LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

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_V\METHOD\SOMVTR071918WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC: VV006673.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.029	28	43	59	rBV	1675731	2189407	100.00%	16.013%
2	1.093	59	63	67	rBV	30550	30063	1.37%	0.220%
3	1.209	92	99	105	rBV	240626	370749	16.93%	2.712%
4	1.318	129	133	151	rVB2	142468	176666	8.07%	1.292%
5	1.469	174	180	191	rBV	2136214	1951176	89.12%	14.270%
6	1.520	191	196	206	rBV	85393	182202	8.32%	1.333%
7	2.054	353	362	377	rBV	340841	472519	21.58%	3.456%
8	2.131	377	386	396	rVB	205045	290139	13.25%	2.122%
9	2.192	398	405	410	rBV	41598	54654	2.50%	0.400%
10	2.231	410	417	434	rVB	167499	246223	11.25%	1.801%
11	2.315	438	443	451	rVB2	24249	32362	1.48%	0.237%
12	2.463	482	489	496	rBV	63481	105323	4.81%	0.770%
13	2.791	585	591	612	rVB	71711	133265	6.09%	0.975%
14	3.726	869	882	896	rBV4	12694	31194	1.42%	0.228%
15	3.951	938	952	969	rBV	102476	255784	11.68%	1.871%
16	4.038	971	979	999	rVB	22821	56380	2.58%	0.412%
17	4.408	1076	1094	1115	rBV	131618	315509	14.41%	2.308%
18	5.099	1291	1309	1325	rBV2	326719	744708	34.01%	5.447%
19	5.668	1472	1486	1511	rBV	280124	582386	26.60%	4.259%
20	6.125	1614	1628	1647	rVB	178755	350183	15.99%	2.561%
21	6.237	1653	1663	1674	rVB	16131	27872	1.27%	0.204%
22	7.035	1899	1911	1928	rBV	87566	152761	6.98%	1.117%
23	7.138	1928	1943	1977	rBV	498035	906606	41.41%	6.631%
24	7.363	2000	2013	2028	rBV	395824	670751	30.64%	4.906%
25	7.668	2096	2108	2124	rBV	54832	92669	4.23%	0.678%
26	8.141	2241	2255	2289	rBV	426173	710468	32.45%	5.196%
27	8.758	2436	2447	2467	rBV	95989	162982	7.44%	1.192%
28	8.900	2470	2491	2525	rBV	413839	748058	34.17%	5.471%
29	10.269	2906	2917	2932	rVB	126661	197590	9.02%	1.445%
30	10.842	3084	3095	3120	rBV	65242	114391	5.22%	0.837%
31	11.089	3160	3172	3190	rBV2	44230	71629	3.27%	0.524%
32	11.301	3225	3238	3258	rBV	381960	600899	27.45%	4.395%
33	11.678	3343	3355	3372	rBV	343954	538948	24.62%	3.942%
34	11.932	3425	3434	3449	rBV2	24444	39277	1.79%	0.287%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

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_V\METHOD\SOMVTR071918WMA.M
Title : TRACE VOA SOM01.0

35	12.285	3533	3544	3553	rBV3	40058	67090	3.06%	0.491%

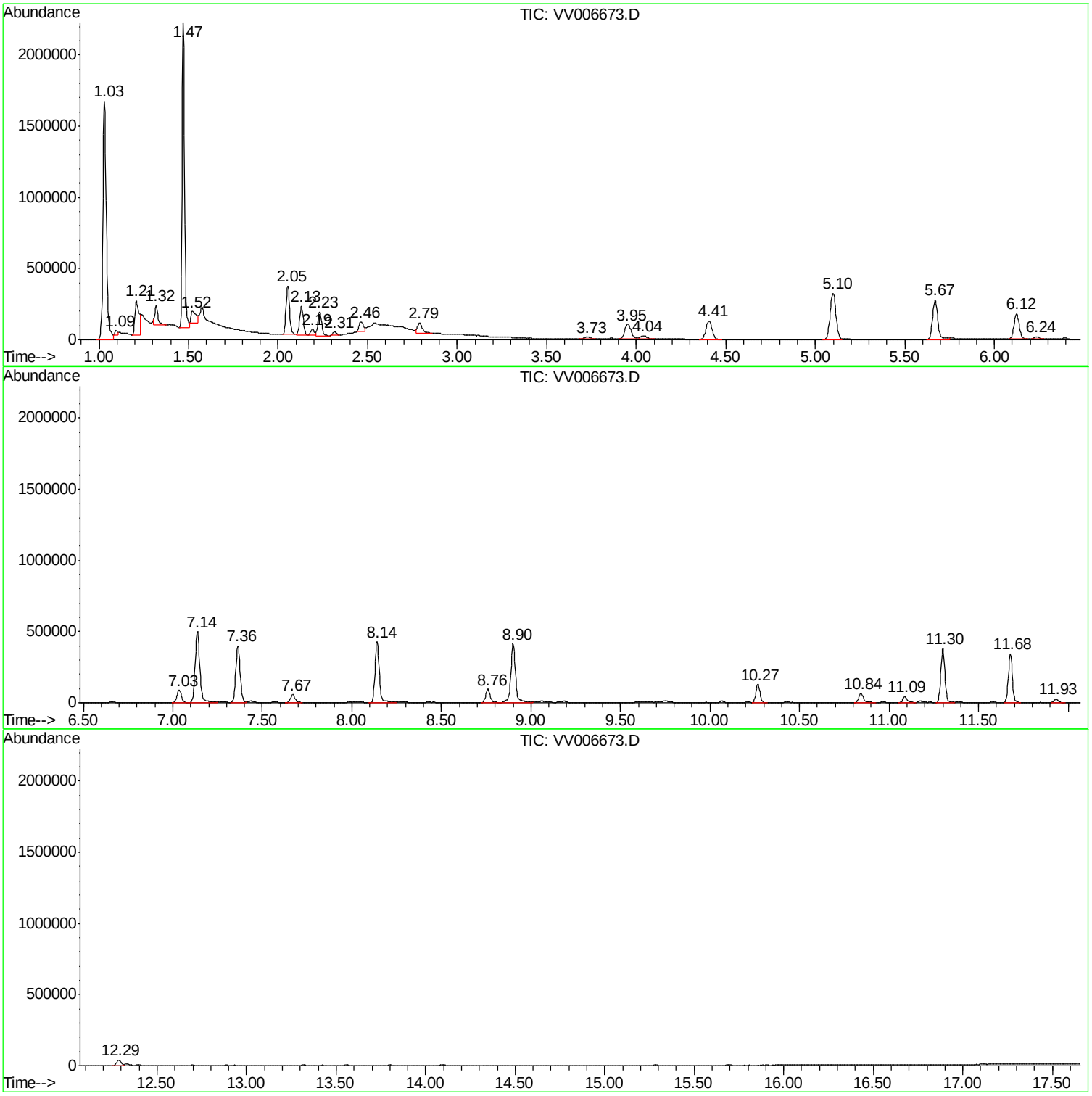
Sum of corrected areas: 13672883

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.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_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

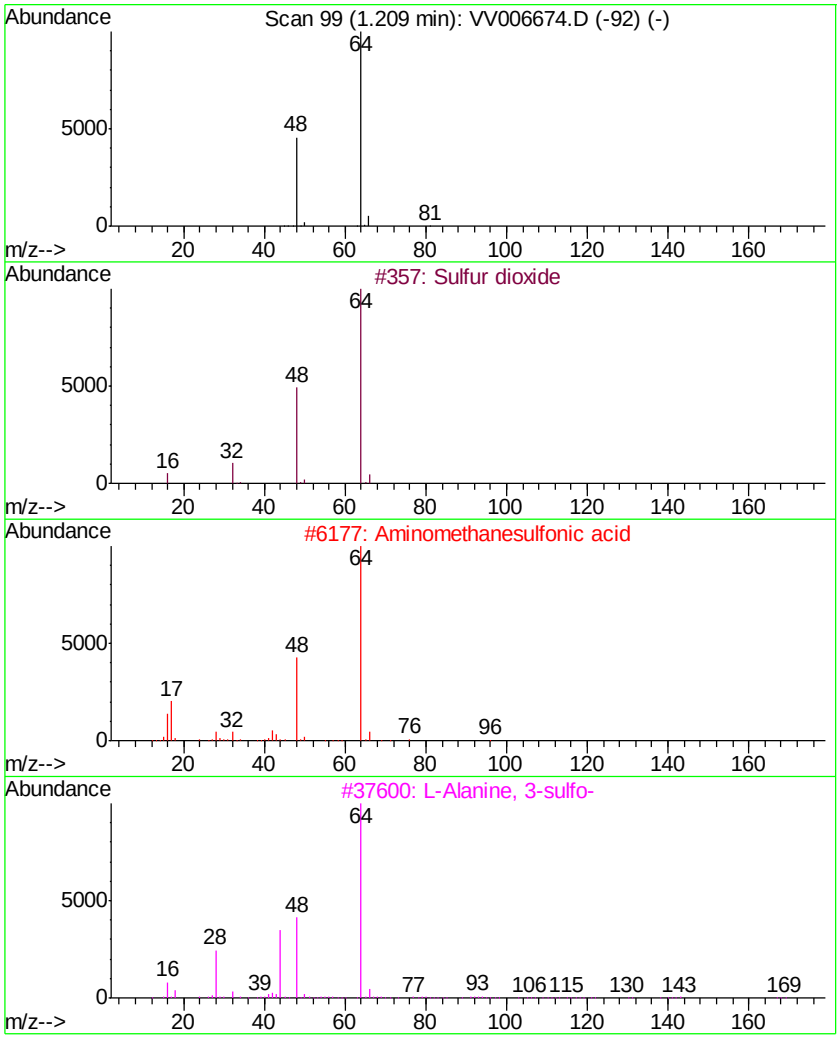
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

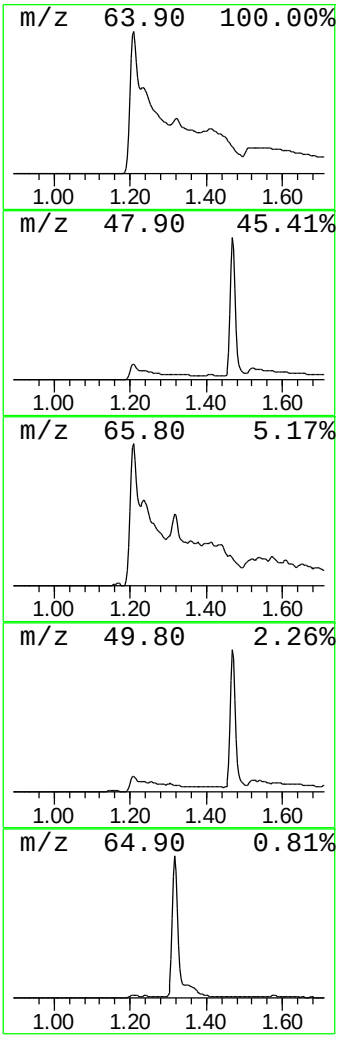
****

Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.21	3.18 ug/L	370749	1,4-Difluorobenzene	5.67

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

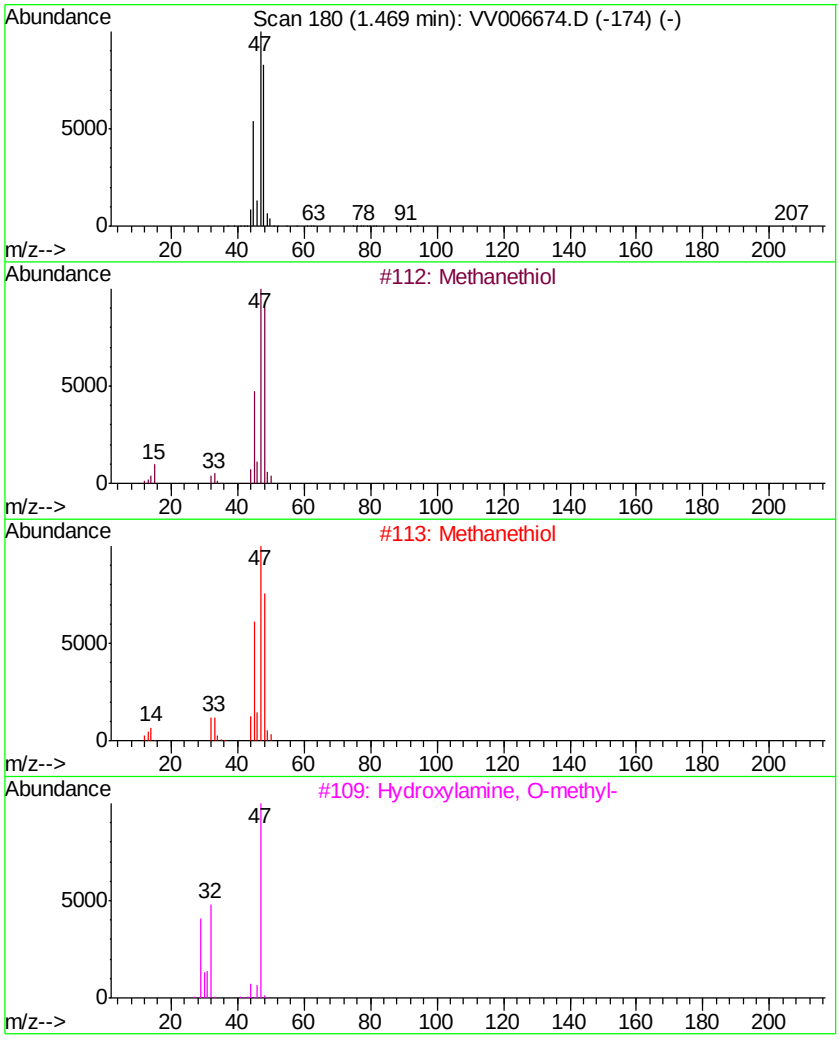
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

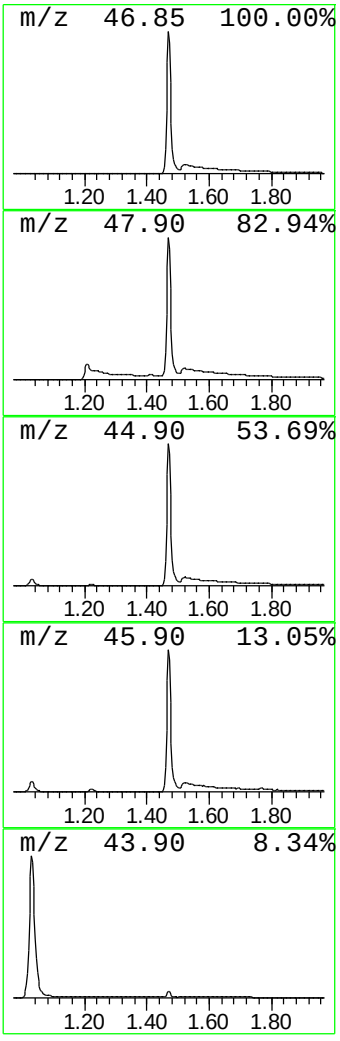
****

Peak Number 3 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	16.75 ug/L	1951180	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Methanethiol	48	CH4S	000074-93-1	90
3	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5	Methane, nitroso-	45	CH3NO	000865-40-7	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

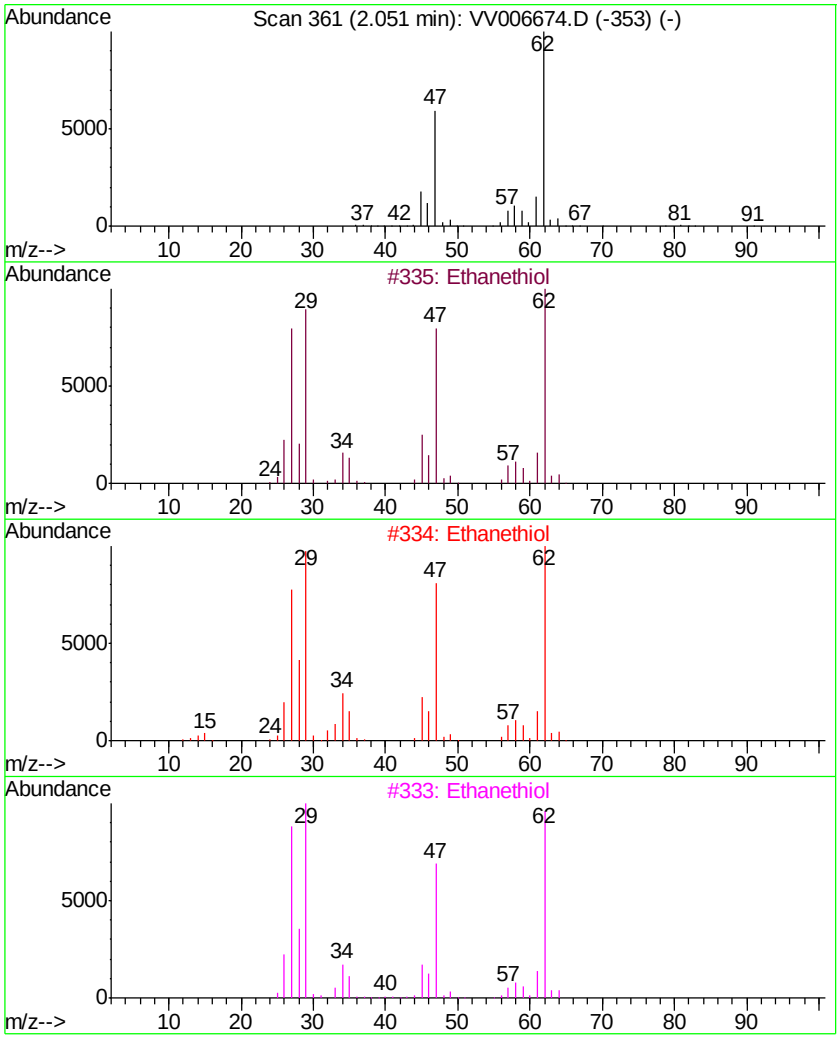
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

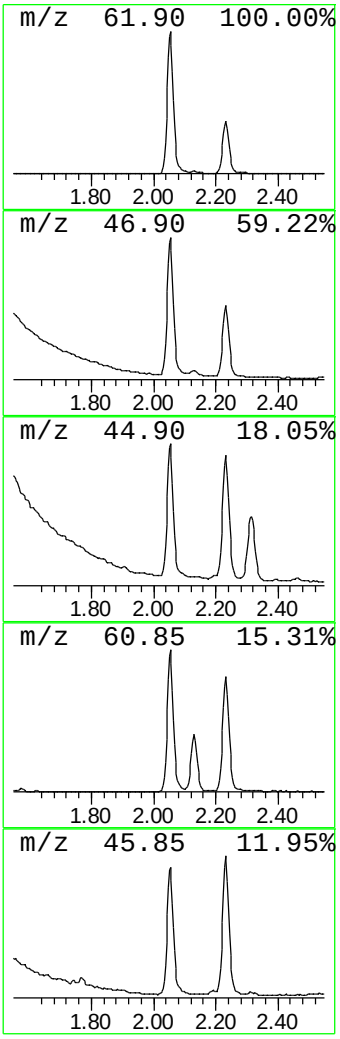
****

Peak Number 5 Ethanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	4.06 ug/L	472519	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91
2	Ethanethiol	62	C2H6S	000075-08-1	91
3	Ethanethiol	62	C2H6S	000075-08-1	91
4	Ethanethiol	62	C2H6S	000075-08-1	91
5	Ethanethiol	62	C2H6S	000075-08-1	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

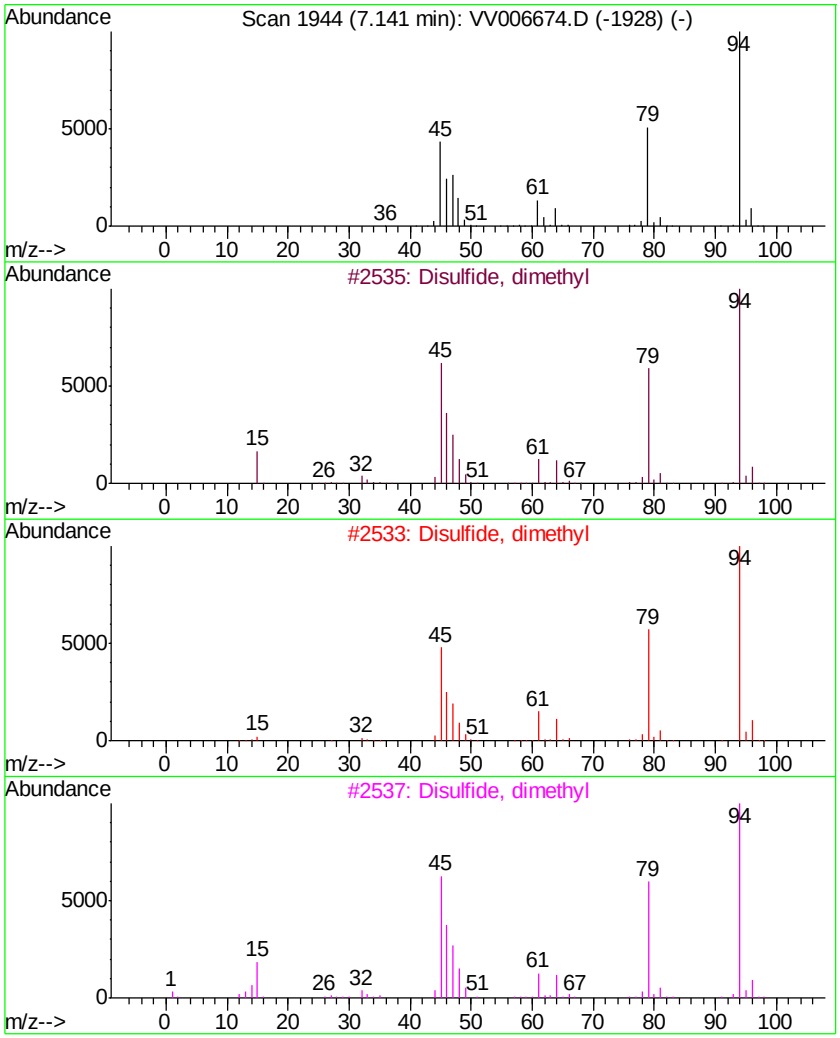
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

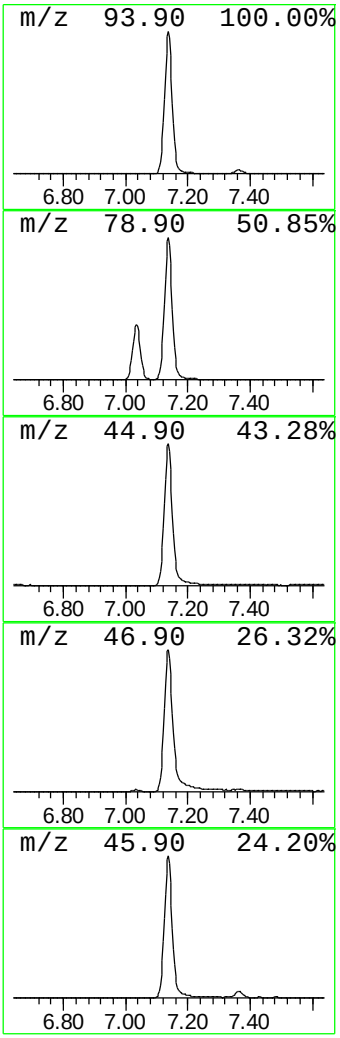
****

Peak Number 7 Disulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	7.78 ug/L	906606	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

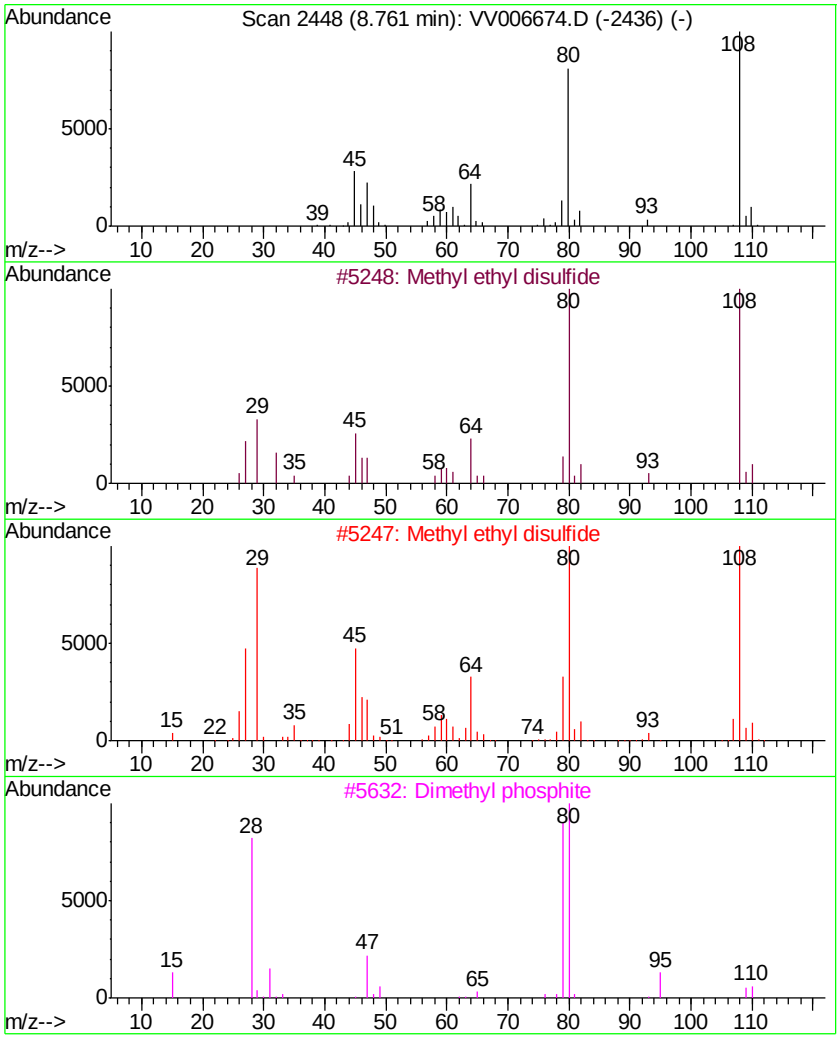
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

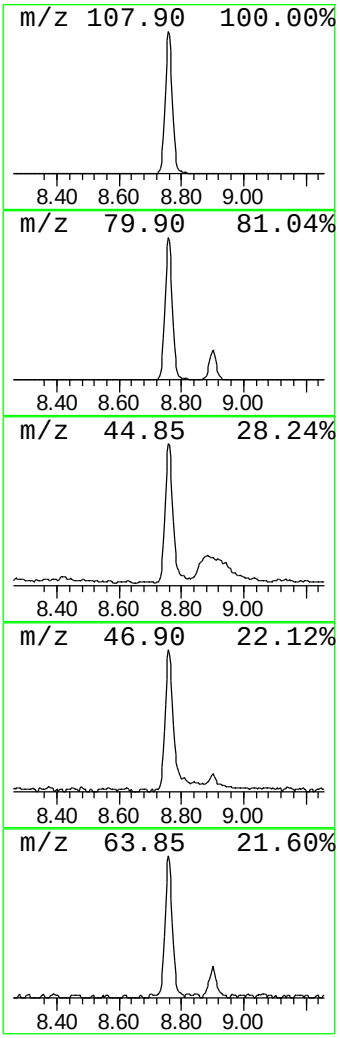
****

Peak Number 8 Methyl ethyl disulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	1.09 ug/L	162982	Chlorobenzene-d5	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	86
2	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	72
3	Dimethyl phosphite	110	C2H7O3P	000868-85-9	53
4	Methanesulfonic acid, methyl ester	110	C2H6O3S	000066-27-3	53
5	Ethene, 1-chloro-2-fluoro-	80	C2H2ClF	000460-16-2	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

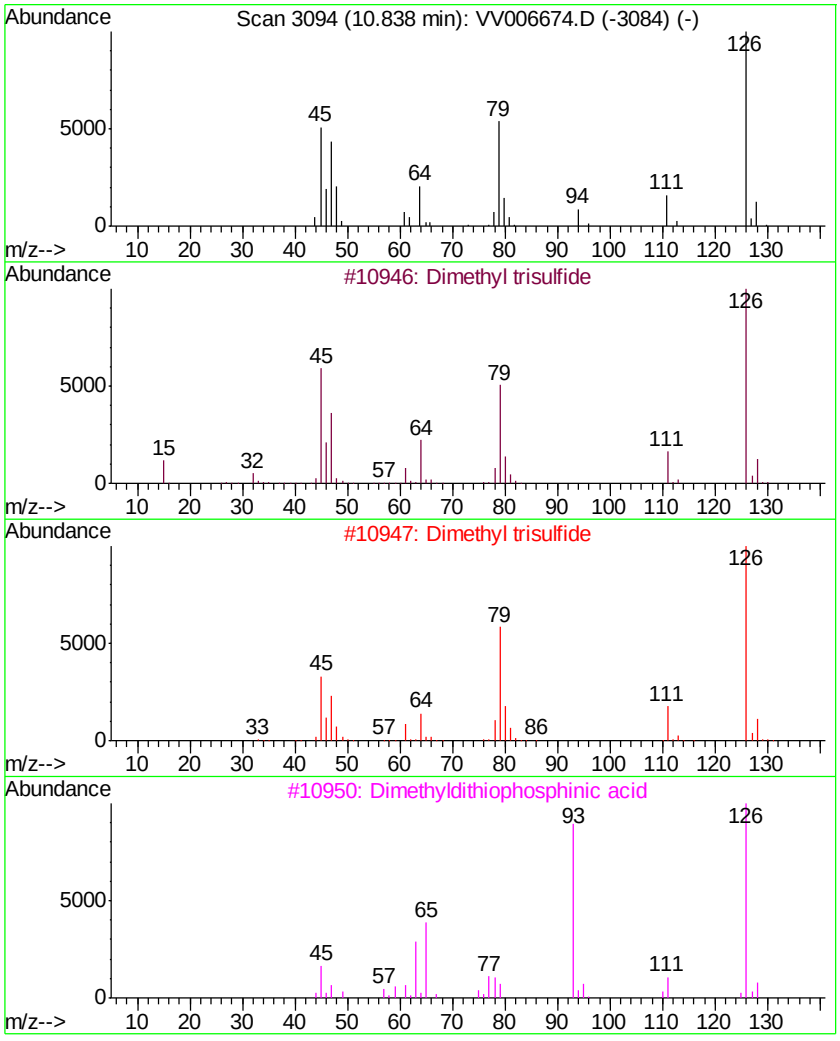
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

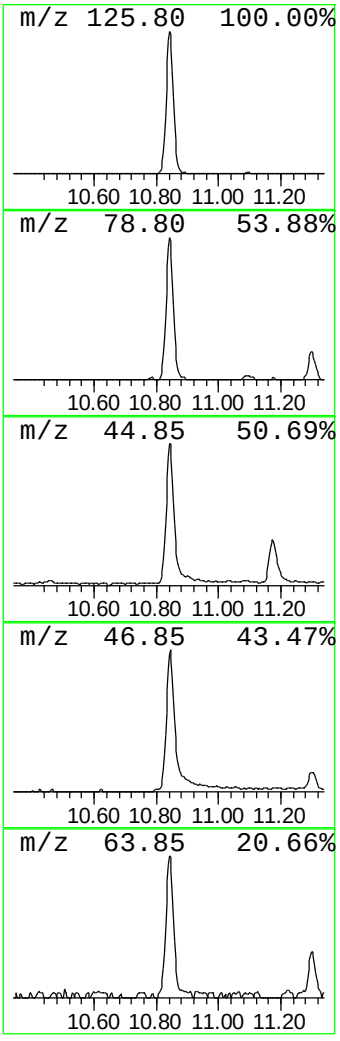
****

Peak Number 9 Dimethyl trisulfide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	0.95 ug/L	114391	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl trisulfide	126	C2H6S3	003658-80-8	96
2	Dimethyl trisulfide	126	C2H6S3	003658-80-8	81
3	Dimethyldithiophosphinic acid	126	C2H7PS2	016367-68-3	22
4	4-Mercaptophenol	126	C6H6OS	000637-89-8	9
5	(2,2,2-Trifluoroethoxy)ethene	126	C4H5F3O	1000306-54-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

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

****

Peak Number 10 2-Octanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	0.60 ug/L	71629	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	91
2	2-Octanone	128	C8H16O	000111-13-7	91
3	2-Octanone	128	C8H16O	000111-13-7	91
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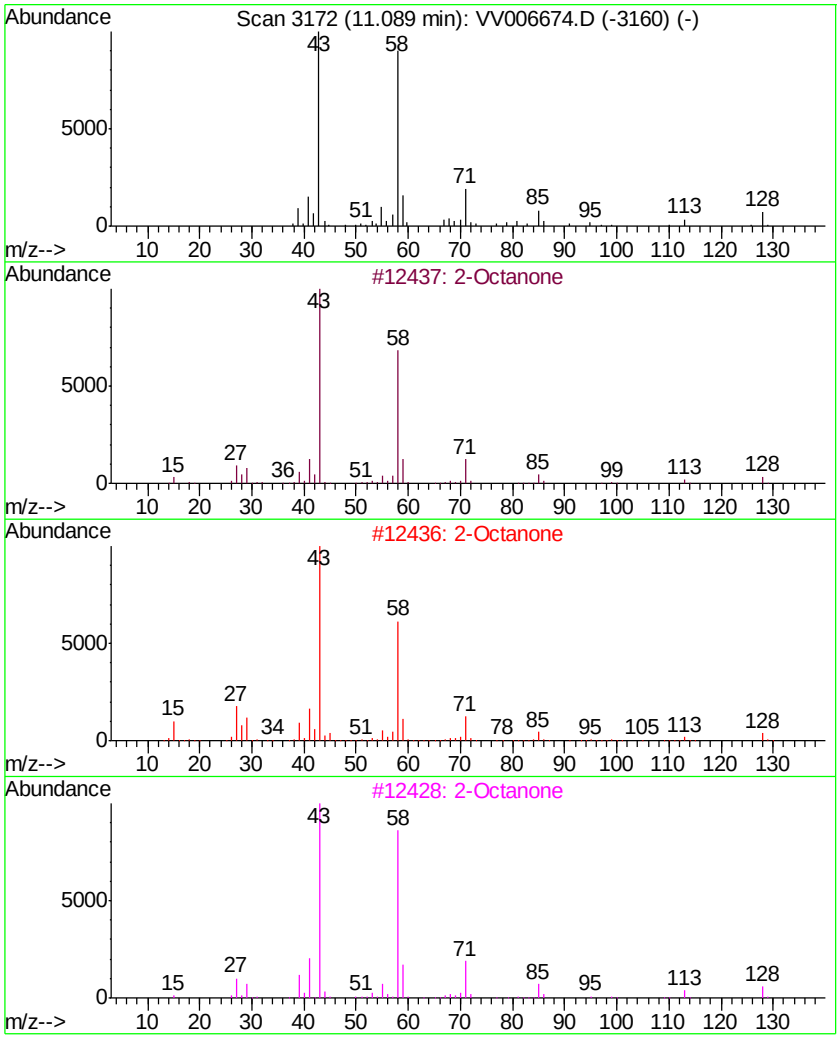
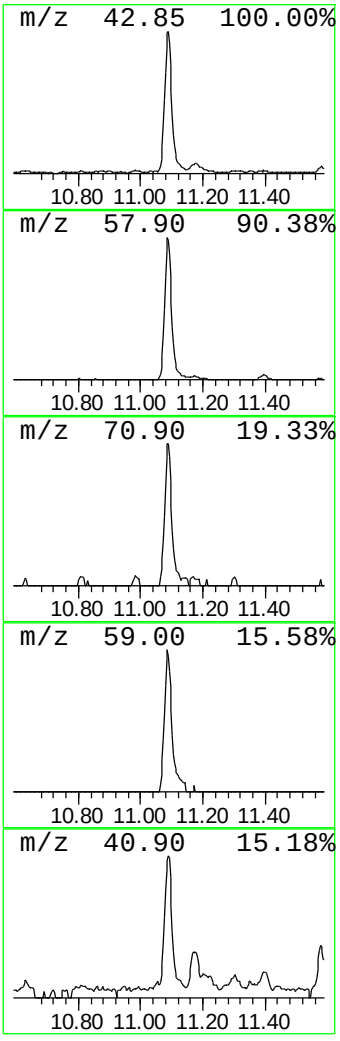
5	2-Octanone	128	C8H16O	000111-13-7	87





Library Search Compound Report

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Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

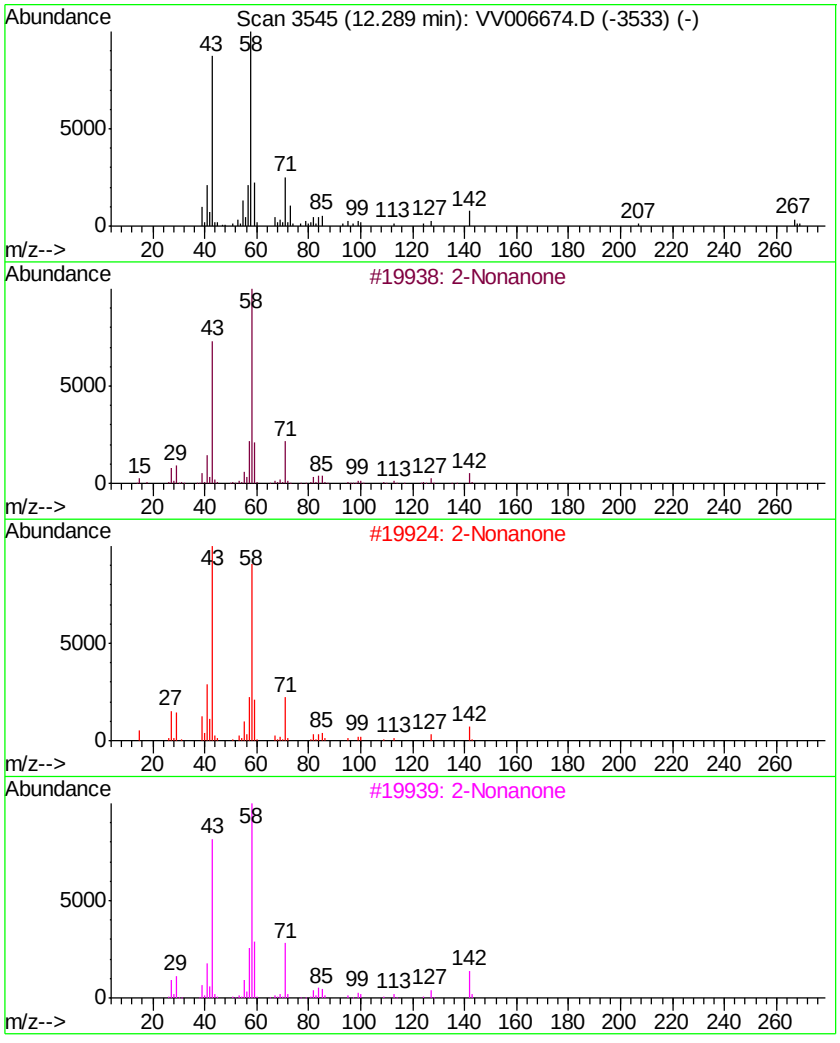
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

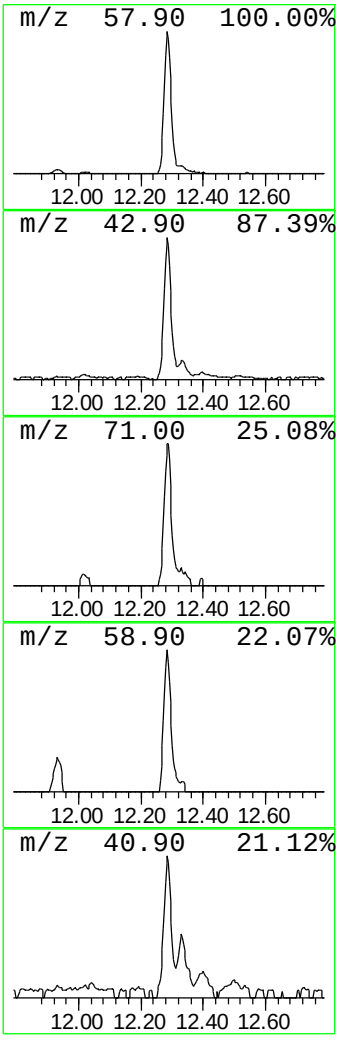
****

Peak Number 11 2-Nonanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	0.56 ug/L	67090	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	94
2	2-Nonanone	142	C9H18O	000821-55-6	90
3	2-Nonanone	142	C9H18O	000821-55-6	87
4	2-Nonanone	142	C9H18O	000821-55-6	87
5	2-Dodecanone	184	C12H24O	006175-49-1	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006674.D
Acq On : 20 Jul 2018 18:16
Operator : SY/MD
Sample : J4078-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AB0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.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
Sulfur dioxide	1.21	3.2	ug/L	370749	1	5.67	582386	5.0
Methanethiol	1.47	16.8	ug/L	1951180	1	5.67	582386	5.0
Ethanethiol	2.05	4.1	ug/L	472519	1	5.67	582386	5.0
Disulfide, dimethyl	7.14	7.8	ug/L	906606	1	5.67	582386	5.0
Methyl ethyl disu...	8.76	1.1	ug/L	162982	2	8.90	748058	5.0
Dimethyl trisulfide	10.84	0.9	ug/L	114391	3	11.30	600899	5.0
2-Octanone	11.09	0.6	ug/L	71629	3	11.30	600899	5.0
2-Nonanone	12.29	0.6	ug/L	67090	3	11.30	600899	5.0