LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004128.D
Acq On : 17 Aug 2018 13:29
Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

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\82X081418W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	75	80	93	rBV	1998582	2611898	100.00%	19.904%
2	1.270	109	112	118	rBV	52768	60080	2.30%	0.458%
3	1.489	143	148	158	rVB	194764	242246	9.27%	1.846%
4	1.581	159	163	168	rBV	156218	166159	6.36%	1.266%
5	2.349	283	289	296	rBV	36397	58603	2.24%	0.447%
6	2.434	298	303	308	rVV	71708	125423	4.80%	0.956%
7	2.483	308	311	322	rVV	53256	94438	3.62%	0.720%
8	2.599	322	330	339	rVB2	30145	61147	2.34%	0.466%
9	3.410	457	463	474	rVB	13404	31341	1.20%	0.239%
10	4.343	607	616	626	rBV2	13111	35569	1.36%	0.271%
11	4.696	664	674	686	rBV2	33927	97942	3.75%	0.746%
12	5.178	741	753	766	rBV4	16001	57481	2.20%	0.438%
13	5.507	794	807	821	rBV2	187635	534538	20.47%	4.073%
14	5.666	821	833	850	rVB2	250560	696099	26.65%	5.305%
15	6.068	888	899	914	rBV	203026	531179	20.34%	4.048%
16	6.867	1020	1030	1041	rBV	388971	906965	34.72%	6.912%
17	7.501	1122	1134	1141	rBV	50442	102760	3.93%	0.783%
18	8.110	1226	1234	1245	rVB	11510	26408	1.01%	0.201%
19	8.488	1288	1296	1313	rBV	105064	253137	9.69%	1.929%
20	8.720	1327	1334	1342	rBV	986397	1559562	59.71%	11.885%
21	8.848	1351	1355	1359	rBV5	31440	69957	2.68%	0.533%
22	9.256	1417	1422	1431	rVB	77157	147543	5.65%	1.124%
23	9.336	1431	1435	1440	rVV	32909	48634	1.86%	0.371%
24	9.397	1440	1445	1454	rVB	18818	29494	1.13%	0.225%
25	9.665	1485	1489	1508	rBV	44317	117189	4.49%	0.893%
26	10.061	1548	1554	1558	rBV	137000	321306	12.30%	2.449%
27	10.116	1558	1563	1576	rVB	914332	1316415	50.40%	10.032%
28	10.683	1653	1656	1664	rBV	51977	91962	3.52%	0.701%
29	10.762	1664	1669	1690	rVB	76296	144456	5.53%	1.101%
30	11.140	1725	1731	1745	rBV	877870	1158582	44.36%	8.829%
31	11.719	1821	1826	1832	rBV	32305	42714	1.64%	0.326%
32	12.079	1879	1885	1895	rBV	1058540	1277511	48.91%	9.735%
33	12.469	1943	1949	1956	rBV	18584	29547	1.13%	0.225%
34	13.213	2066	2071	2079	rBV	57883	74094	2.84%	0.565%

LSC Area Percent Report

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Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

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\82X081418W.M
Title : SW846 8260

Sum of corrected areas: 13122379

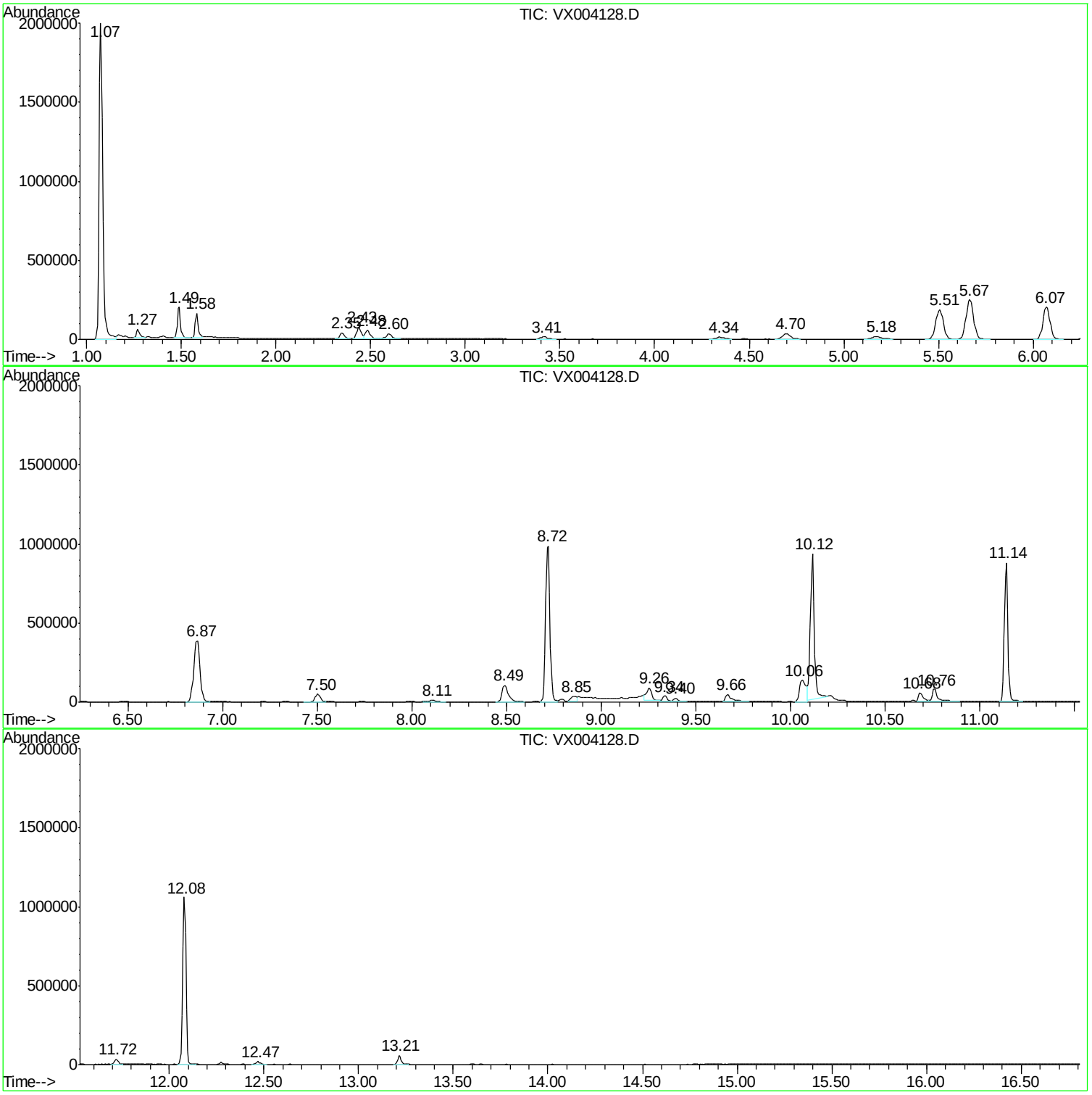
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004128.D
Acq On : 17 Aug 2018 13:29
Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081718\
Data File : VX004128.D
Acq On : 17 Aug 2018 13:29
Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

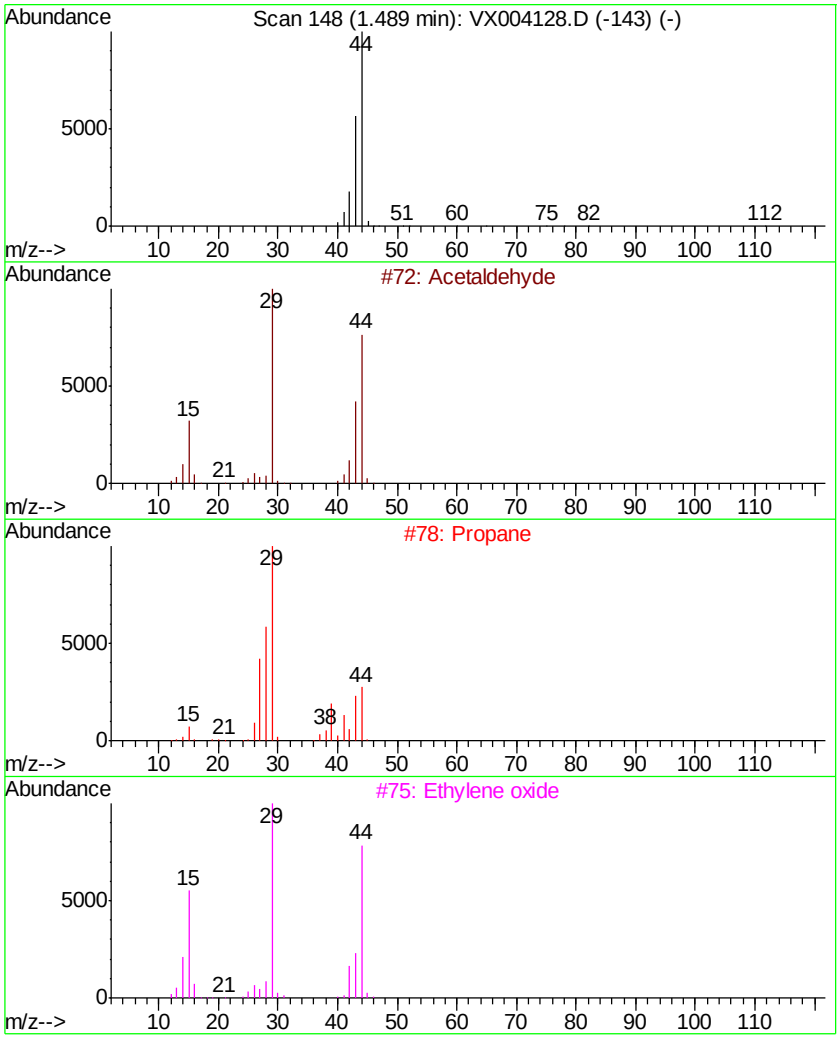
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

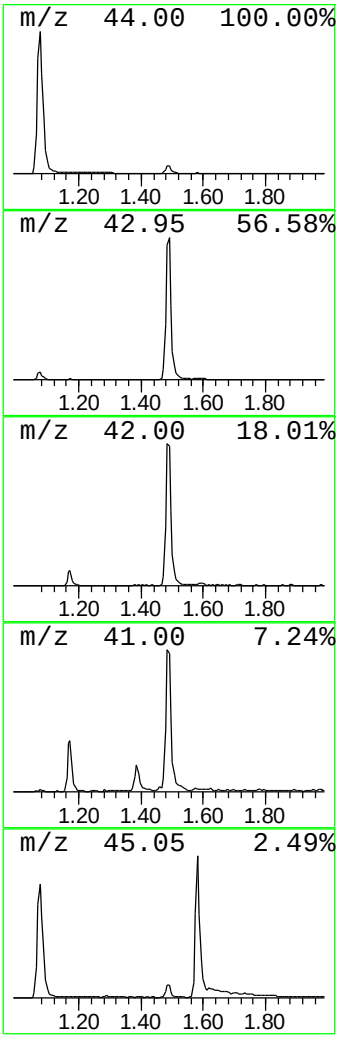
****

Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	17.40 ug/l	242246	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Carbon dioxide	44	CO2	000124-38-9	3





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081718\
Data File : VX004128.D
Acq On : 17 Aug 2018 13:29
Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

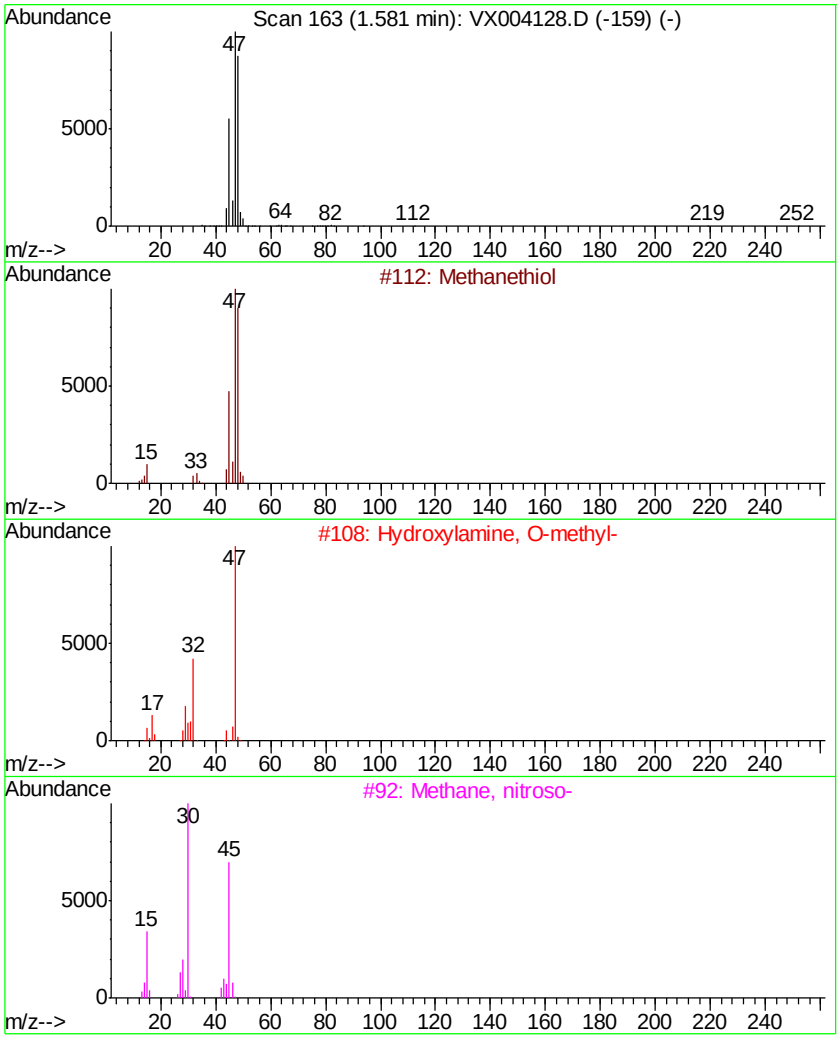
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

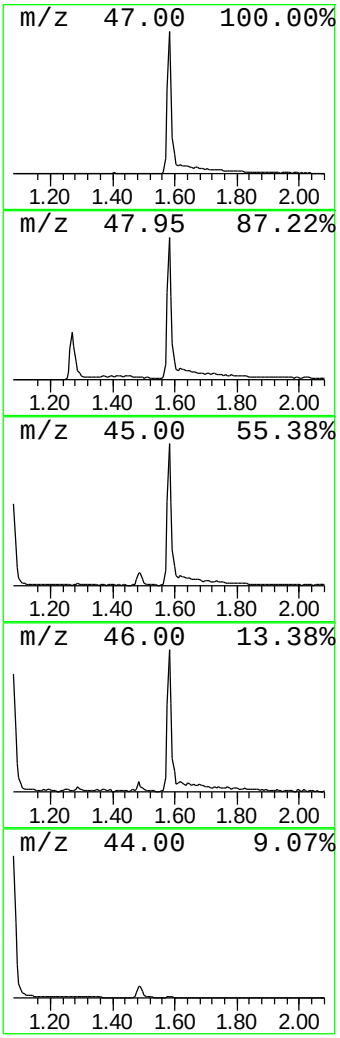
****

Peak Number 3 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.58	11.94 ug/l	166159	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
3	Methane, nitroso-	45	CH3NO	000865-40-7	5
4	Ethane, fluoro-	48	C2H5F	000353-36-6	4
5	Taurine	125	C2H7NO3S	000107-35-7	2





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004128.D
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Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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

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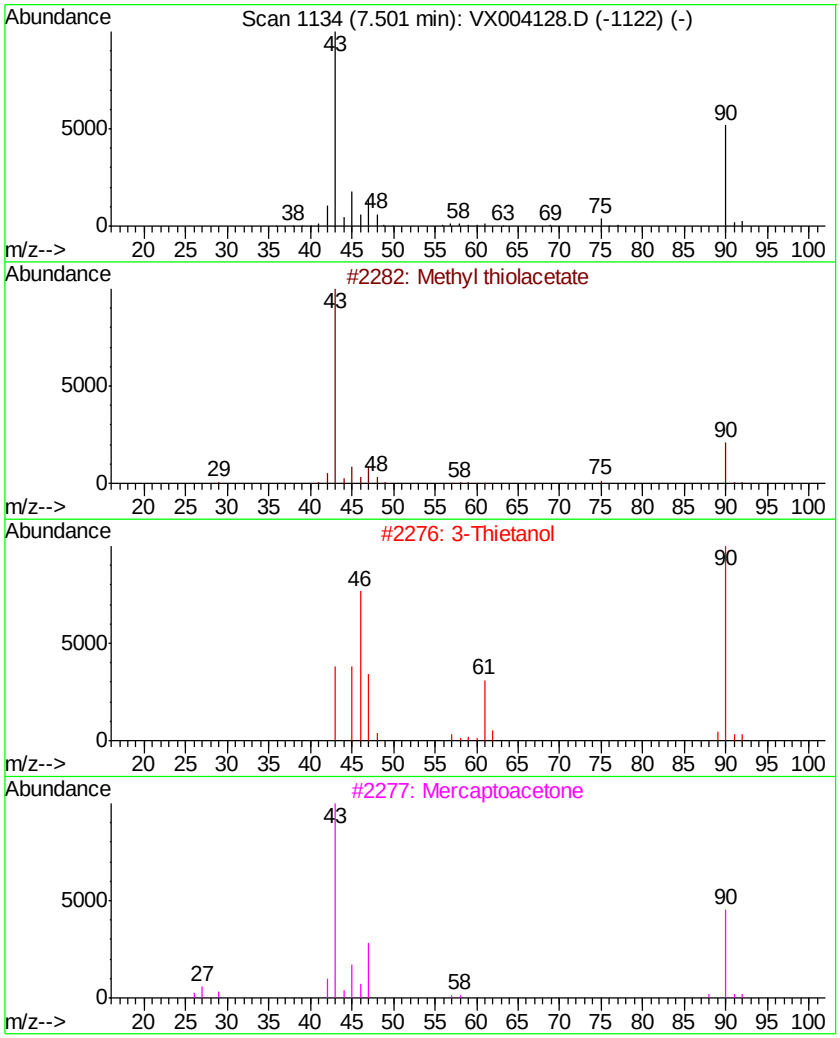
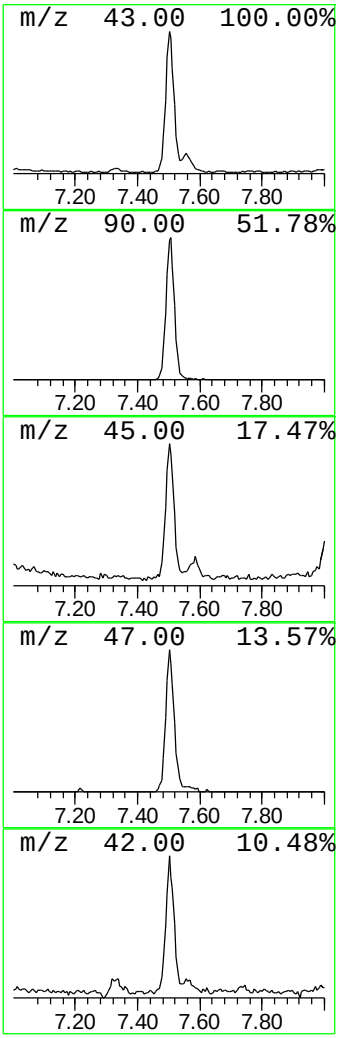
Peak Number 4 Methyl thiolacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	5.67 ug/l	102760	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl thiolacetate	90	C3H6OS	001534-08-3	58
2	3-Thietanol	90	C3H6OS	010304-16-2	50
3	Mercaptoacetone	90	C3H6OS	024653-75-6	42
4	Carbamimidothioic acid, methyl e...	90	C2H6N2S	002986-19-8	42
5	1,3-Oxathiolane	90	C3H6OS	002094-97-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081718\
Data File : VX004128.D
Acq On : 17 Aug 2018 13:29
Operator : JC/MD
Sample : J4520-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

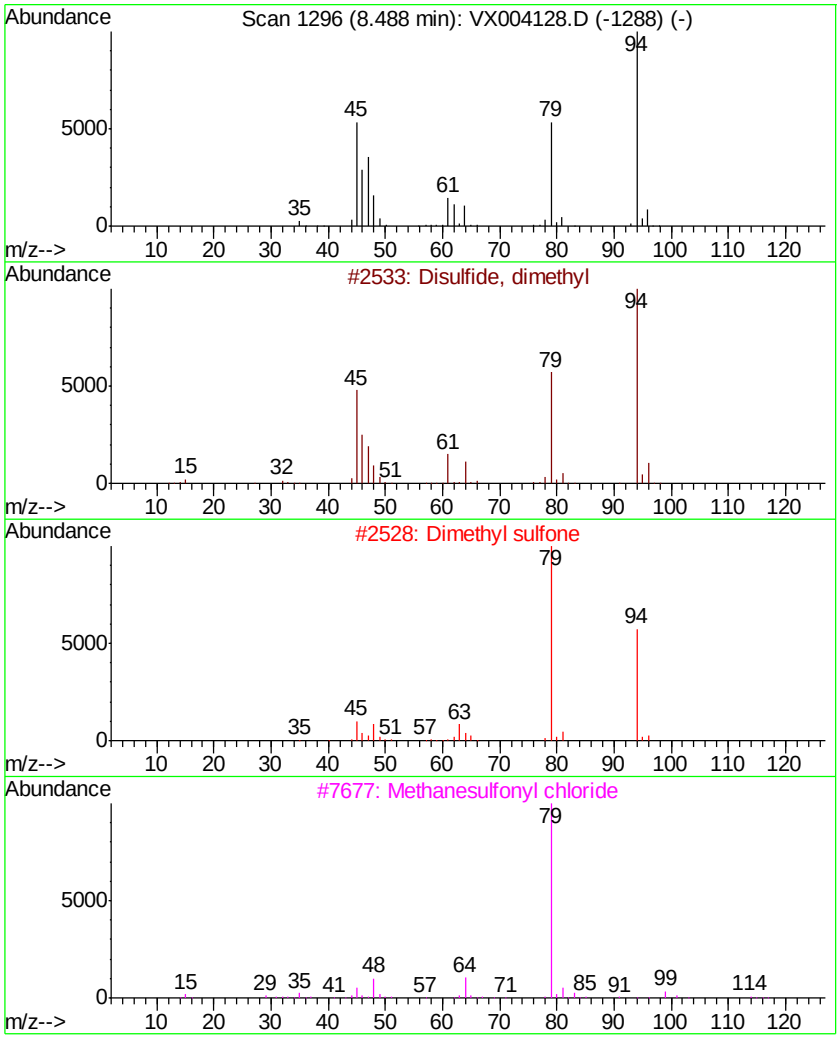
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

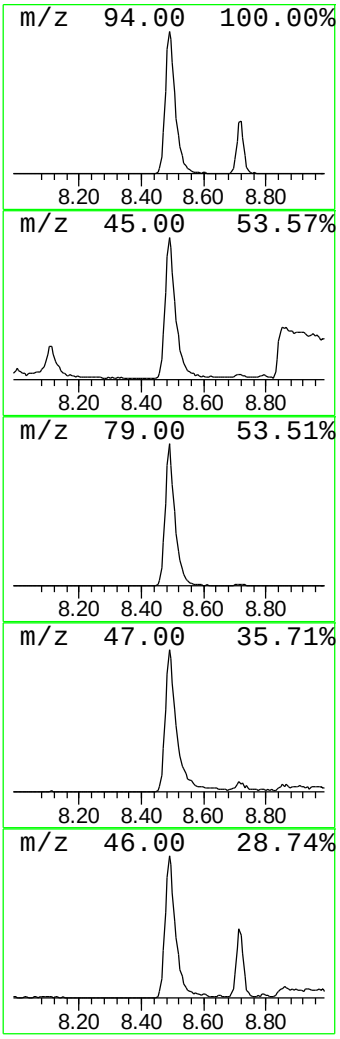
****

Peak Number 5 Disulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.49	13.96 ug/l	253137	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2	Dimethyl sulfone	94	C2H6O2S	000067-71-0	35
3	Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	9
4	Methanesulfonylacetic acid	138	C3H6O4S	002516-97-4	9
5	Ethyne, dichloro-	94	C2Cl2	007572-29-4	5





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Sample : J4520-01
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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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

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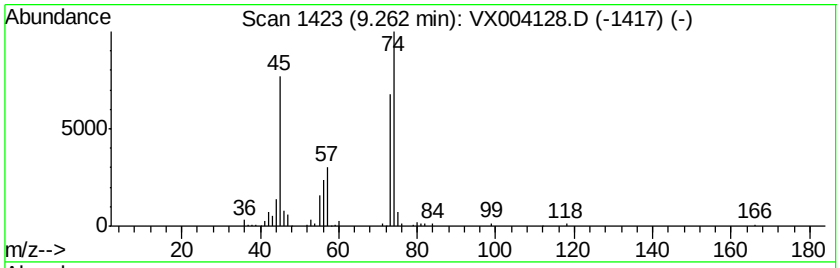
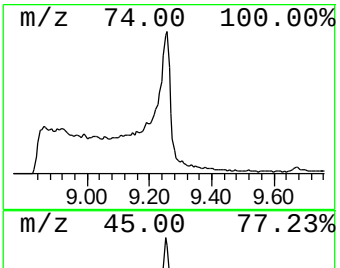
Peak Number 6 Propanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.26	5.60 ug/l	147543	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid	74	C3H6O2	000079-09-4	86
2	Ethanol, 2-nitro-, propionate (e...	147	C5H9NO4	005390-28-3	72
3	Propanedioic acid, oxo-, diethyl...	174	C7H10O5	000609-09-6	64
4	N,N-Dimethylformamide diisopropy...	175	C9H21NO2	018503-89-4	40
5	Methylmalonic acid	118	C4H6O4	000516-05-2	36





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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : F-8-15-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

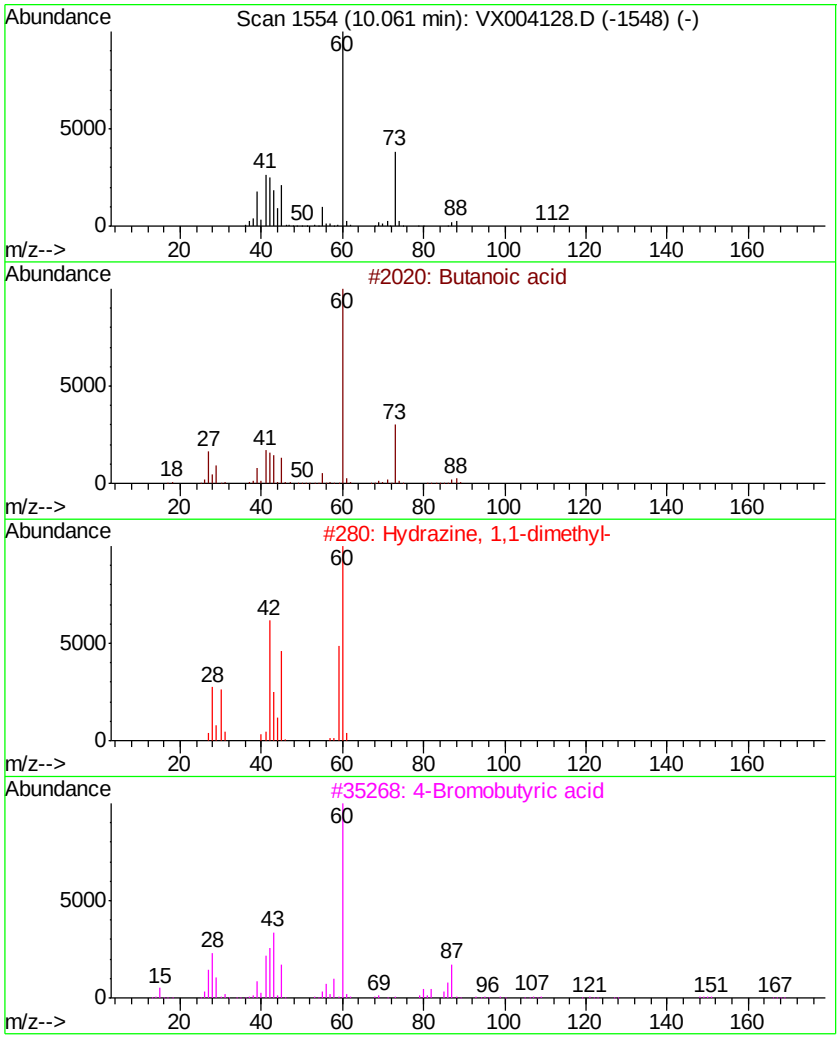
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

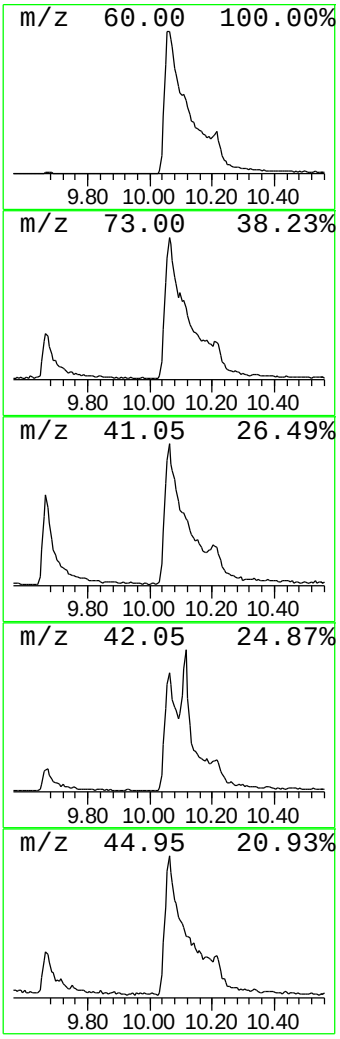
****

Peak Number 7 Butanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	12.20 ug/l	321306	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	74
2	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	47
3	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	Benserazide	257	C10H15N3O5	000322-35-0	9





Library Search Compound Report

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

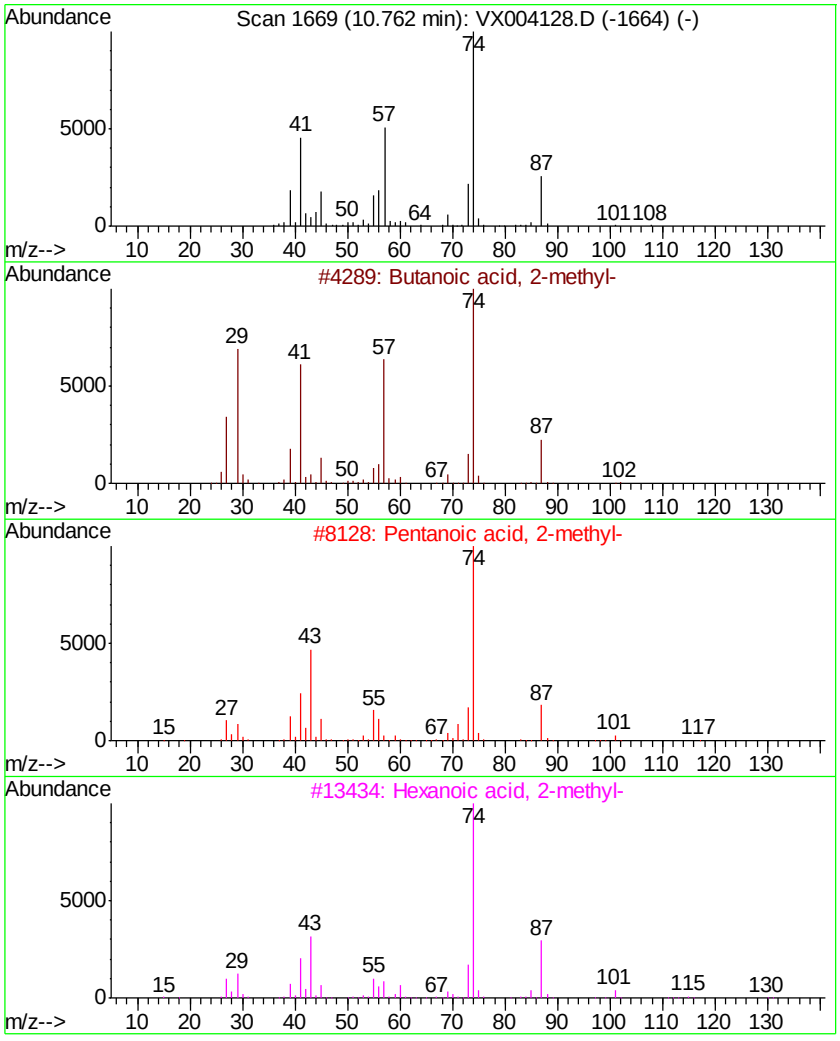
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

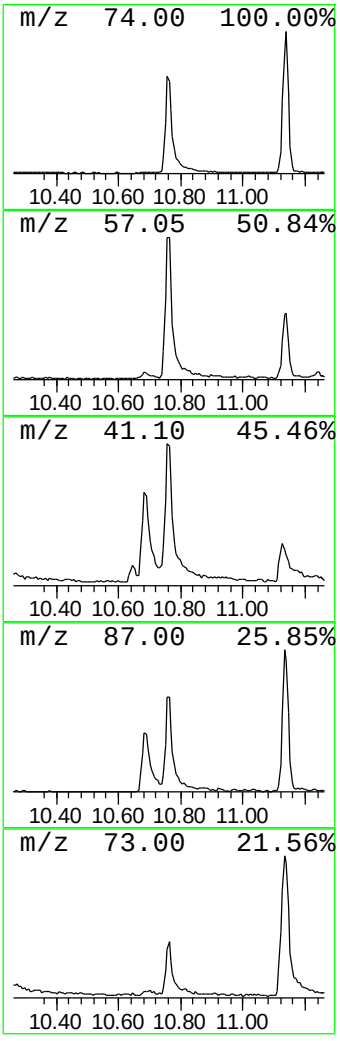
****

Peak Number 8 Butanoic acid, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	5.49 ug/l	144456	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
2	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	78
3	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	40
4	Propanoic acid	74	C3H6O2	000079-09-4	28
5	Diethanolamine	105	C4H11NO2	000111-42-2	25





Tentatively Identified Compound (LSC) summary

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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
Acetaldehyde	1.49	17.4	ug/l	242246	1	5.67	696099	50.0
Methanethiol	1.58	11.9	ug/l	166159	1	5.67	696099	50.0
Methyl thiolacetate	7.50	5.7	ug/l	102760	2	6.87	906965	50.0
Disulfide, dimethyl	8.49	14.0	ug/l	253137	2	6.87	906965	50.0
Propanoic acid	9.26	5.6	ug/l	147543	3	10.12	1316420	50.0
Butanoic acid	10.06	12.2	ug/l	321306	3	10.12	1316420	50.0
Butanoic acid, 2-...	10.76	5.5	ug/l	144456	3	10.12	1316420	50.0