LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

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\SFAMUTR061422WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU049250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.391	10	16	24	rBV	45141	46687	7.71%	0.738%
2	1.520	52	56	61	rBV2	7412	6079	1.00%	0.096%
3	1.578	62	74	79	rBV2	32216	70900	11.70%	1.121%
4	1.629	81	90	104	rVB2	83459	167237	27.60%	2.644%
5	1.951	184	190	202	rVB	52333	72108	11.90%	1.140%
6	2.607	384	394	408	rVB	94829	154042	25.42%	2.436%
7	2.729	423	432	457	rBV3	53524	157295	25.96%	2.487%
8	3.092	534	545	560	rVB2	109172	207543	34.25%	3.281%
9	3.912	787	800	816	rVV	41702	94862	15.66%	1.500%
10	4.005	817	829	844	rVB4	12077	31130	5.14%	0.492%
11	4.742	1031	1058	1074	rBV2	51642	211475	34.90%	3.344%
12	5.121	1160	1176	1193	rBV	87621	215403	35.55%	3.406%
13	5.661	1338	1344	1357	rBV	7256	14090	2.33%	0.223%
14	5.787	1364	1383	1417	rBV2	193338	477500	78.81%	7.550%
15	6.230	1509	1521	1530	rBV3	4460	9804	1.62%	0.155%
16	6.301	1530	1543	1557	rVB	177451	324626	53.58%	5.133%
17	6.735	1664	1678	1695	rBV	123191	243224	40.14%	3.846%
18	6.832	1700	1708	1725	rVB3	11880	26018	4.29%	0.411%
19	7.198	1803	1822	1824	rBV7	6424	14425	2.38%	0.228%
20	7.282	1842	1848	1856	rVB4	5932	8398	1.39%	0.133%
21	7.594	1933	1945	1962	rBV	62259	109203	18.02%	1.727%
22	7.828	2004	2018	2036	rBV3	70831	164798	27.20%	2.606%
23	7.922	2036	2047	2060	rVV	227651	396762	65.49%	6.273%
24	7.992	2060	2069	2082	rVV	57993	102390	16.90%	1.619%
25	8.063	2083	2091	2102	rVB3	5245	9706	1.60%	0.153%
26	8.201	2123	2134	2144	rBV	38202	62784	10.36%	0.993%
27	8.266	2144	2154	2176	rVB2	19315	42875	7.08%	0.678%
28	8.655	2261	2275	2308	rBV	308988	605877	100.00%	9.579%
29	9.057	2391	2400	2410	rVB4	6591	9595	1.58%	0.152%
30	9.430	2503	2516	2533	rBV	242744	394172	65.06%	6.232%
31	9.584	2554	2564	2572	rBV2	9430	15997	2.64%	0.253%
32	9.703	2586	2601	2614	rBV2	26864	45912	7.58%	0.726%
33	10.108	2719	2727	2734	rBV2	9801	15707	2.59%	0.248%
34	10.243	2758	2769	2777	rVB	8747	12986	2.14%	0.205%
35	10.372	2797	2809	2831	rVB5	8202	20393	3.37%	0.322%
36	10.761	2919	2930	2942	rBV	95701	153445	25.33%	2.426%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

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\SFAMUTR061422WMA.M
Title : TRACE VOA SFAM1.0

37	11.217	3063	3072	3083	rBV5	4792	8815	1.45%	0.139%
38	11.471	3139	3151	3159	rBV3	11805	18884	3.12%	0.299%
39	11.578	3175	3184	3190	rBV6	4251	7446	1.23%	0.118%
40	11.648	3197	3206	3216	rBV6	8652	16220	2.68%	0.256%
41	11.815	3245	3258	3275	rVB	253053	404181	66.71%	6.390%
42	11.899	3275	3284	3291	rBV3	5303	7562	1.25%	0.120%
43	12.060	3319	3334	3353	rBV	217243	384349	63.44%	6.077%
44	12.195	3366	3376	3395	rVB	227406	364103	60.10%	5.757%
45	12.301	3406	3409	3423	rVB8	3666	7024	1.16%	0.111%
46	12.536	3472	3482	3503	rBV	58906	105187	17.36%	1.663%
47	12.950	3602	3611	3623	rBV2	20634	34194	5.64%	0.541%
48	13.295	3707	3718	3731	rVB3	12470	22410	3.70%	0.354%
49	13.449	3757	3766	3778	rVV5	4434	8376	1.38%	0.132%
50	13.520	3778	3788	3801	rVB3	12564	20179	3.33%	0.319%
51	13.738	3846	3856	3865	rBV6	11369	20407	3.37%	0.323%
52	13.838	3882	3887	3898	rVB6	4136	6653	1.10%	0.105%
53	13.934	3911	3917	3925	rVB4	5881	8122	1.34%	0.128%
54	14.037	3942	3949	3957	rVB7	5064	6871	1.13%	0.109%
55	14.423	4060	4069	4083	rVB2	7260	12311	2.03%	0.195%
56	16.236	4625	4633	4641	rBV2	7663	11000	1.82%	0.174%
57	16.519	4715	4721	4732	rVB9	5474	8291	1.37%	0.131%
58	16.770	4788	4799	4816	rBV2	73990	126698	20.91%	2.003%

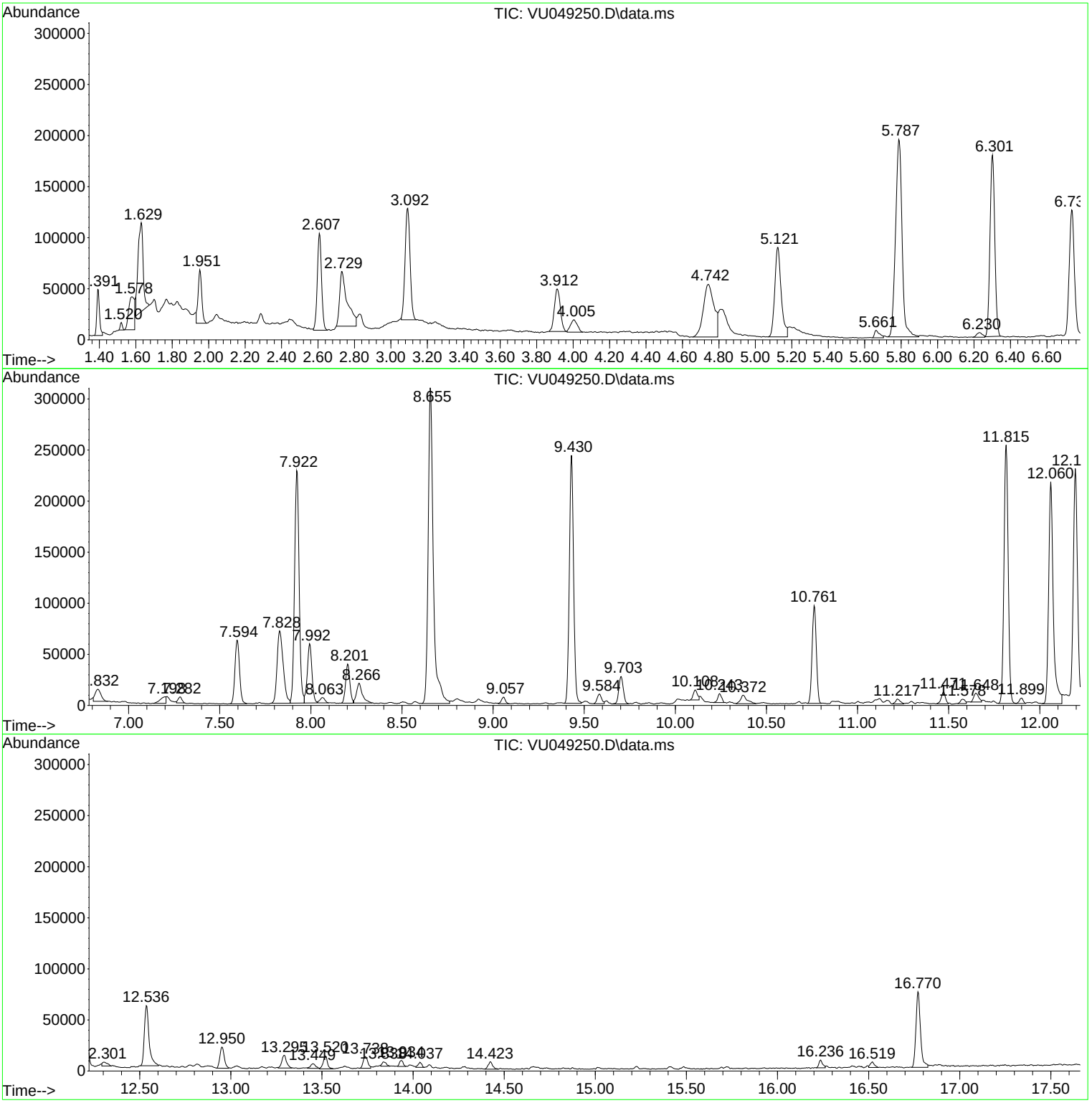
Sum of corrected areas: 6324731

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

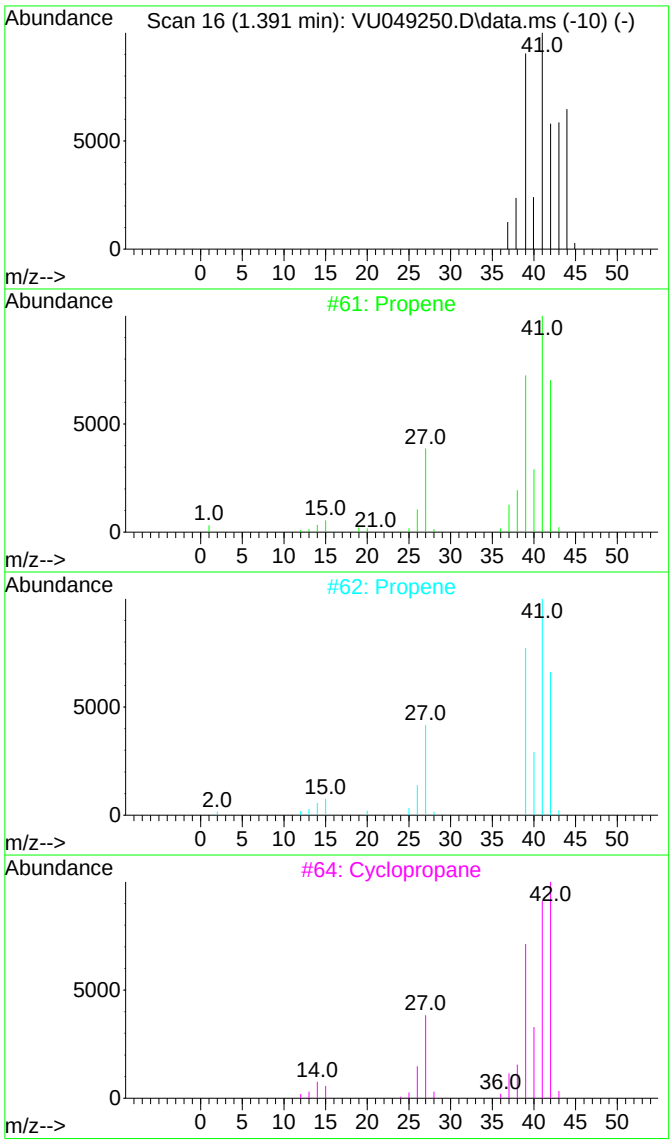
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

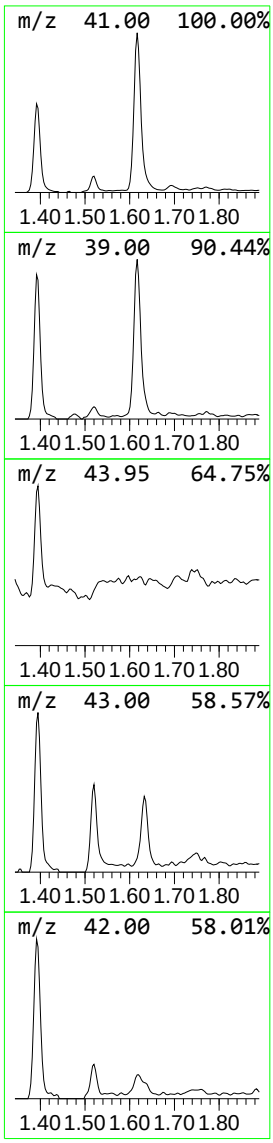
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.391	0.72 ug/L	46687	1,4-Difluorobenzene	6.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropane	42	C3H6	000075-19-4	9
5	Cyclopropene	40	C3H4	002781-85-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

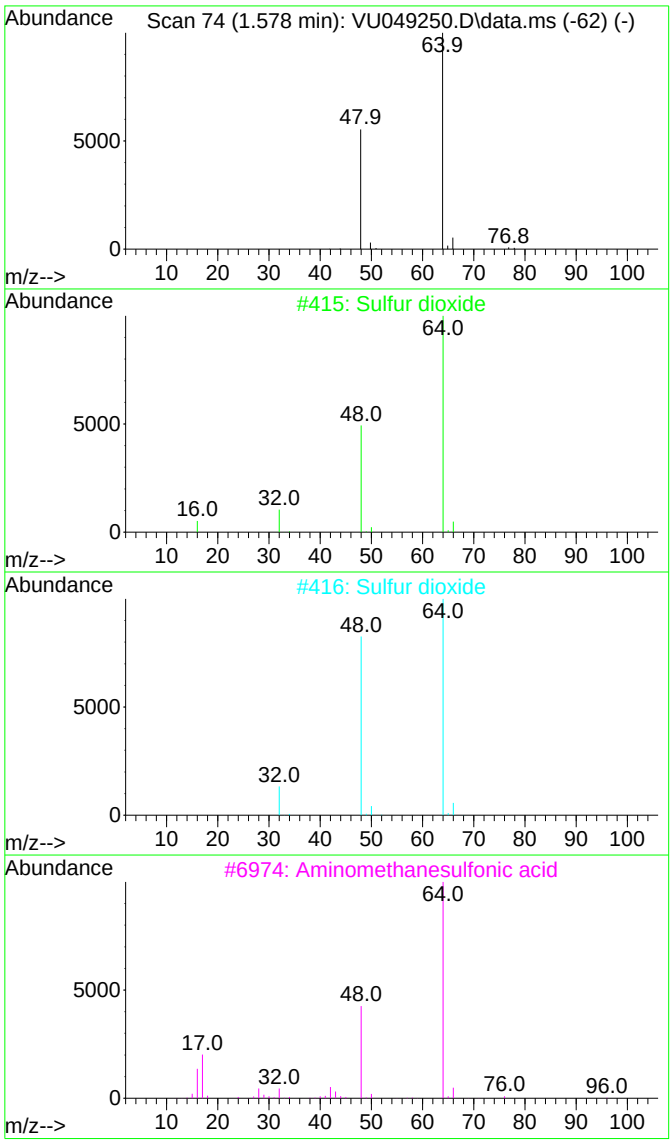
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

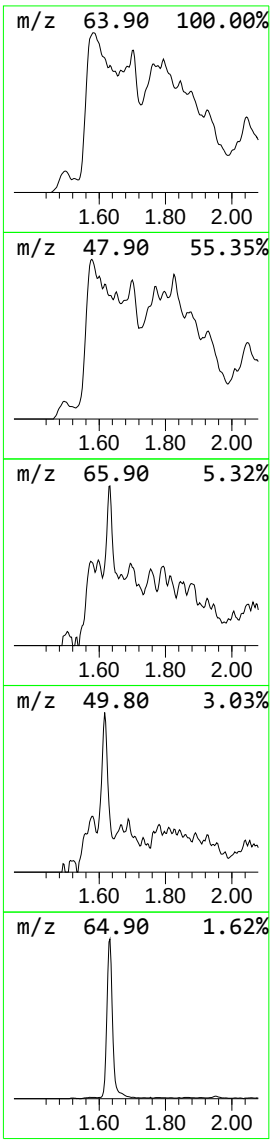
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.578	1.09 ug/L	70900	1,4-Difluorobenzene	6.301

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

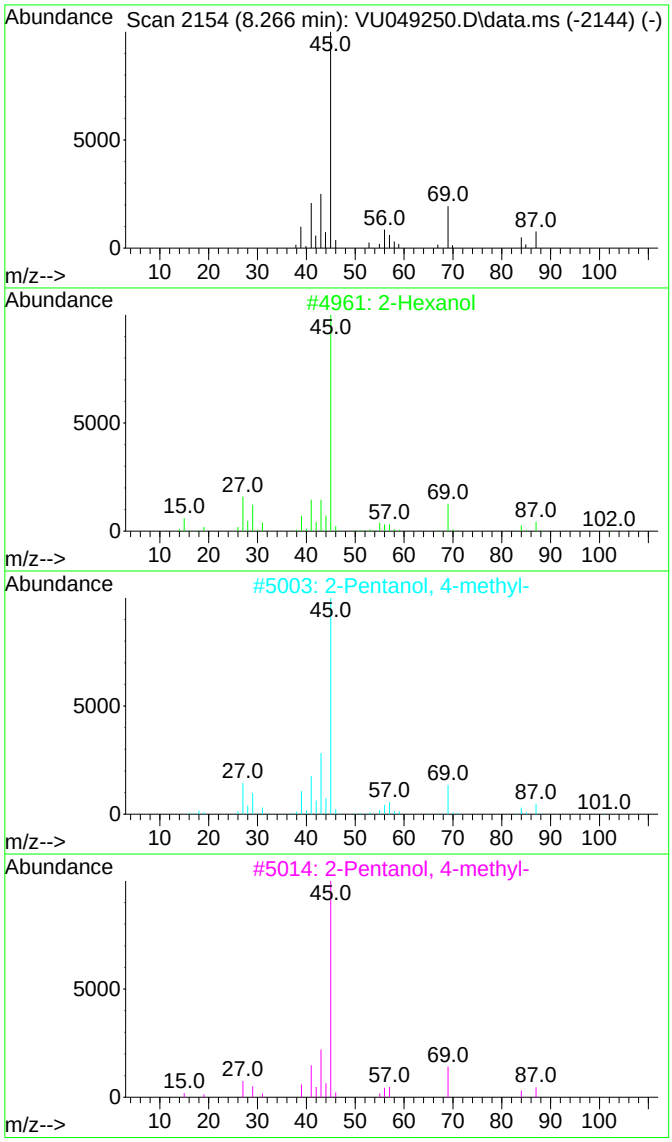
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

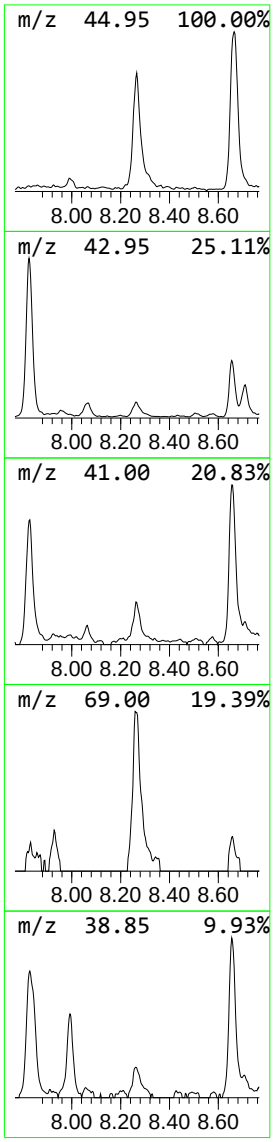
****

Peak Number 4 2-Hexanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.266	0.54 ug/L	42875	Chlorobenzene-d5	9.430

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol	102	C6H14O	000626-93-7	83
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
4	2-Hexanol	102	C6H14O	000626-93-7	83
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

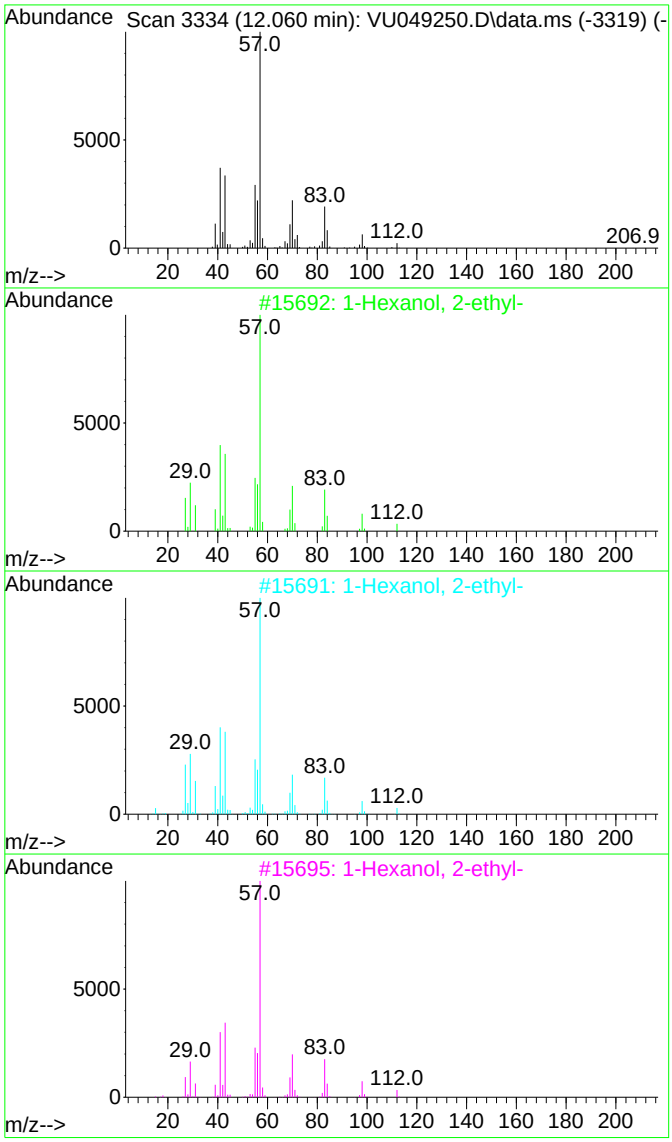
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

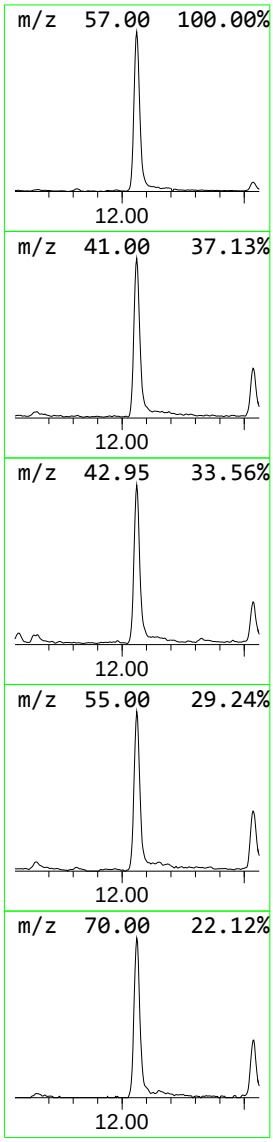
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	4.75 ug/L	384349	1,4-Dichlorobenzene-d4	11.816

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	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

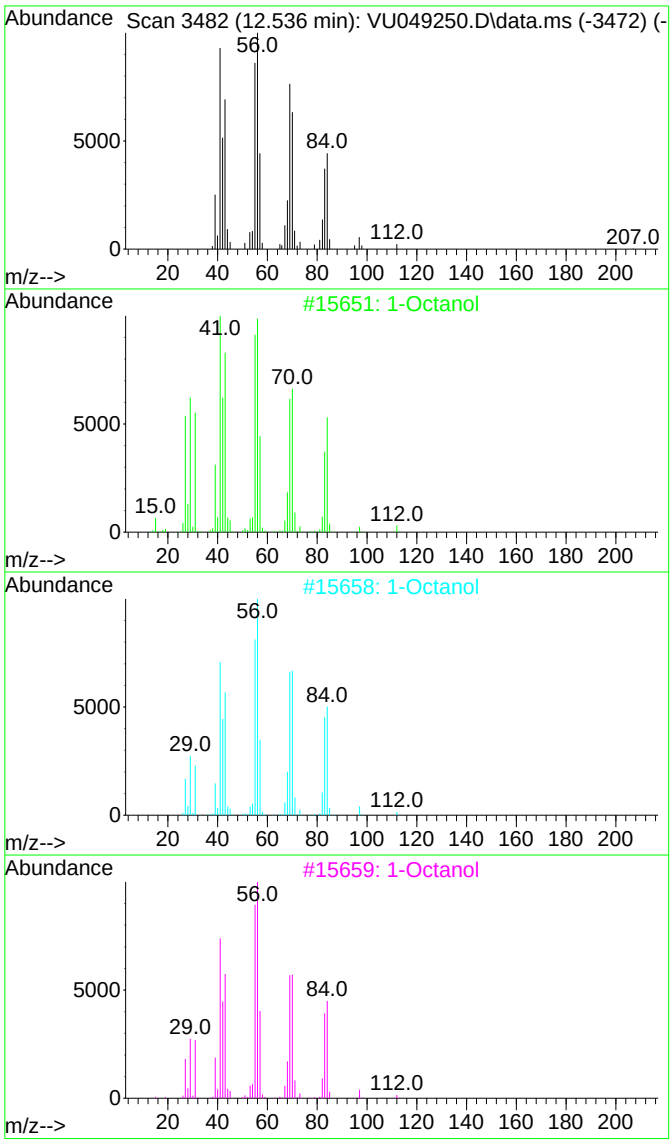
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

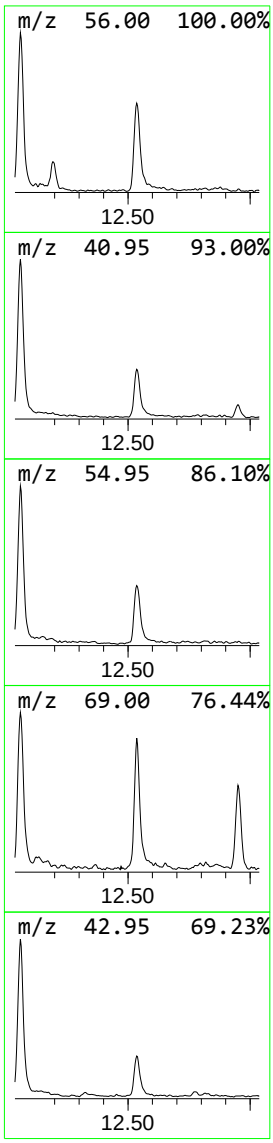
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.536	1.30 ug/L	105187	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	91
2	1-Octanol	130	C8H18O	000111-87-5	91
3	1-Octanol	130	C8H18O	000111-87-5	91
4	1-Octanol	130	C8H18O	000111-87-5	90
5	Formic acid, octyl ester	158	C9H18O2	000112-32-3	72





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

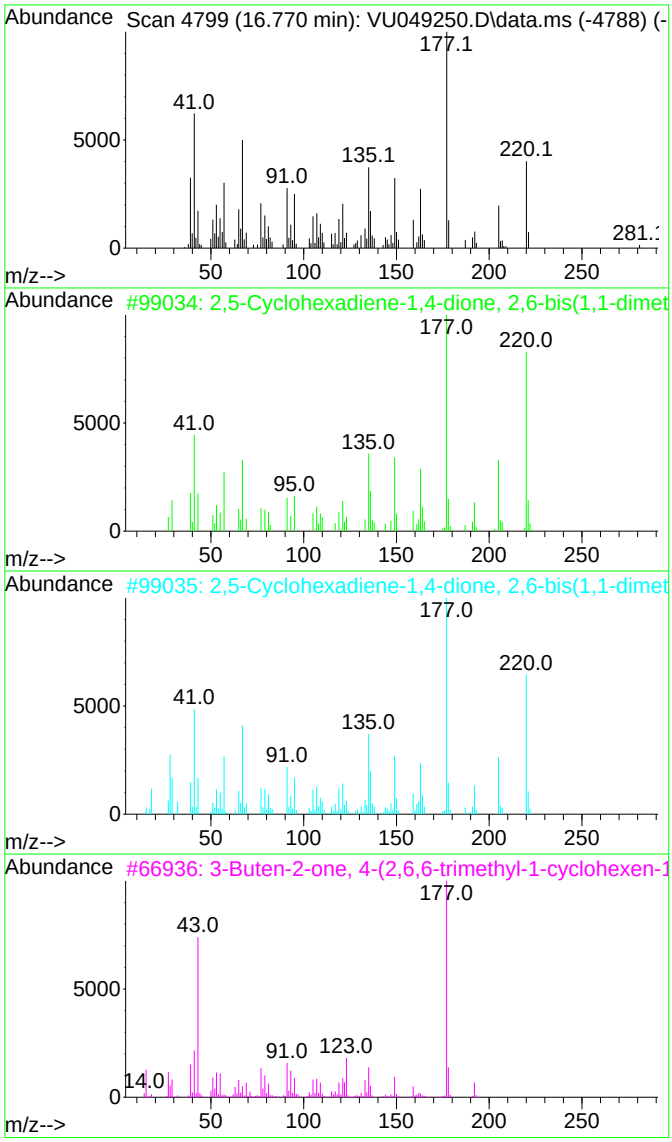
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

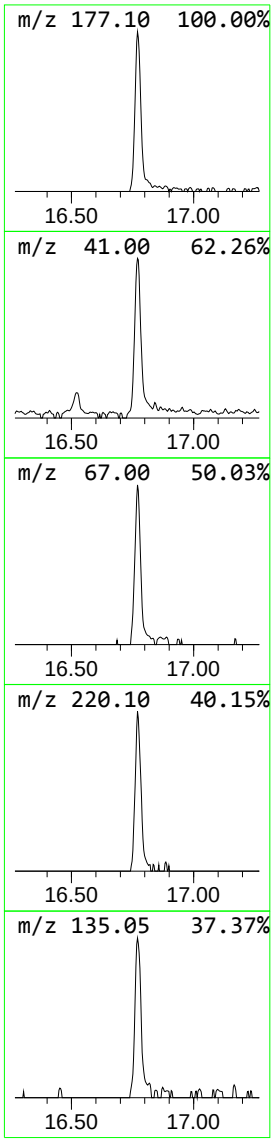
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.770	1.57 ug/L	126698	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	70
3	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	50
4	.beta.-Oplopenone	220	C15H24O	028305-60-4	50
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
Data File : VU049250.D
Acq On : 17 Jun 2022 16:40
Operator : SY/MD
Sample : N3285-01DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4P5DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
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...	1.391	0.7	ug/L	46687	1	6.301	324626	5.0
Sulfur dioxide	1.578	1.1	ug/L	70900	1	6.301	324626	5.0
2-Hexanol	8.266	0.5	ug/L	42875	2	9.430	394172	5.0
1-Hexanol, 2-et...	12.060	4.8	ug/L	384349	3	11.816	404181	5.0
1-Octanol	12.536	1.3	ug/L	105187	3	11.816	404181	5.0
2,5-Cyclohexadi...	16.770	1.6	ug/L	126698	3	11.816	404181	5.0