide	64	O2S	007446-09-5	4
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB3

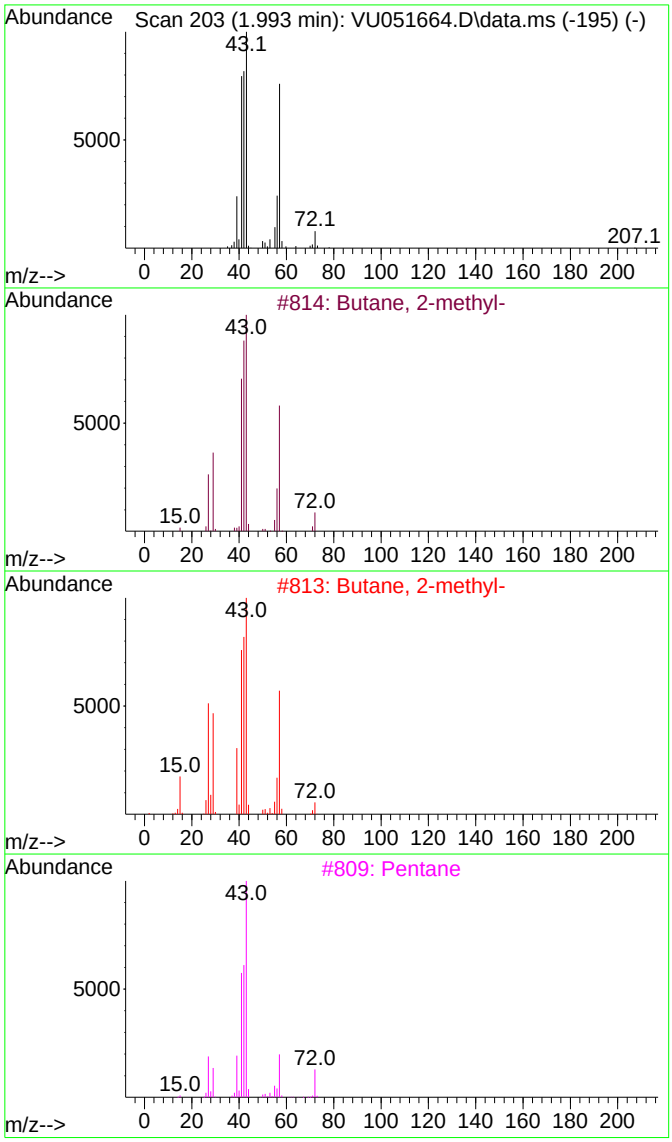
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

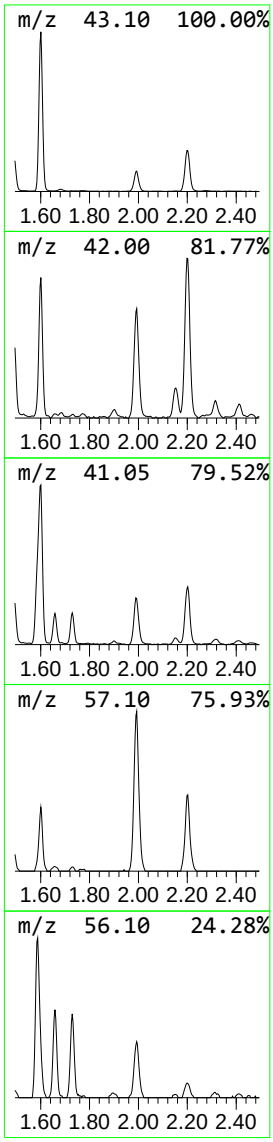
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.993	1.00 ug/L	95569	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Butane, 2-methyl-	72	C5H12	000078-78-4	80
3	Pentane	72	C5H12	000109-66-0	45
4	3-Buten-1-ol	72	C4H8O	000627-27-0	43
5	1-Butene	56	C4H8	000106-98-9	10





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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB3

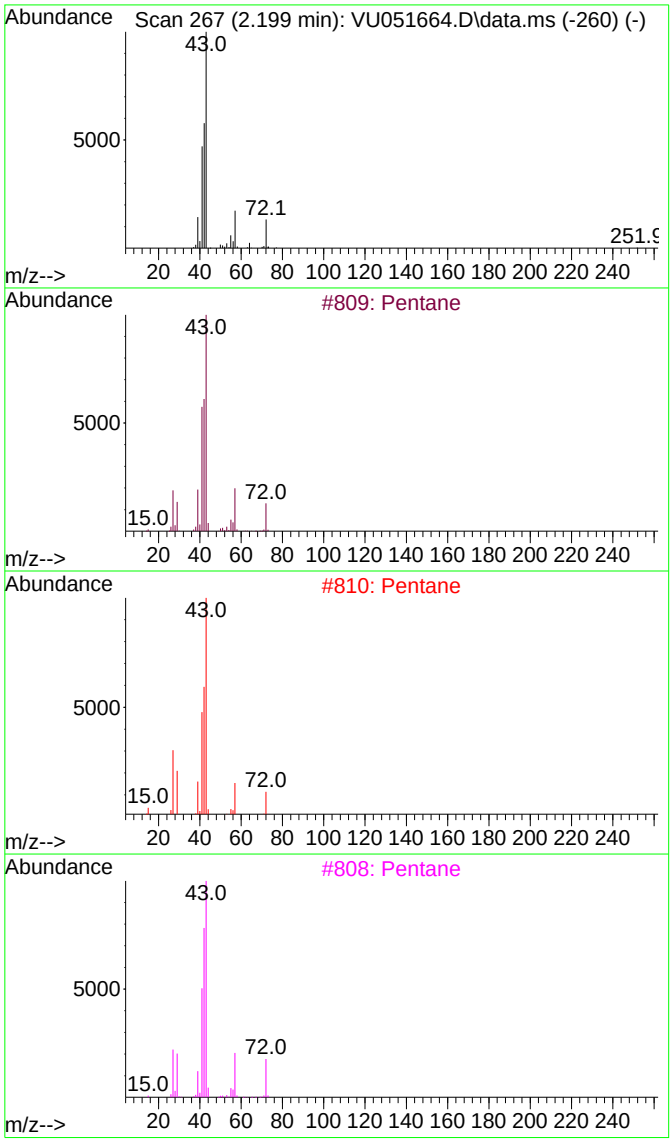
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

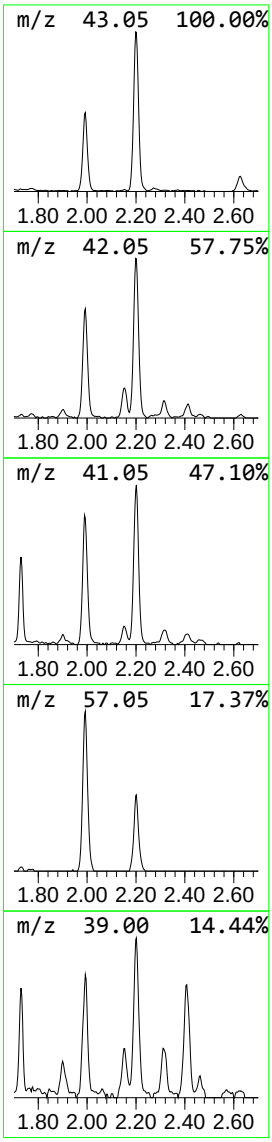
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	1.36 ug/L	129624	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	87
2	Pentane	72	C5H12	000109-66-0	86
3	Pentane	72	C5H12	000109-66-0	86
4	Pentane	72	C5H12	000109-66-0	86
5	Pentane	72	C5H12	000109-66-0	86





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Operator : JC/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB3

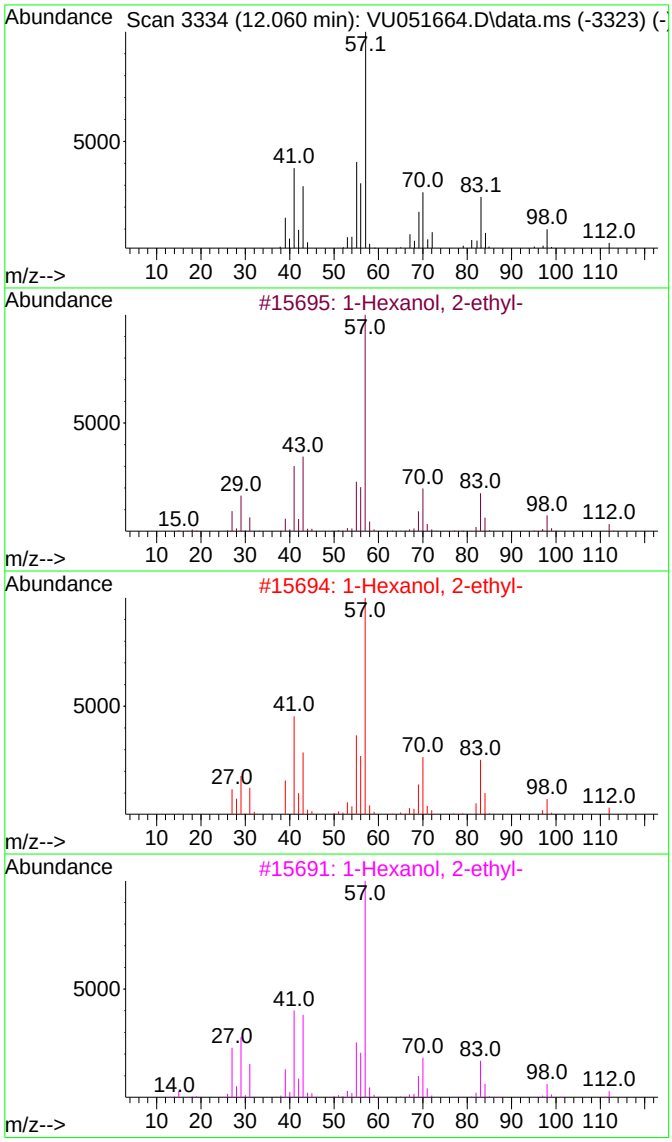
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

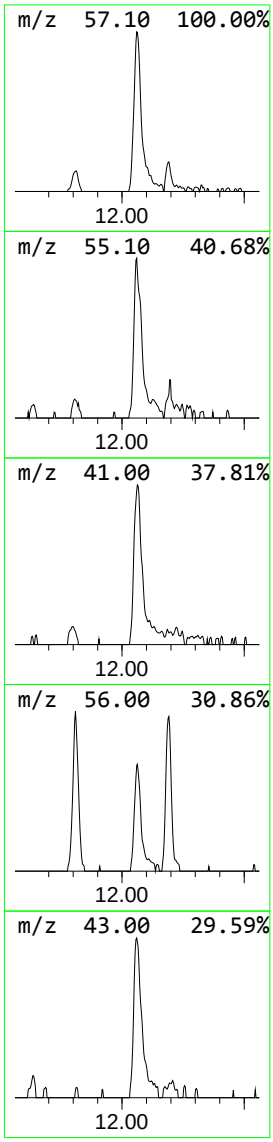
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	0.78 ug/L	82677	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	3.0	ug/L	281322	1	6.247	477046	5.0
Sulfur dioxide	1.465	4.9	ug/L	467044	1	6.247	477046	5.0
(DEL) Alkane: S...	1.993	1.0	ug/L	95569	1	6.247	477046	5.0
(DEL) Alkane: S...	2.199	1.4	ug/L	129624	1	6.247	477046	5.0
1-Hexanol, 2-et...	12.060	0.8	ug/L	82677	3	11.809	527840	5.0