LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100120\
Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

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\SOMUTR092920WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.366	3	8	17	rVB3	33801	33613	4.45%	0.503%
2	1.450	28	34	38	rBV2	7998	8179	1.08%	0.122%
3	1.495	38	48	74	rBV	105344	404602	53.59%	6.051%
4	1.604	77	82	95	rVB3	52220	79864	10.58%	1.194%
5	1.922	175	181	199	rVB	43926	61712	8.17%	0.923%
6	2.581	374	386	401	rBV	77095	127146	16.84%	1.901%
7	2.658	401	410	433	rVB3	4341	12327	1.63%	0.184%
8	3.099	521	547	565	rVB2	56625	139691	18.50%	2.089%
9	3.379	617	634	655	rBV	115071	254699	33.73%	3.809%
10	3.720	721	740	759	rBV	178828	396964	52.57%	5.937%
11	4.314	909	925	944	rBV3	12383	32213	4.27%	0.482%
12	4.459	953	970	983	rBV5	10086	27517	3.64%	0.412%
13	4.552	983	999	1016	rVB2	63862	151494	20.06%	2.266%
14	4.658	1016	1032	1073	rBV	96015	322149	42.67%	4.818%
15	4.829	1073	1085	1100	rVB2	10254	24077	3.19%	0.360%
16	5.083	1148	1164	1180	rBV2	90233	196219	25.99%	2.934%
17	5.404	1251	1264	1278	rBV8	6680	15107	2.00%	0.226%
18	5.742	1349	1369	1399	rVB2	165070	439853	58.26%	6.578%
19	6.263	1516	1531	1548	rBV	200961	382905	50.71%	5.726%
20	6.703	1655	1668	1684	rBV2	115989	224110	29.68%	3.352%
21	7.575	1924	1939	1955	rBV2	54287	95555	12.66%	1.429%
22	7.906	2029	2042	2055	rBV	182065	311457	41.25%	4.658%
23	7.973	2055	2063	2076	rVB	13338	22653	3.00%	0.339%
24	8.186	2117	2129	2146	rBV	35418	61948	8.20%	0.926%
25	8.639	2256	2270	2299	rBV	409986	755047	100.00%	11.292%
26	9.420	2500	2513	2540	rBV	285191	502645	66.57%	7.517%
27	9.694	2585	2598	2610	rVB2	10041	16636	2.20%	0.249%
28	10.099	2716	2724	2734	rBV3	6495	10029	1.33%	0.150%
29	10.755	2915	2928	2940	rBV	104029	167576	22.19%	2.506%
30	10.903	2962	2974	2986	rVB	16088	24474	3.24%	0.366%
31	10.993	2991	3002	3022	rVV	51439	110550	14.64%	1.653%
32	11.086	3022	3031	3041	rVB2	18029	27329	3.62%	0.409%
33	11.227	3066	3075	3085	rBV2	24230	37931	5.02%	0.567%
34	11.288	3085	3094	3103	rVB2	26092	39386	5.22%	0.589%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100120\
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Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

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\SOMUTR092920WMA.M
Title : TRACE VOA SOM01.0

35	11.462	3137	3148	3161	rBV	56222	86984	11.52%	1.301%
36	11.806	3241	3255	3270	rBV	306605	483508	64.04%	7.231%
37	11.890	3270	3281	3293	rVV	22608	34128	4.52%	0.510%
38	12.089	3334	3343	3348	rBV3	11073	16899	2.24%	0.253%
39	12.185	3361	3373	3387	rVB	242732	397457	52.64%	5.944%
40	12.459	3449	3458	3462	rBV2	5960	8384	1.11%	0.125%
41	12.491	3462	3468	3481	rVV2	5548	8130	1.08%	0.122%
42	12.562	3481	3490	3500	rVV2	11597	16525	2.19%	0.247%
43	12.877	3577	3588	3595	rBV7	6446	10403	1.38%	0.156%
44	12.964	3607	3615	3623	rBV2	6733	9152	1.21%	0.137%
45	13.018	3624	3632	3641	rVB	7101	10763	1.43%	0.161%
46	13.446	3757	3765	3779	rVB8	7875	14760	1.95%	0.221%
47	13.828	3874	3884	3897	rBV3	30331	46860	6.21%	0.701%
48	14.076	3949	3961	3971	rBV	8690	13805	1.83%	0.206%
49	14.317	4028	4036	4046	rVB4	7976	11329	1.50%	0.169%

Sum of corrected areas: 6686744

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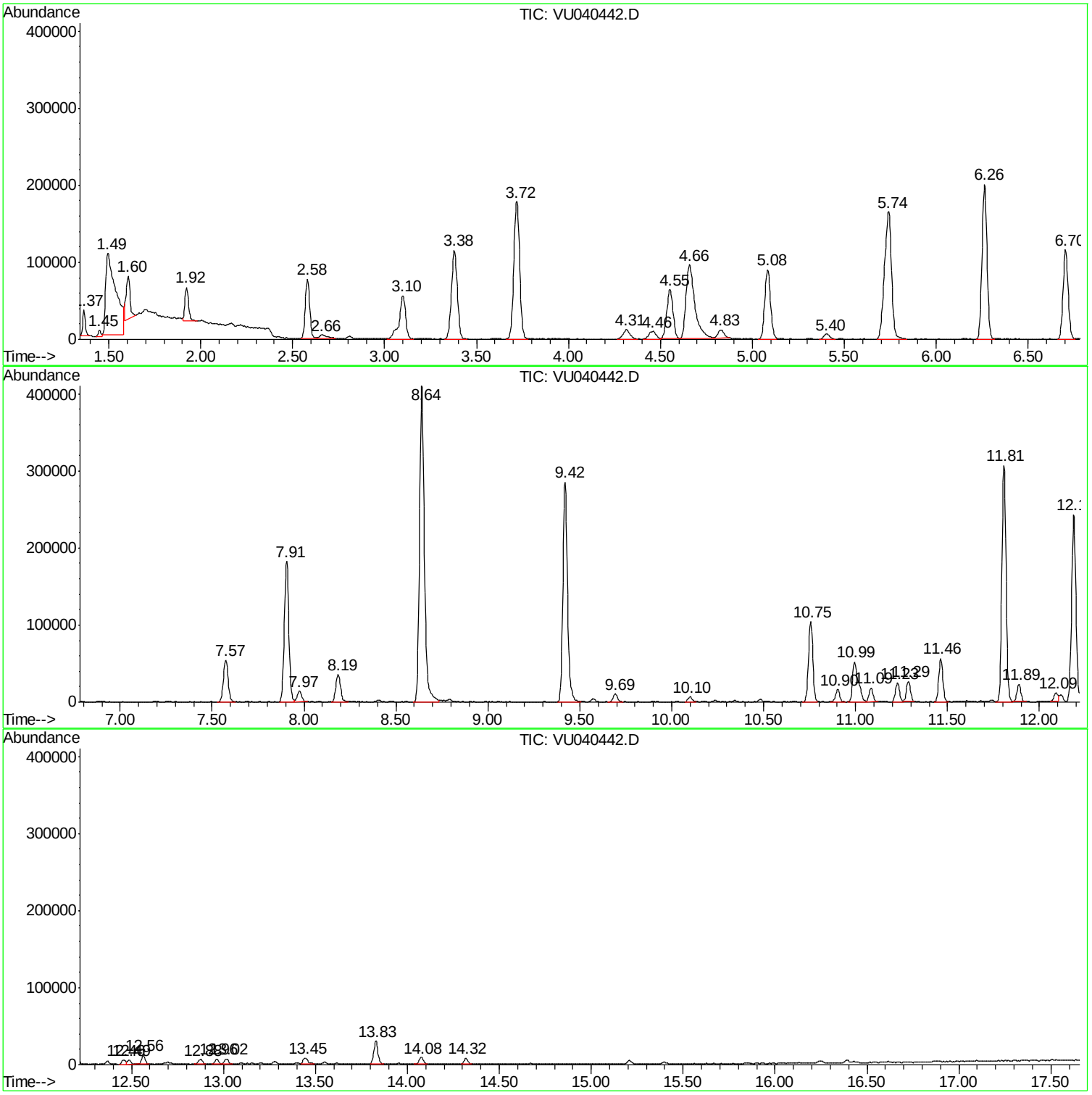
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100120\
Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

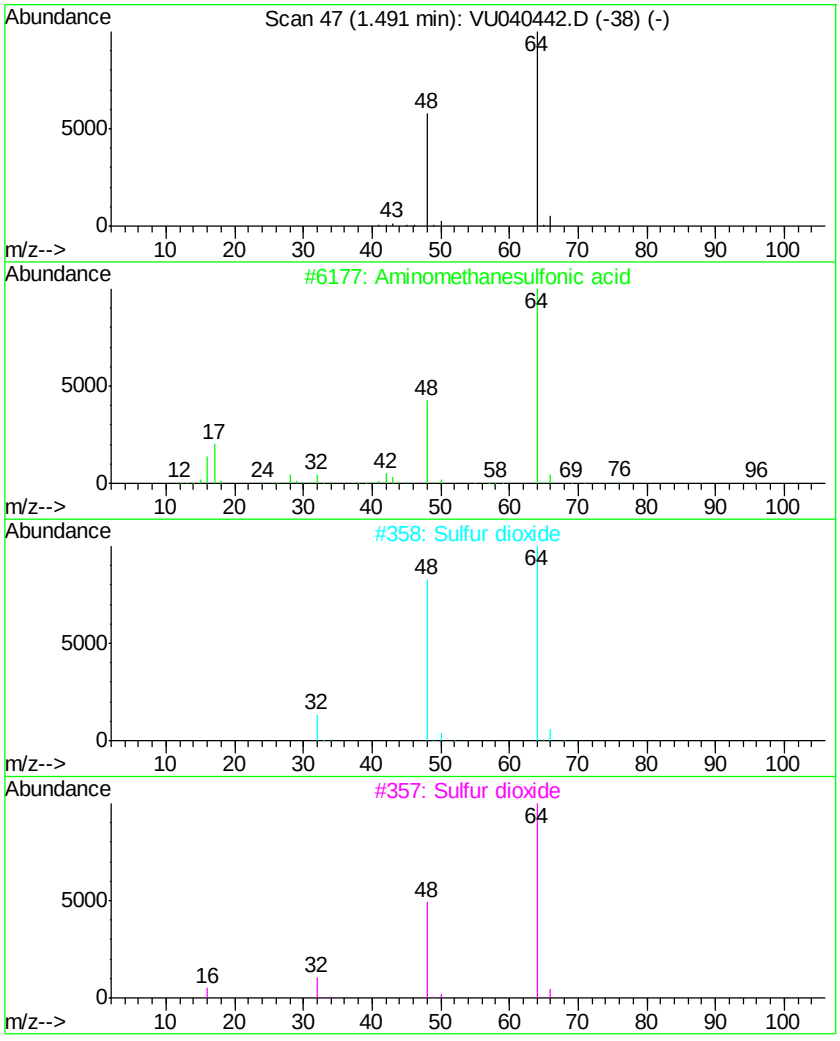
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

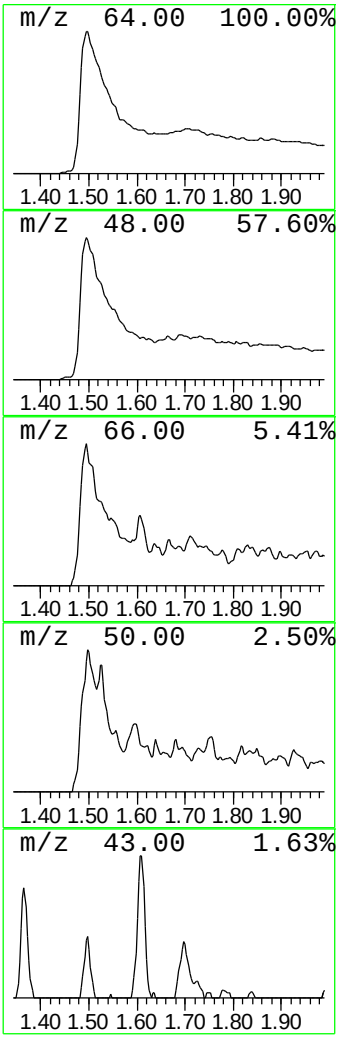
****

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	5.28 ug/L	404602	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	83
3	Sulfur dioxide	64	O2S	007446-09-5	83
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100120\
Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

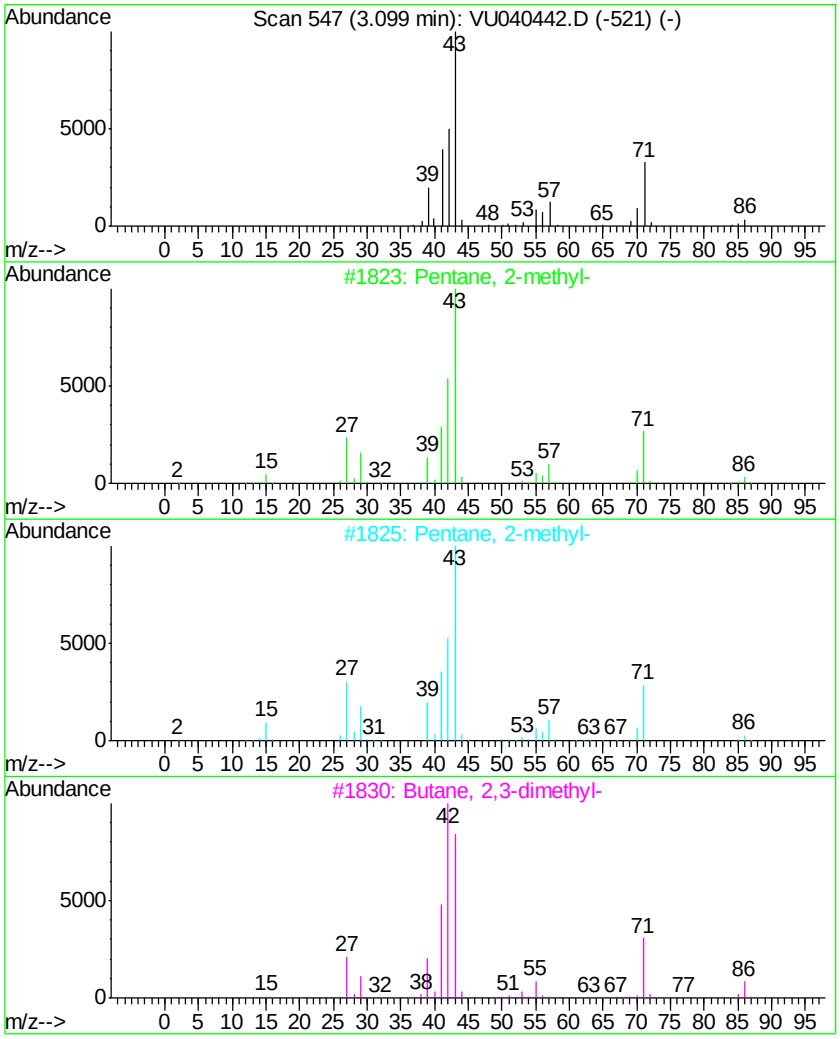
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

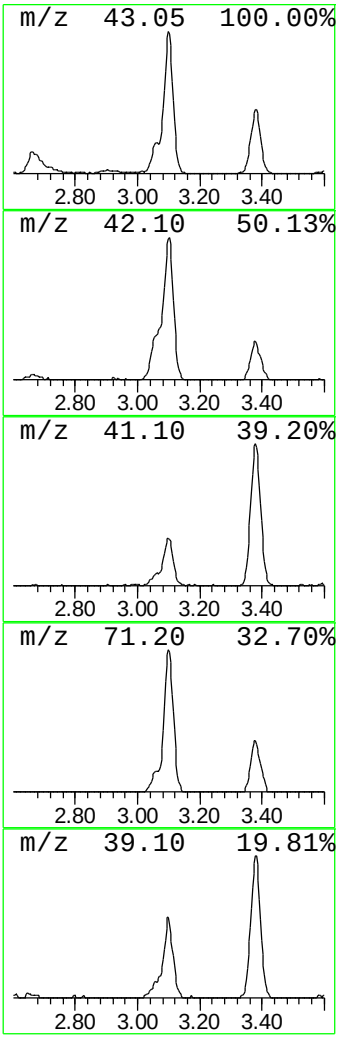
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	1.82 ug/L	139691	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100120\
Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

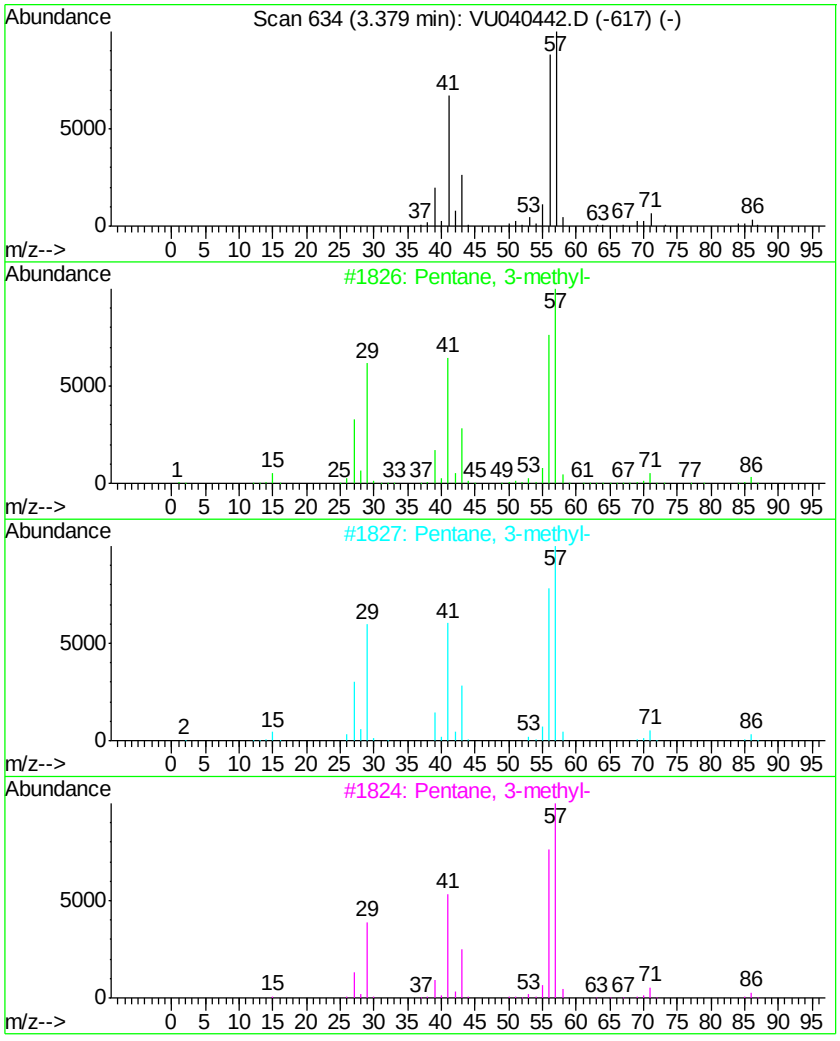
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

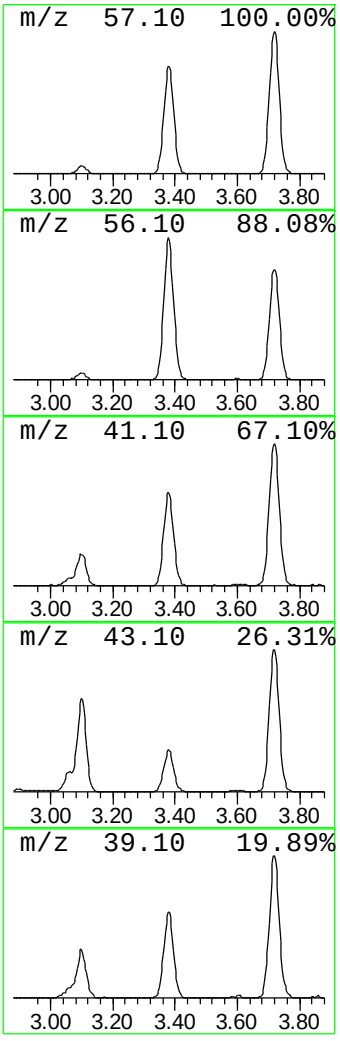
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	3.33 ug/L	254699	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
3	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	83
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100120\
Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

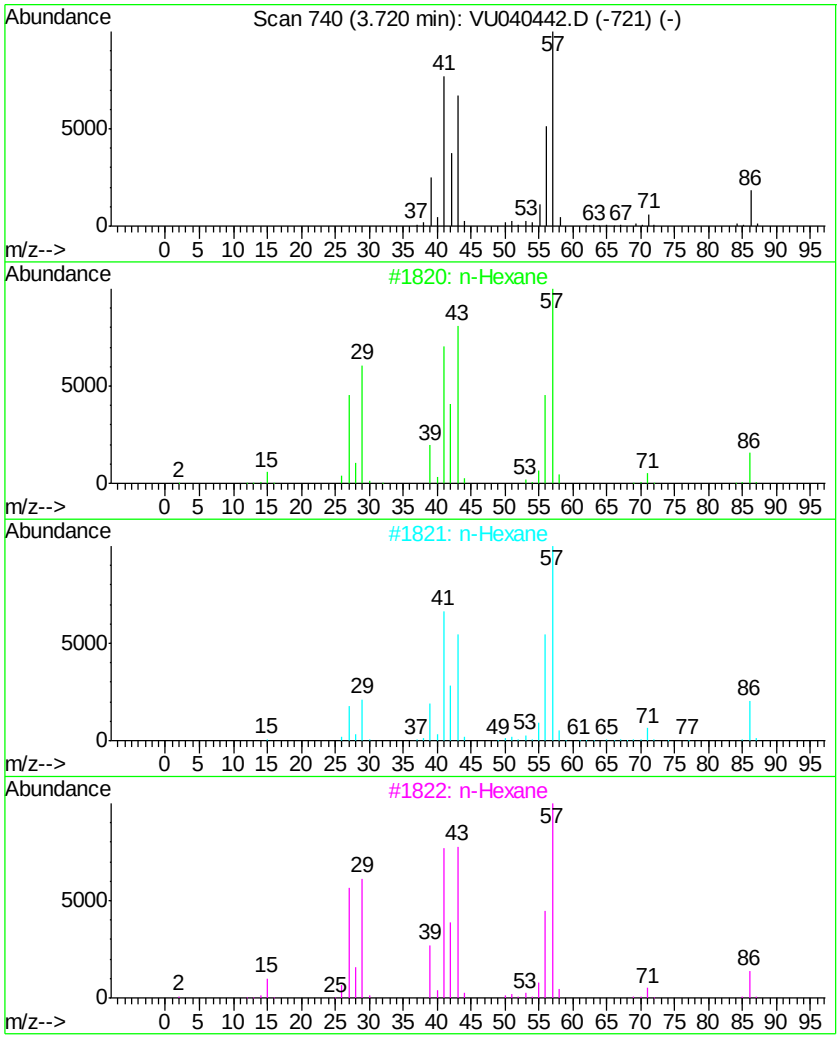
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

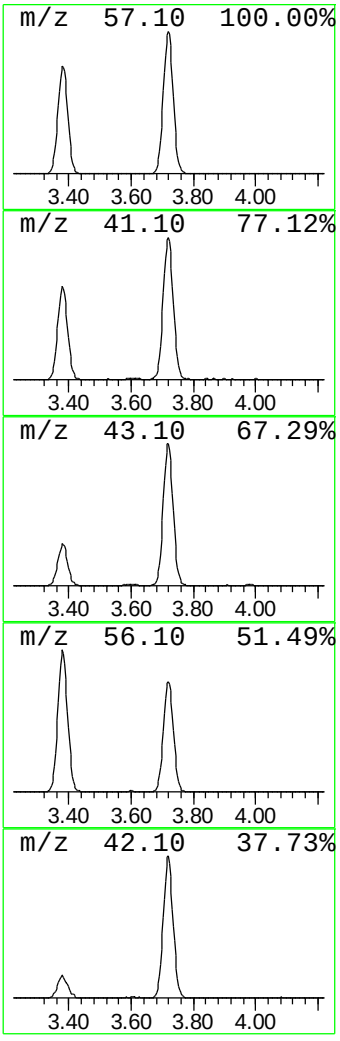
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	5.18 ug/L	396964	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	n-Hexane	86	C6H14	000110-54-3	87
3	n-Hexane	86	C6H14	000110-54-3	78
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	47
5	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38





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Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

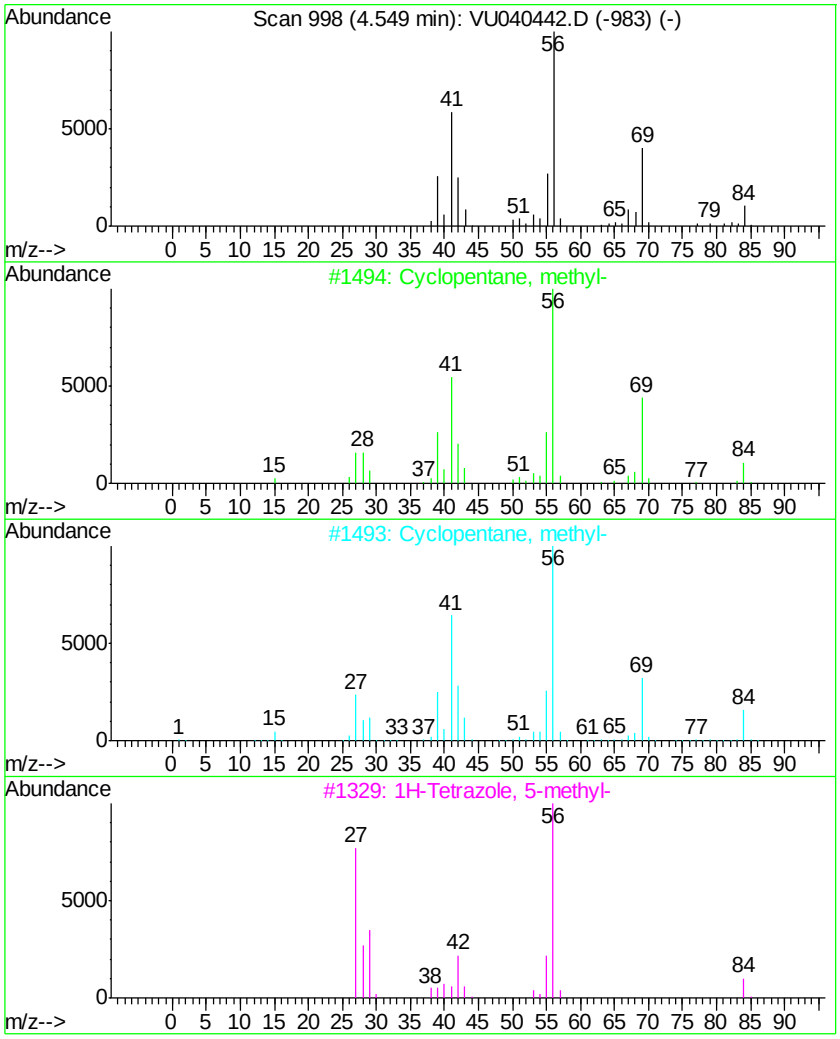
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

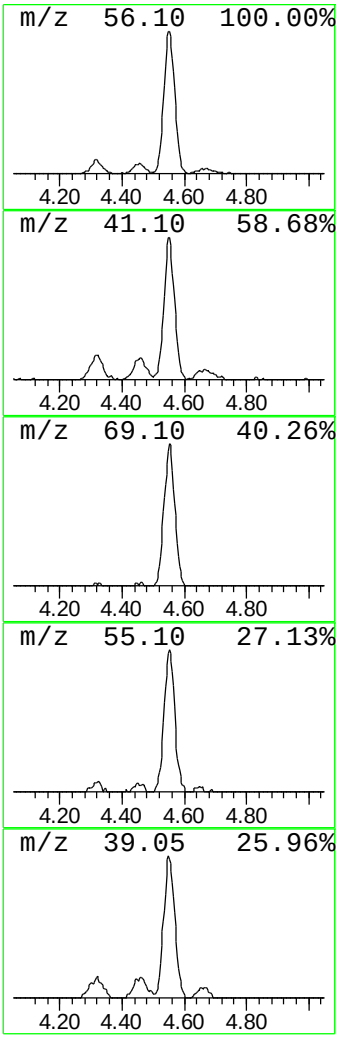
****

Peak Number 5 (DEL) Alkane: Cyclic4.55 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	1.98 ug/L	151494	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclohexane	84	C6H12	000110-82-7	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64





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Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

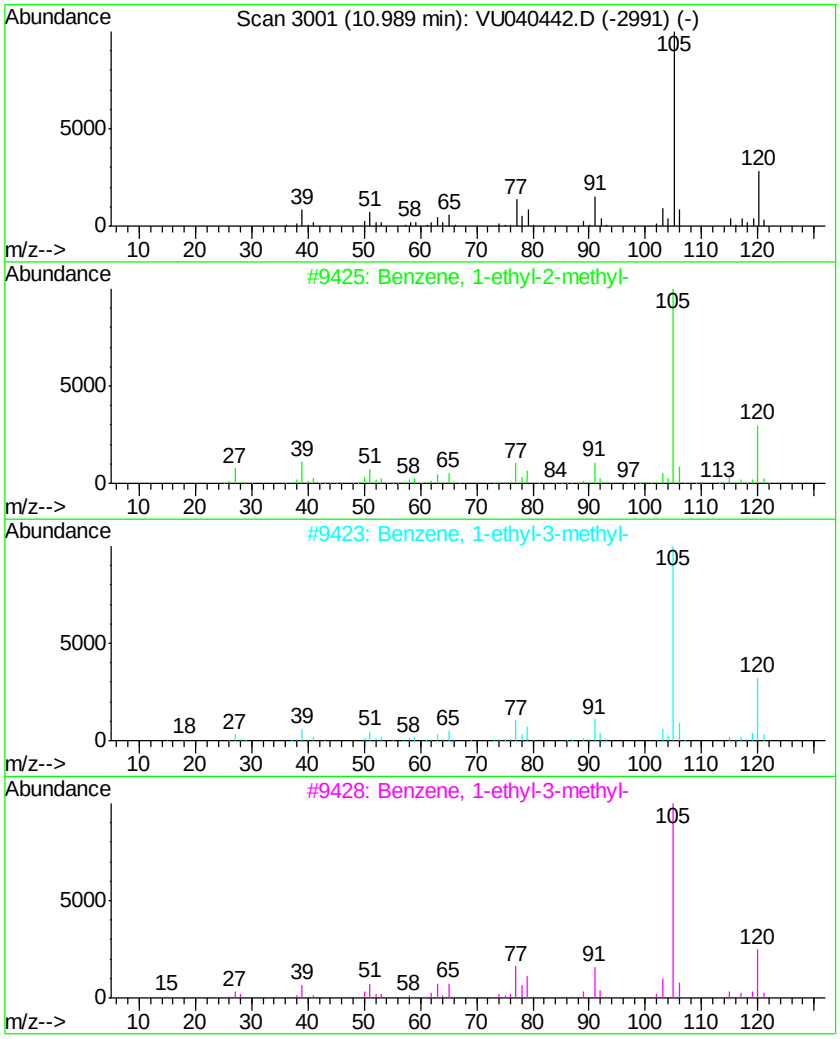
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

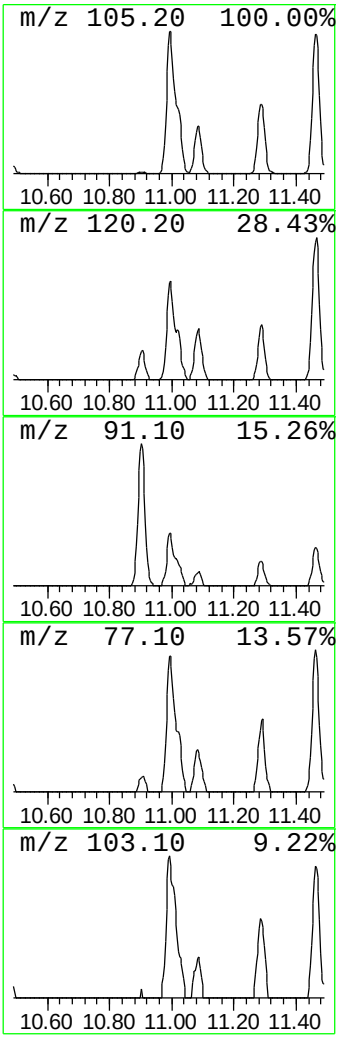
****

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	1.14 ug/L	110550	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Library Search Compound Report

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ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

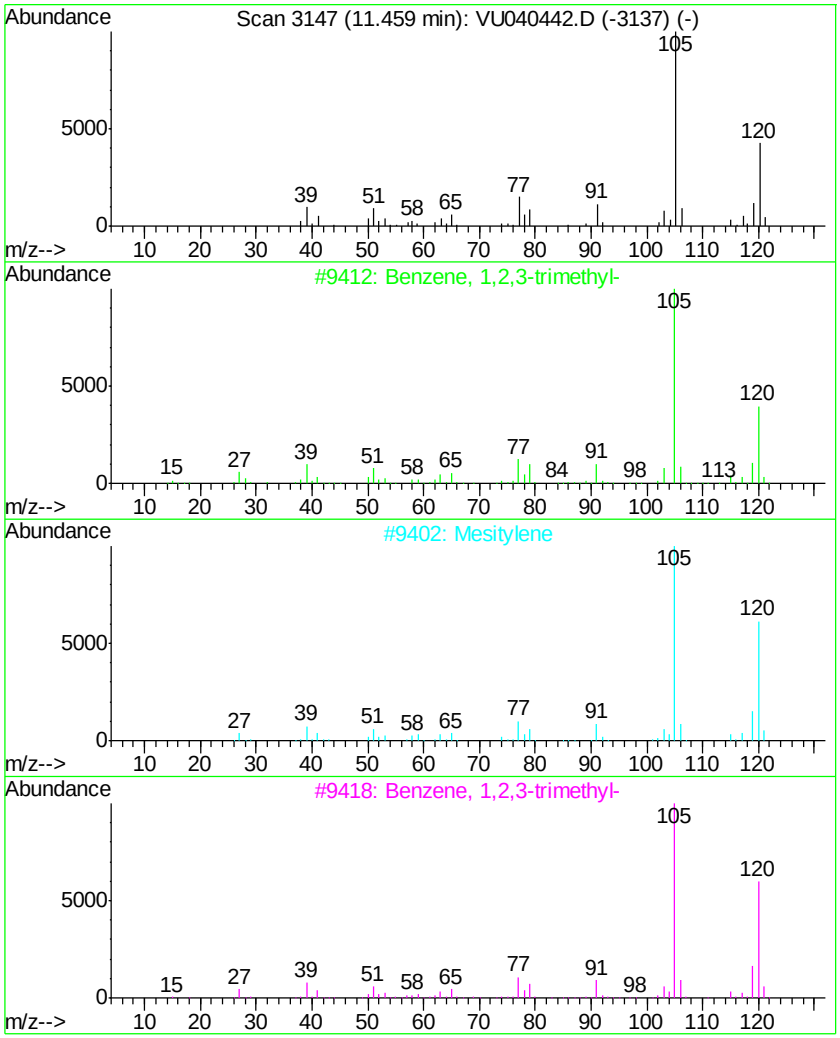
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

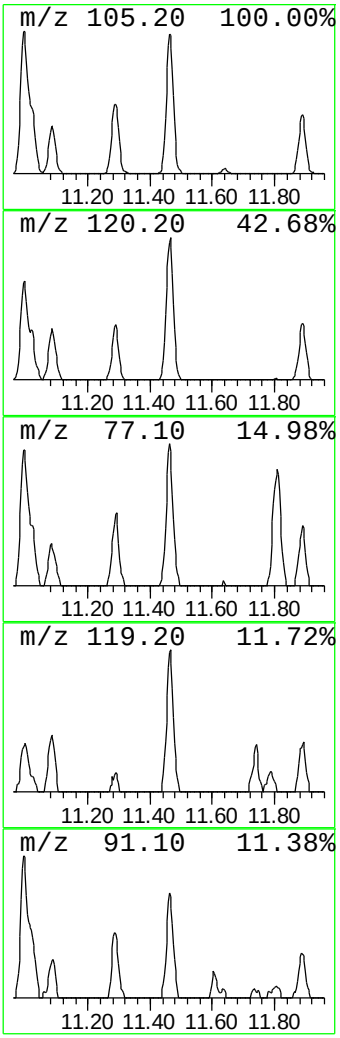
****

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	0.90 ug/L	86984	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100120\
Data File : VU040442.D
Acq On : 02 Oct 2020 00:10
Operator : SY/MD
Sample : L4240-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BG3T3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Aminomethanesulfo...	1.49	5.3	ug/L	404602	1	6.26	382905	5.0
(DEL) Alkane: Str...	3.10	1.8	ug/L	139691	1	6.26	382905	5.0
(DEL) Alkane: Str...	3.38	3.3	ug/L	254699	1	6.26	382905	5.0
(DEL) Alkane: Str...	3.72	5.2	ug/L	396964	1	6.26	382905	5.0
(DEL) Alkane: Cyc...	4.55	2.0	ug/L	151494	1	6.26	382905	5.0
Benzene, 1-ethyl-...	10.99	1.1	ug/L	110550	3	11.81	483508	5.0
Benzene, 1,2,3-tr...	11.46	0.9	ug/L	86984	3	11.81	483508	5.0