LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_X\Method\82X061021W.M
Title : SW846 8260

Signal : TIC: VX022678.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	7	10	15	rVB	62748	57213	1.04%	0.407%
2	1.300	27	35	54	rBV	212569	1375168	25.11%	9.774%
3	1.544	73	75	86	rVB	47604	81212	1.48%	0.577%
4	2.300	193	199	208	rVB	90509	143399	2.62%	1.019%
5	2.386	208	213	226	rVB	89983	146295	2.67%	1.040%
6	2.550	228	240	249	rBV	55722	119080	2.17%	0.846%
7	4.239	506	517	535	rBV	51599	142564	2.60%	1.013%
8	4.574	564	572	591	rVB3	18716	58319	1.06%	0.415%
9	5.397	693	707	717	rBV	42418	120572	2.20%	0.857%
10	5.562	722	734	746	rBV2	69671	194885	3.56%	1.385%
11	5.964	788	800	807	rBV2	53601	142999	2.61%	1.016%
12	6.043	807	813	823	rVB	52687	138193	2.52%	0.982%
13	6.647	900	912	922	rBV	27014	74010	1.35%	0.526%
14	6.769	922	932	945	rBV	120708	295848	5.40%	2.103%
15	7.220	998	1006	1015	rBV	33023	76888	1.40%	0.546%
16	7.464	1039	1046	1058	rVB2	38022	80460	1.47%	0.572%
17	8.653	1234	1241	1247	rBV	260314	396614	7.24%	2.819%
18	10.055	1459	1471	1477	rBV	256395	359912	6.57%	2.558%
19	11.000	1620	1626	1636	rBV	4160988	5476796	100.00%	38.927%
20	11.085	1636	1640	1652	rVB	227186	341235	6.23%	2.425%
21	11.975	1781	1786	1790	rBV	200063	238454	4.35%	1.695%
22	12.024	1790	1794	1799	rVB	258211	312640	5.71%	2.222%
23	12.219	1821	1826	1837	rBV	422275	556099	10.15%	3.953%
24	12.579	1879	1885	1892	rBV2	50820	98292	1.79%	0.699%
25	13.420	2018	2023	2027	rBV4	43074	82499	1.51%	0.586%
26	13.756	2073	2078	2085	rBV	1391921	1801760	32.90%	12.806%
27	14.231	2151	2156	2160	rBV4	61319	93600	1.71%	0.665%
28	14.487	2194	2198	2206	rVB5	64995	134537	2.46%	0.956%
29	14.621	2216	2220	2226	rVV2	87117	157669	2.88%	1.121%
30	14.676	2226	2229	2233	rVV	82454	97682	1.78%	0.694%
31	14.761	2240	2243	2245	rBV	63329	66148	1.21%	0.470%
32	14.853	2255	2258	2263	rVB6	52254	67999	1.24%	0.483%
33	15.316	2331	2334	2340	rVB6	48872	84688	1.55%	0.602%
34	15.383	2341	2345	2347	rBV5	49475	68995	1.26%	0.490%
35	16.097	2457	2462	2474	rVB	219509	386503	7.06%	2.747%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_X\Method\82X061021W.M
Title : SW846 8260

Sum of corrected areas: 14069227

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
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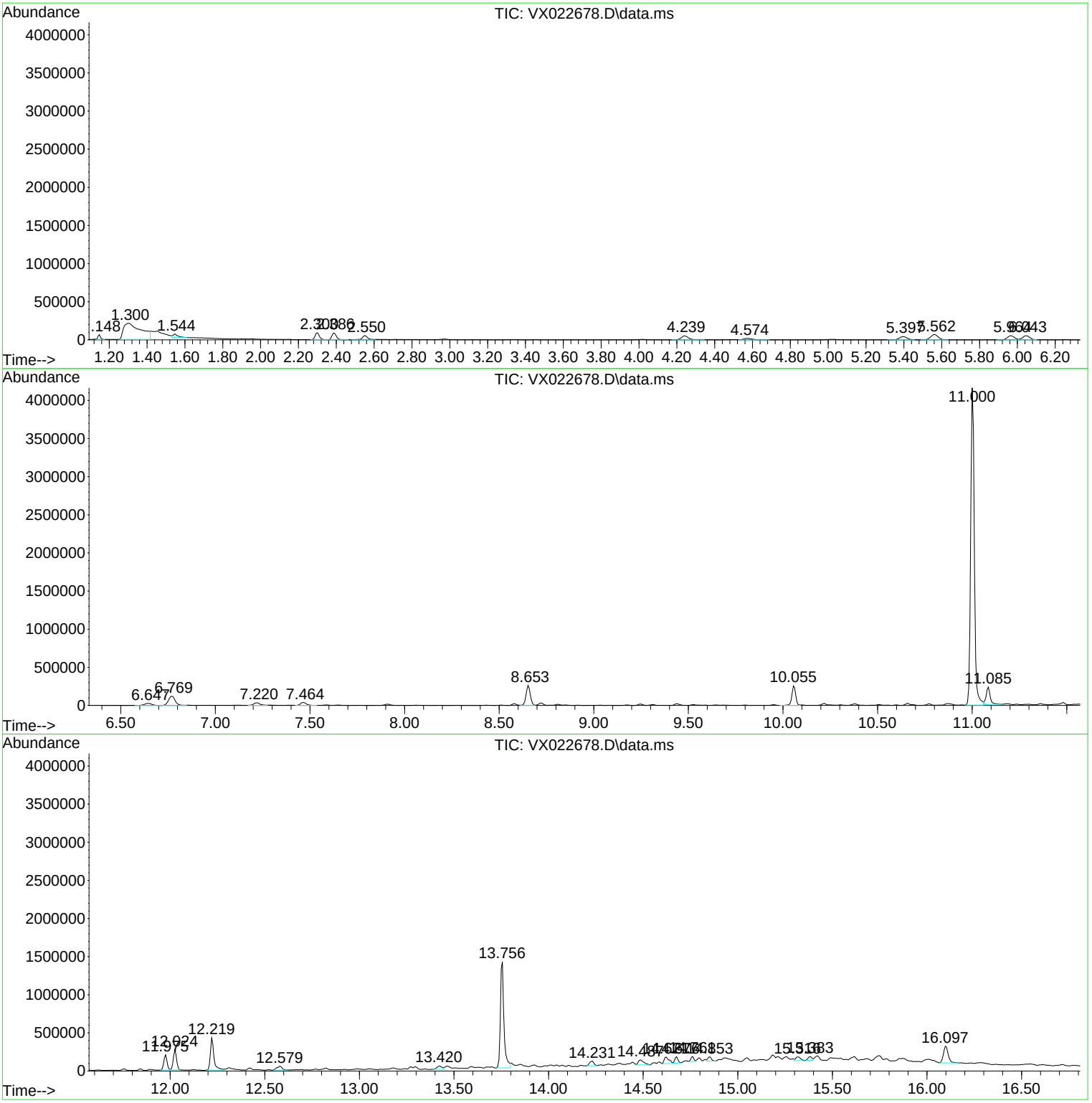
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
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MSVOA_X
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1847

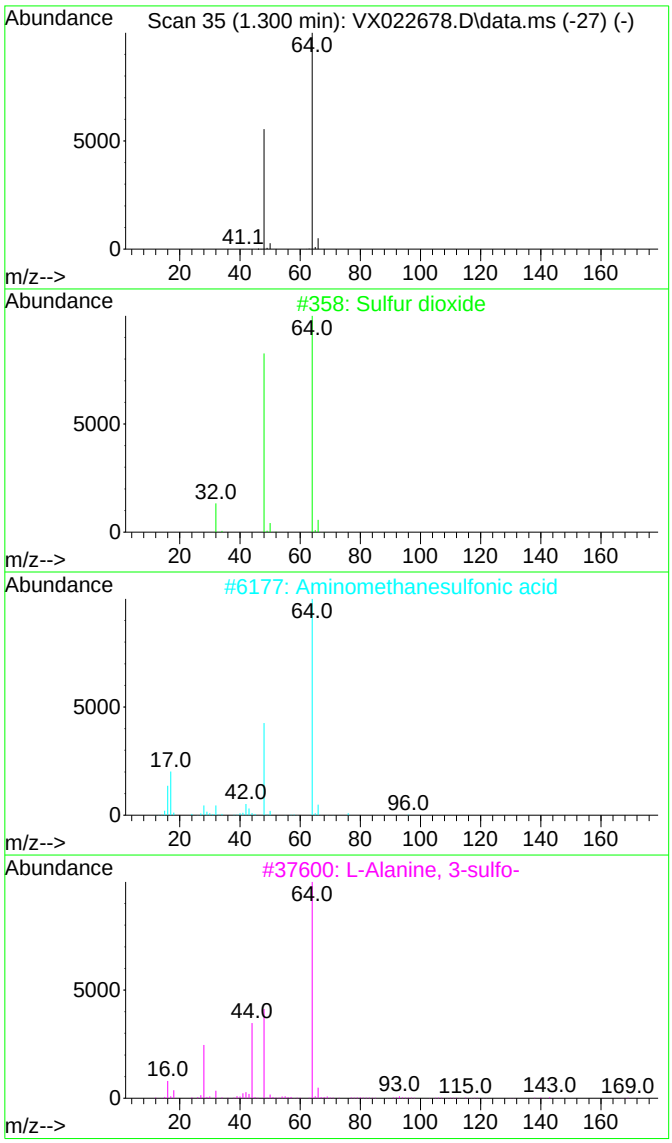
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

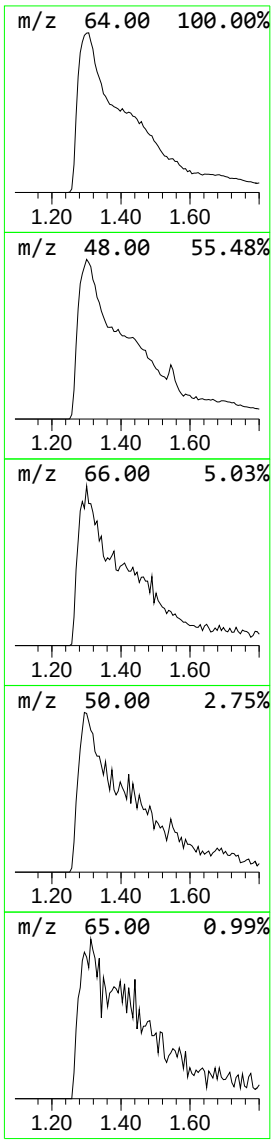
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.300	352.82 ug/l	1375170	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

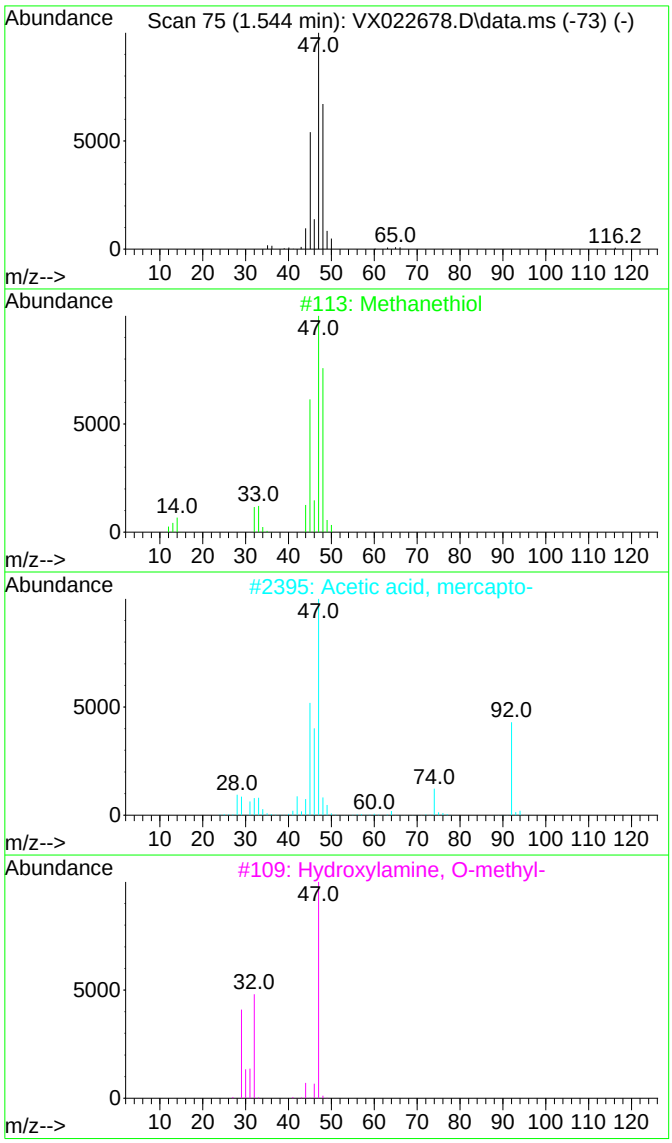
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

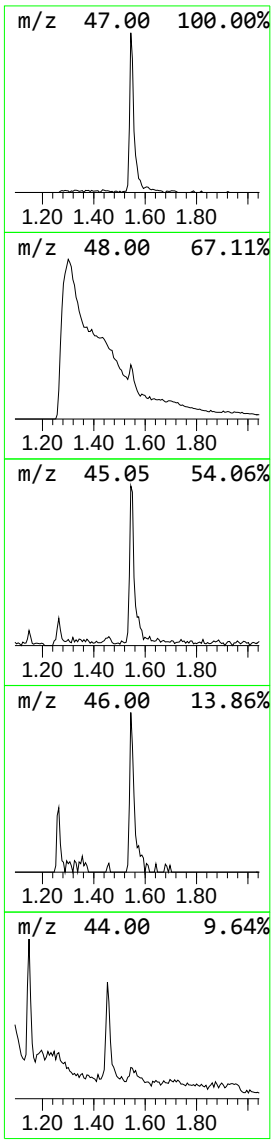
****

Peak Number 2 Methanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.544	20.84 ug/l	81212	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	36
3	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4	Methional	104	C4H8OS	003268-49-3	4
5	Methoxyacetaldehyde diethyl acetal	148	C7H16O3	004819-75-4	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

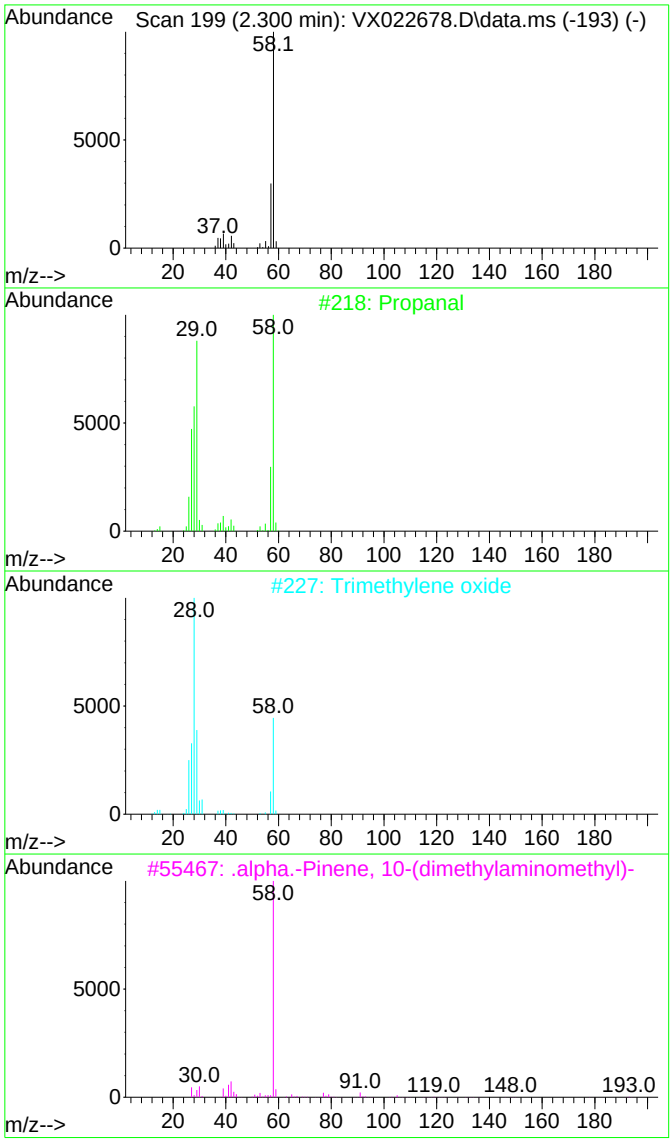
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

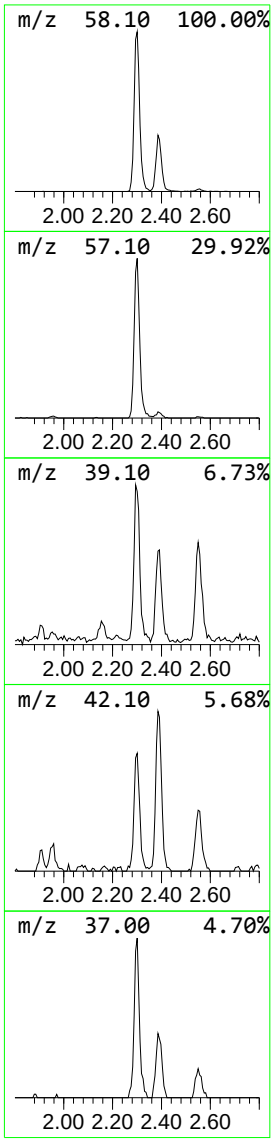
****

Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.300	36.79 ug/l	143399	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

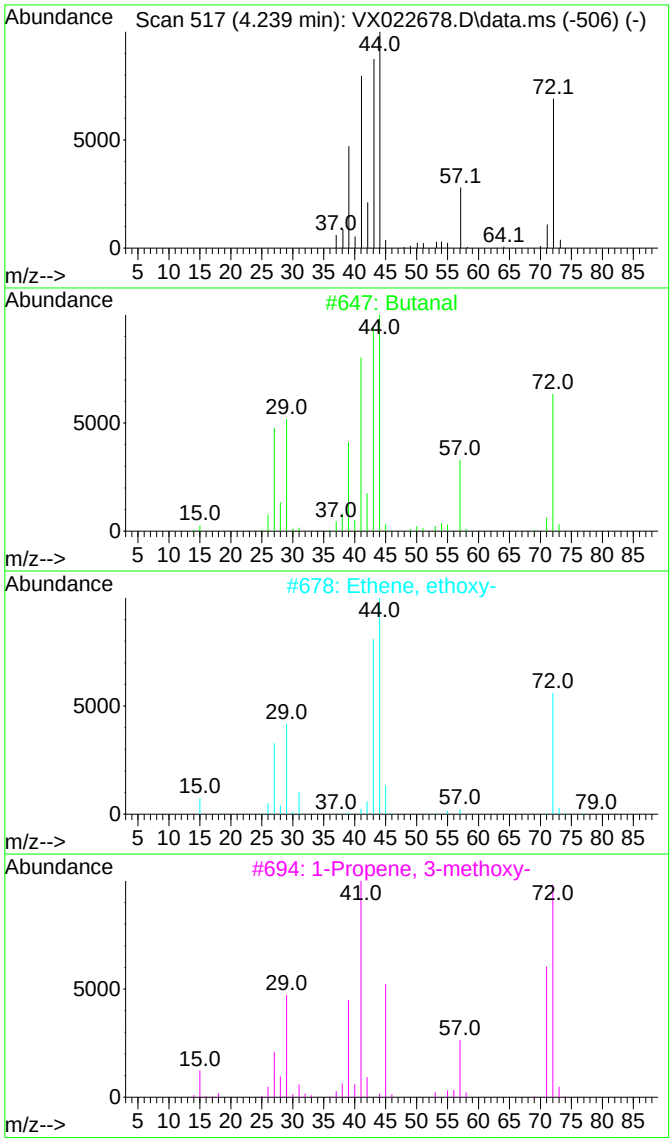
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

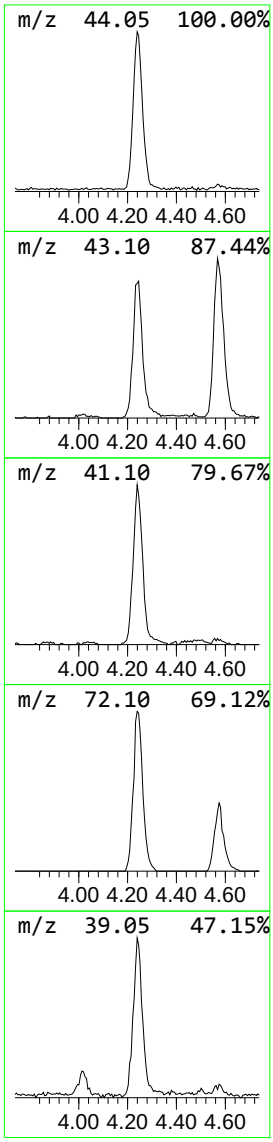
****

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.239	36.58 ug/l	142564	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	30
5	Dimethylketene	70	C4H6O	000598-26-5	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

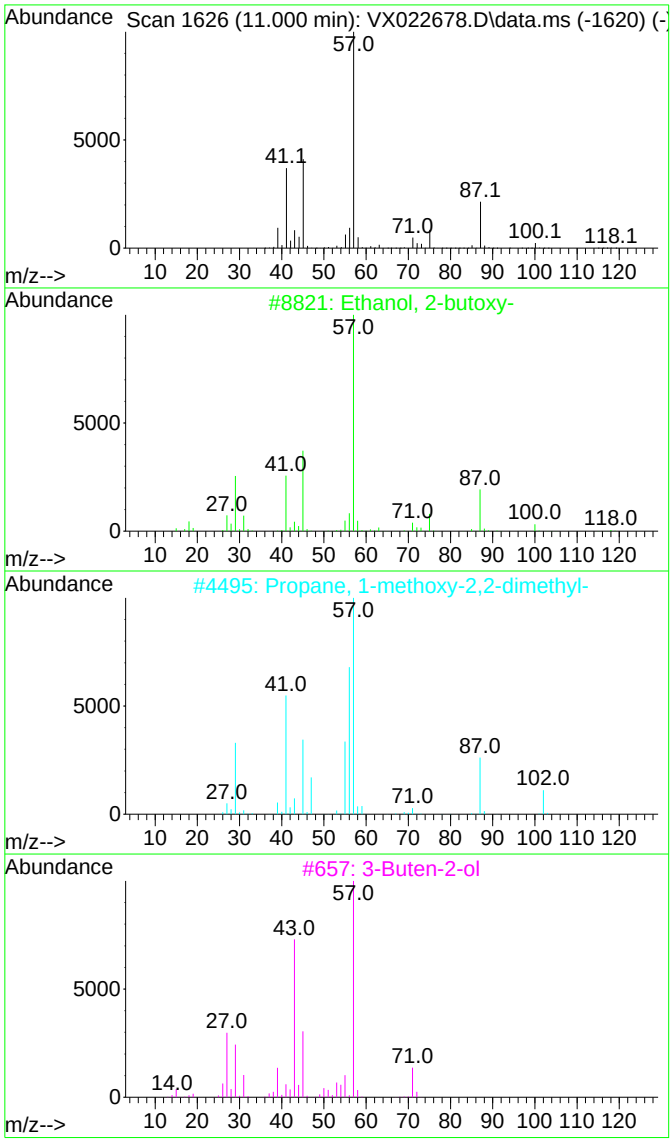
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

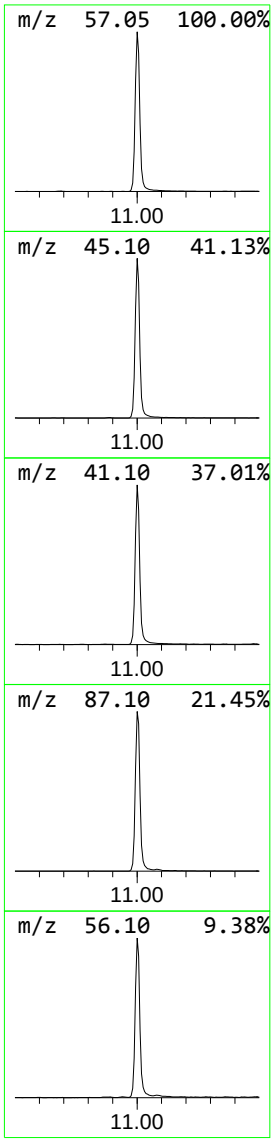
****

Peak Number 5 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.000	760.85 ug/l	5476800	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	52
2	Propane, 1-methoxy-2,2-dimethyl-	102	C6H14O	001118-00-9	50
3	3-Buten-2-ol	72	C4H8O	000598-32-3	43
4	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	32
5	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	25





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Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1847

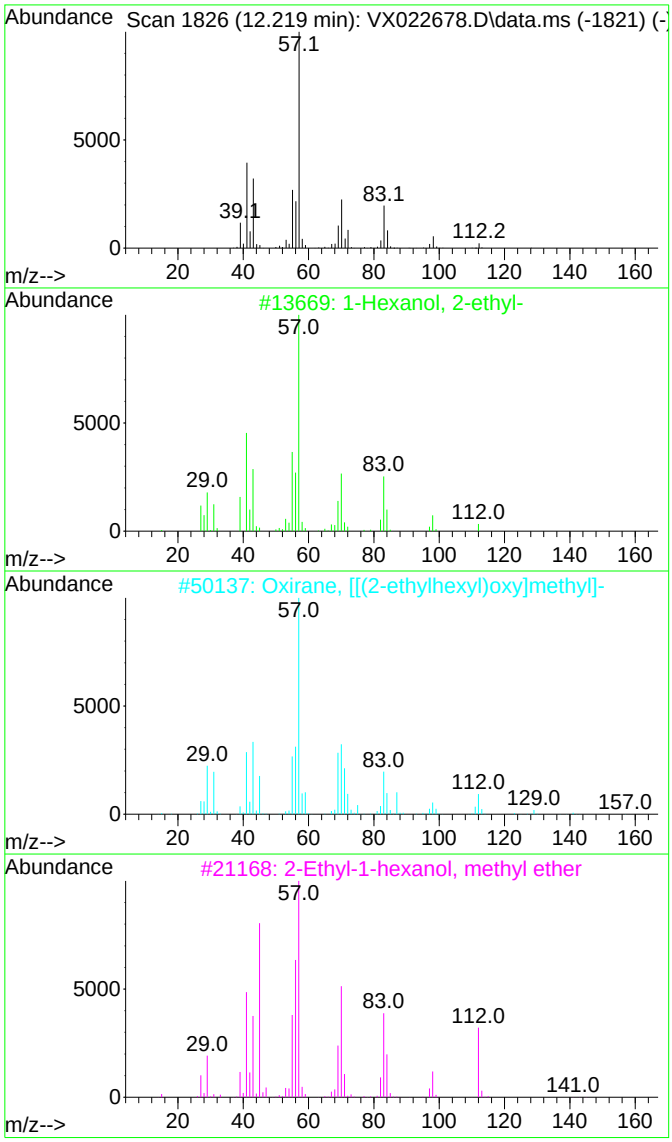
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

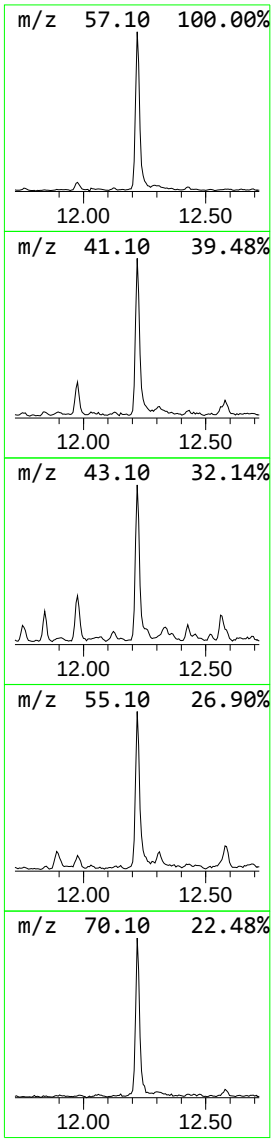
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	88.94 ug/l	556099	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	56
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47





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Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

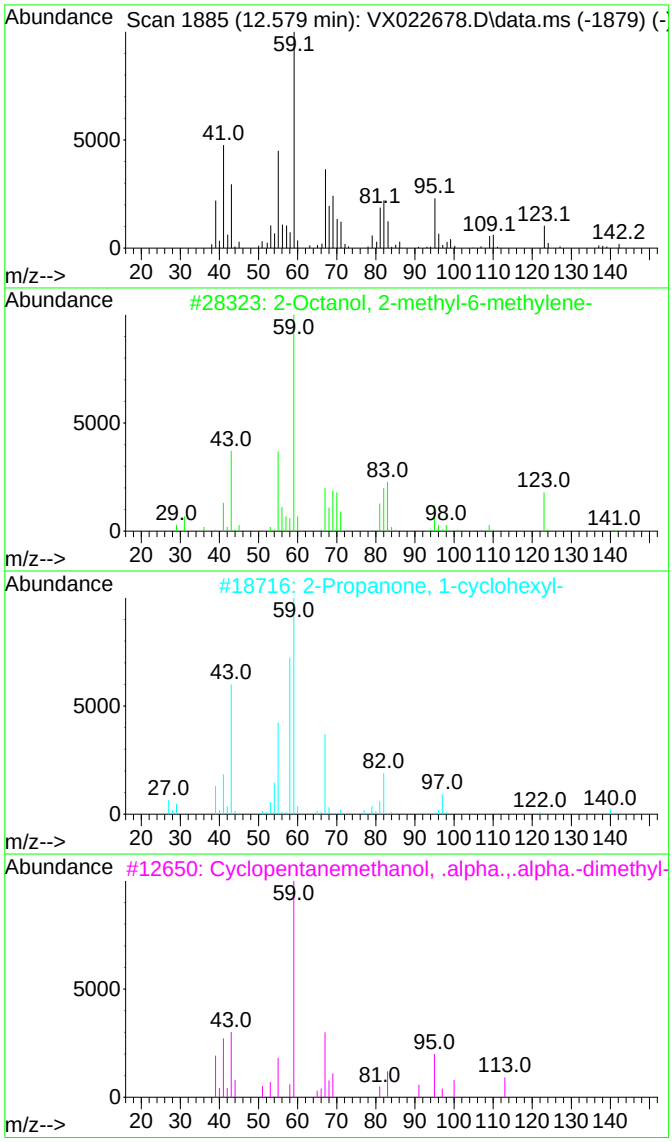
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

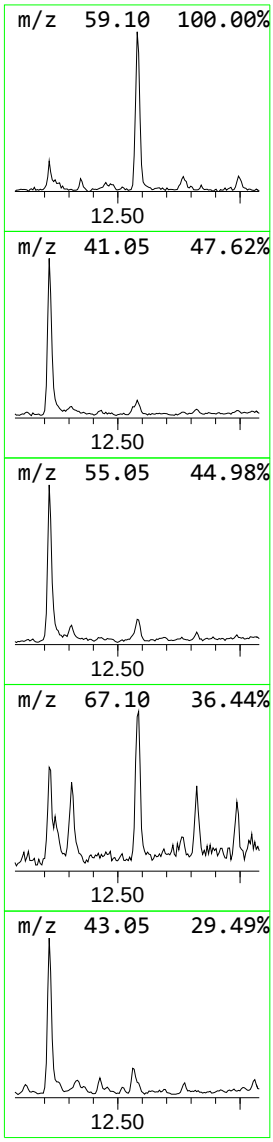
****

Peak Number 7 unknown12.579 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.579	15.72 ug/l	98292	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	45
2	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	40
3	Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	40
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	38
5	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	37





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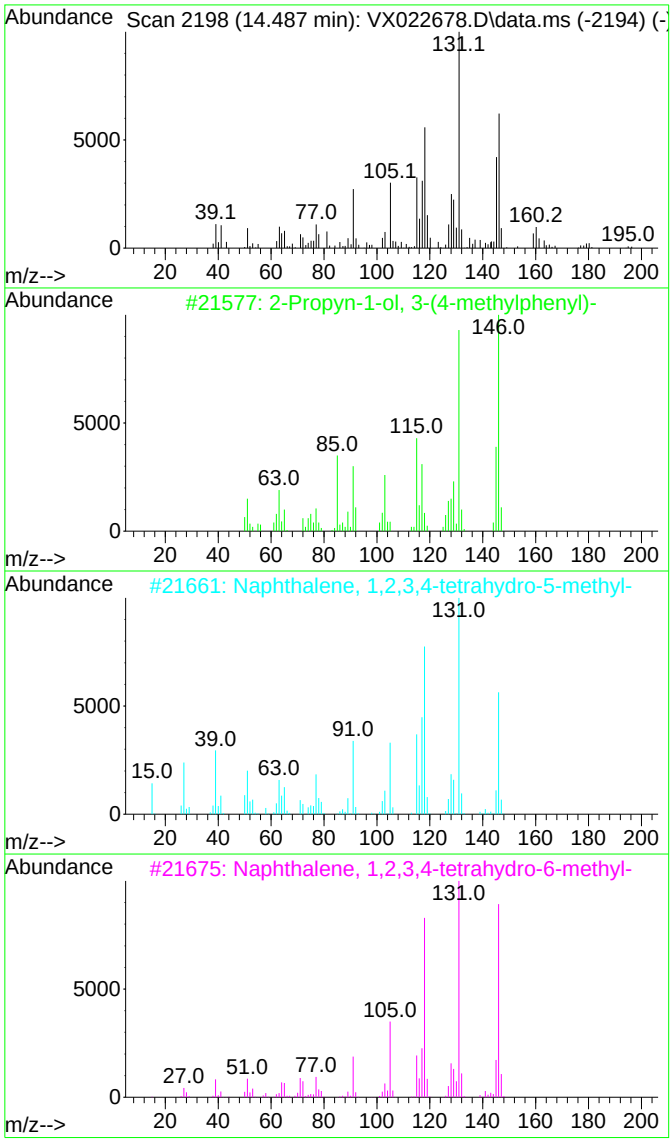
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

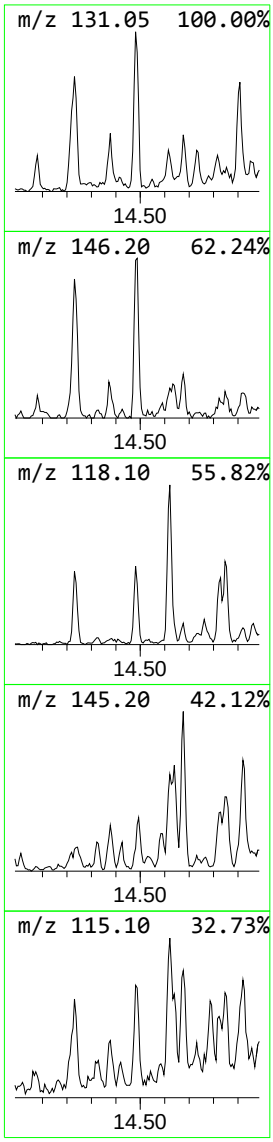
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Propyn-1-ol, 3-(4-methylp... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.487	21.52 ug/l	134537	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	83
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	68
4	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
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Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

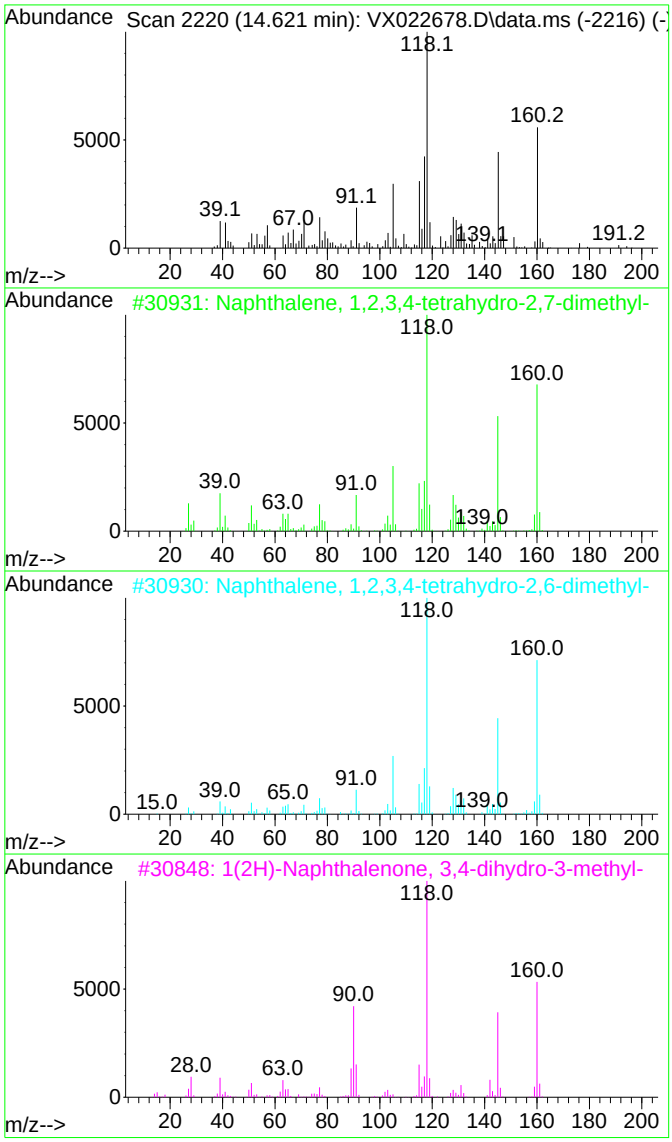
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

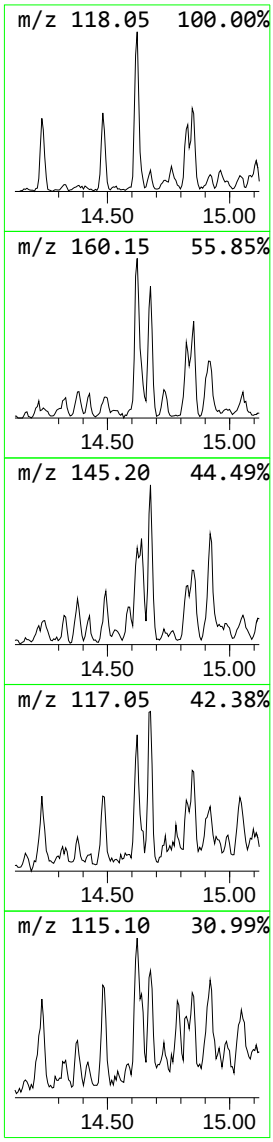
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	25.22 ug/l	157669	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	91
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	76
3	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	62
4	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	58
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1847

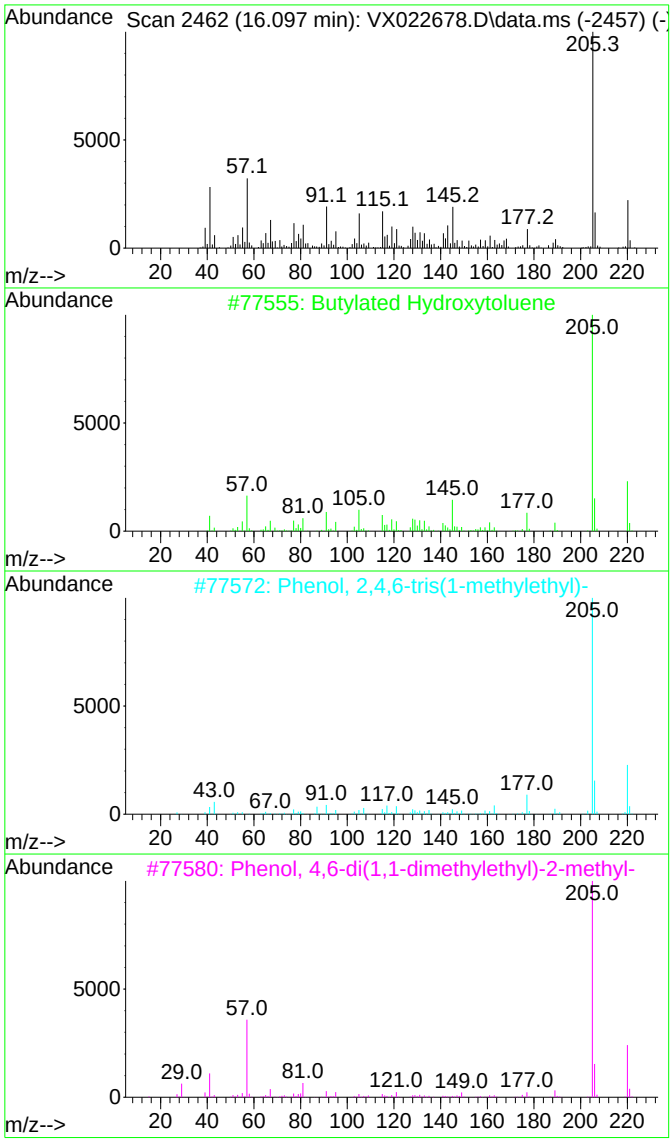
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

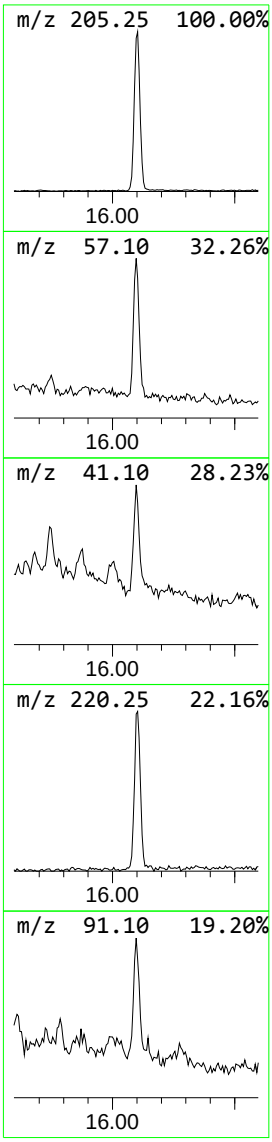
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Butylated Hydroxytoluene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.097	61.81 ug/l	386503	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	70
3	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	62
4	4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	53
5	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022678.D
Acq On : 11 Jun 2021 19:28
Operator : JC/MD
Sample : M2644-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1847

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.300	352.8	ug/l	1375170	1	5.562	194885	50.0
Methanethiol	1.544	20.8	ug/l	81212	1	5.562	194885	50.0
Propanal	2.300	36.8	ug/l	143399	1	5.562	194885	50.0
Butanal	4.239	36.6	ug/l	142564	1	5.562	194885	50.0
Ethanol, 2-butoxy-	11.000	760.9	ug/l	5476800	3	10.055	359912	50.0
1-Hexanol, 2-et...	12.219	88.9	ug/l	556099	4	12.024	312640	50.0
unknown12.579	12.579	15.7	ug/l	98292	4	12.024	312640	50.0
2-Propyn-1-ol, ...	14.487	21.5	ug/l	134537	4	12.024	312640	50.0
Naphthalene, 1,...	14.621	25.2	ug/l	157669	4	12.024	312640	50.0
Butylated Hydro...	16.097	61.8	ug/l	386503	4	12.024	312640	50.0