LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

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_R\METHODS\SOMRTR092718WMA.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	1.794	15	19	46	rVB	290872	1255812	14.33%	4.143%
2	2.172	75	81	96	rVB3	60218	240792	2.75%	0.794%
3	2.433	111	124	148	rBV	2945373	8765974	100.00%	28.917%
4	2.634	151	157	168	rVB2	126122	350319	4.00%	1.156%
5	3.461	284	293	300	rBV	1816782	4535816	51.74%	14.963%
6	3.772	338	344	352	rVB	140192	347354	3.96%	1.146%
7	4.191	404	413	426	rVB	183552	519277	5.92%	1.713%
8	4.404	437	448	456	rBV3	105376	341924	3.90%	1.128%
9	6.369	762	771	783	rBV4	89429	268428	3.06%	0.885%
10	6.497	783	792	800	rVV	128583	364267	4.16%	1.202%
11	6.594	800	808	818	rVV2	118491	363652	4.15%	1.200%
12	7.203	898	908	909	rBV	406224	662759	7.56%	2.186%
13	7.641	969	980	985	rBV3	34279	93952	1.07%	0.310%
14	7.854	1005	1015	1029	rBV2	670677	1880593	21.45%	6.204%
15	8.462	1106	1115	1122	rBV	715483	1335665	15.24%	4.406%
16	8.541	1122	1128	1133	rVB	67349	125934	1.44%	0.415%
17	8.900	1180	1187	1195	rBV	426474	862051	9.83%	2.844%
18	9.034	1201	1209	1222	rVB2	135081	272471	3.11%	0.899%
19	9.289	1245	1251	1260	rBV	120946	207708	2.37%	0.685%
20	9.685	1310	1316	1321	rBV	167347	273114	3.12%	0.901%
21	9.837	1332	1341	1352	rVB2	82520	224883	2.57%	0.742%
22	9.971	1356	1363	1370	rBV	1051697	1697299	19.36%	5.599%
23	10.232	1401	1406	1413	rVB	74827	120006	1.37%	0.396%
24	10.591	1459	1465	1475	rBV	622758	980423	11.18%	3.234%
25	10.871	1502	1511	1518	rBV	67708	106956	1.22%	0.353%
26	11.200	1556	1565	1573	rBV3	43883	98385	1.12%	0.325%
27	11.285	1573	1579	1588	rBV	929030	1400270	15.97%	4.619%
28	12.070	1703	1708	1716	rBV	123543	167897	1.92%	0.554%
29	12.362	1751	1756	1763	rVB	166771	251267	2.87%	0.829%
30	13.086	1869	1875	1881	rBV	63942	91432	1.04%	0.302%
31	13.219	1890	1897	1907	rBV	746612	1094008	12.48%	3.609%
32	13.511	1939	1945	1956	rVB	590457	855044	9.75%	2.821%
33	13.986	2018	2023	2032	rVB	97171	158509	1.81%	0.523%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

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_R\METHODS\SOMRTR092718WMA.M
Title : TRACE VOA SOM01.0

Sum of corrected areas: 30314241

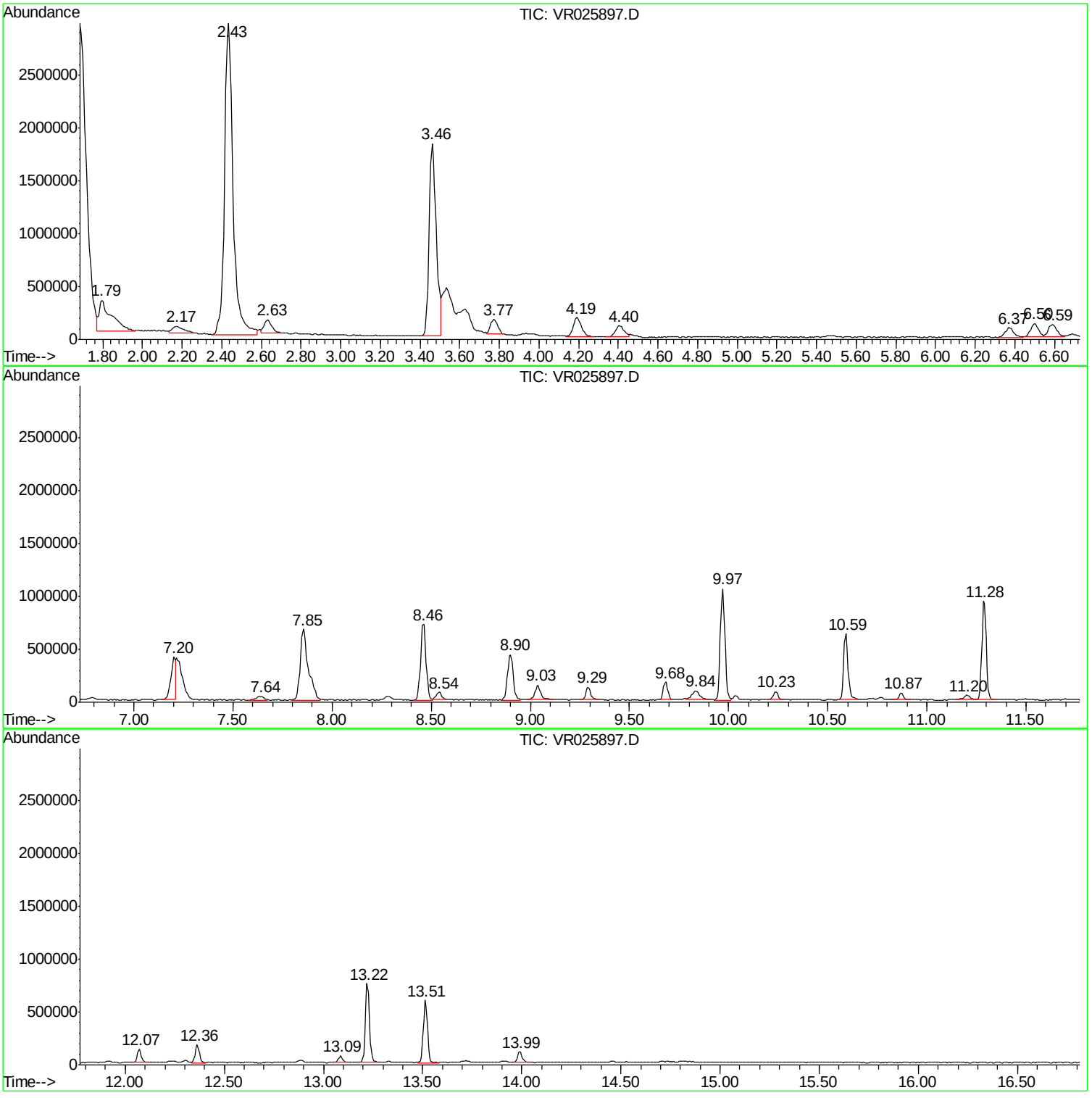
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.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 R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

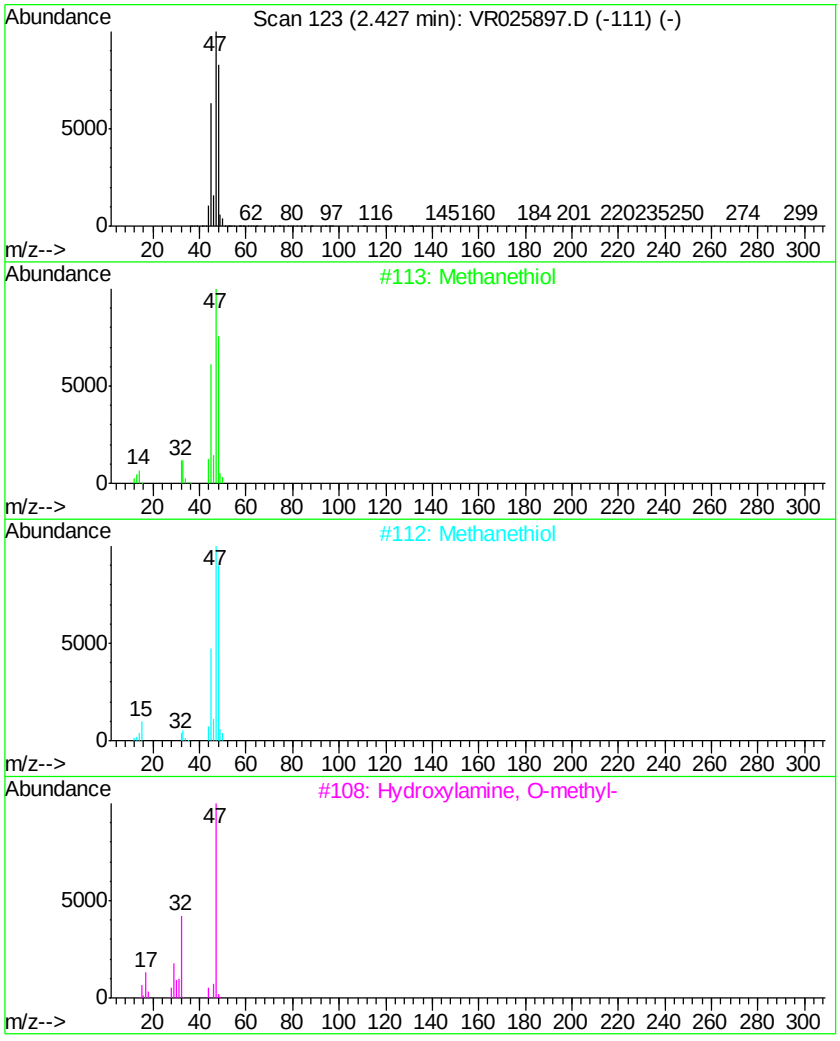
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

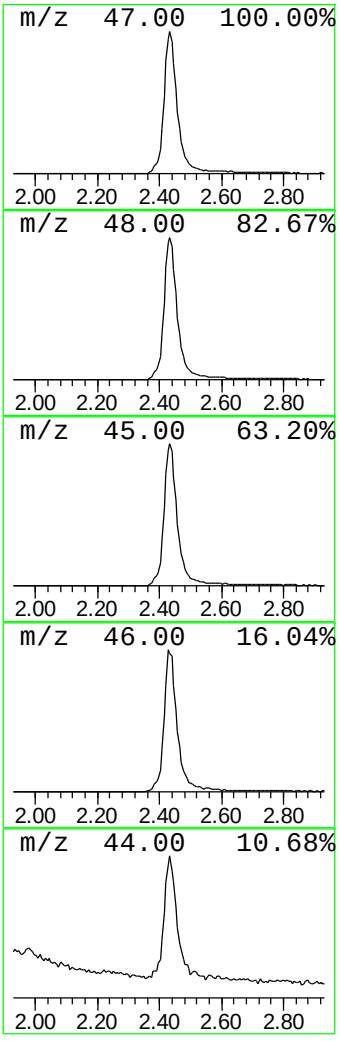
****

Peak Number 2 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	32.82 ug/L	8765970	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Methanethiol	48	CH4S	000074-93-1	90
3	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4	Methane, nitroso-	45	CH3NO	000865-40-7	5
5	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

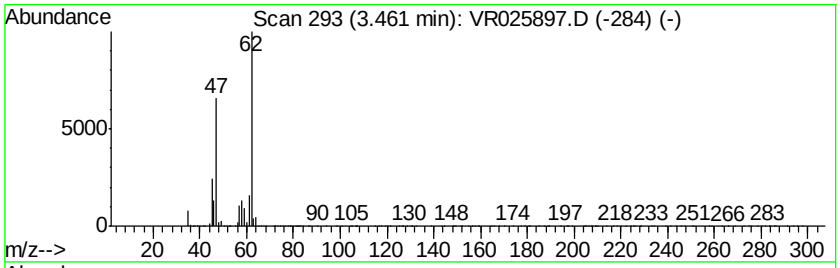
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

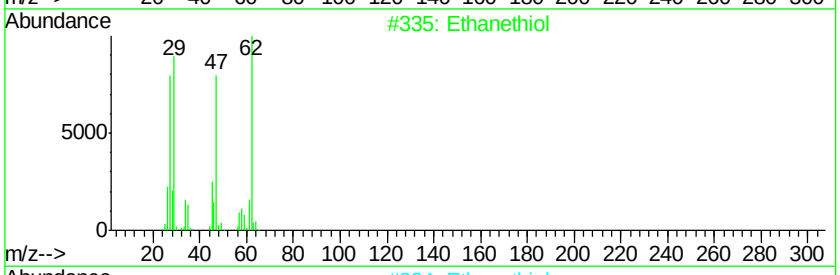
****

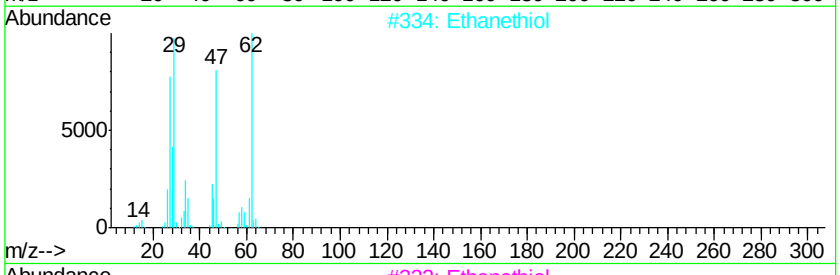
Peak Number 3 Ethanethiol Concentration Rank 2

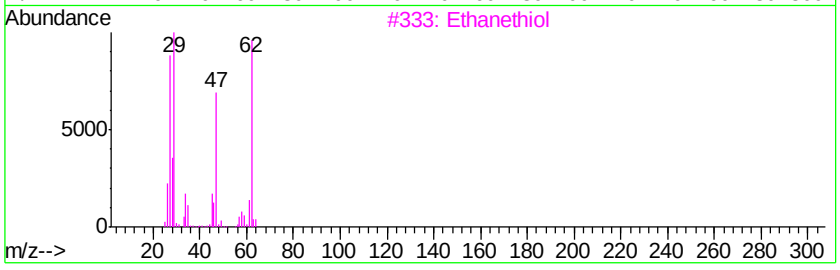
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.46	16.98 ug/L	4535820	1,4-Difluorobenzene	8.46

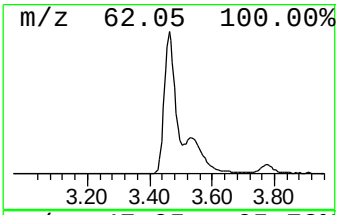
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91
2	Ethanethiol	62	C2H6S	000075-08-1	91
3	Ethanethiol	62	C2H6S	000075-08-1	91
4	Ethanethiol	62	C2H6S	000075-08-1	91
5	Ethanethiol	62	C2H6S	000075-08-1	91

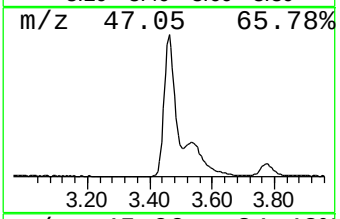


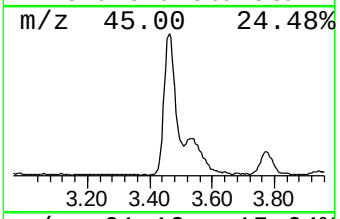


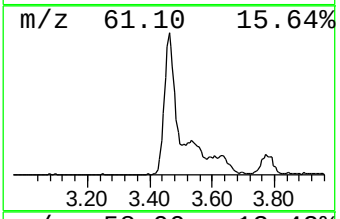


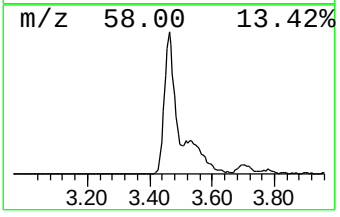












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

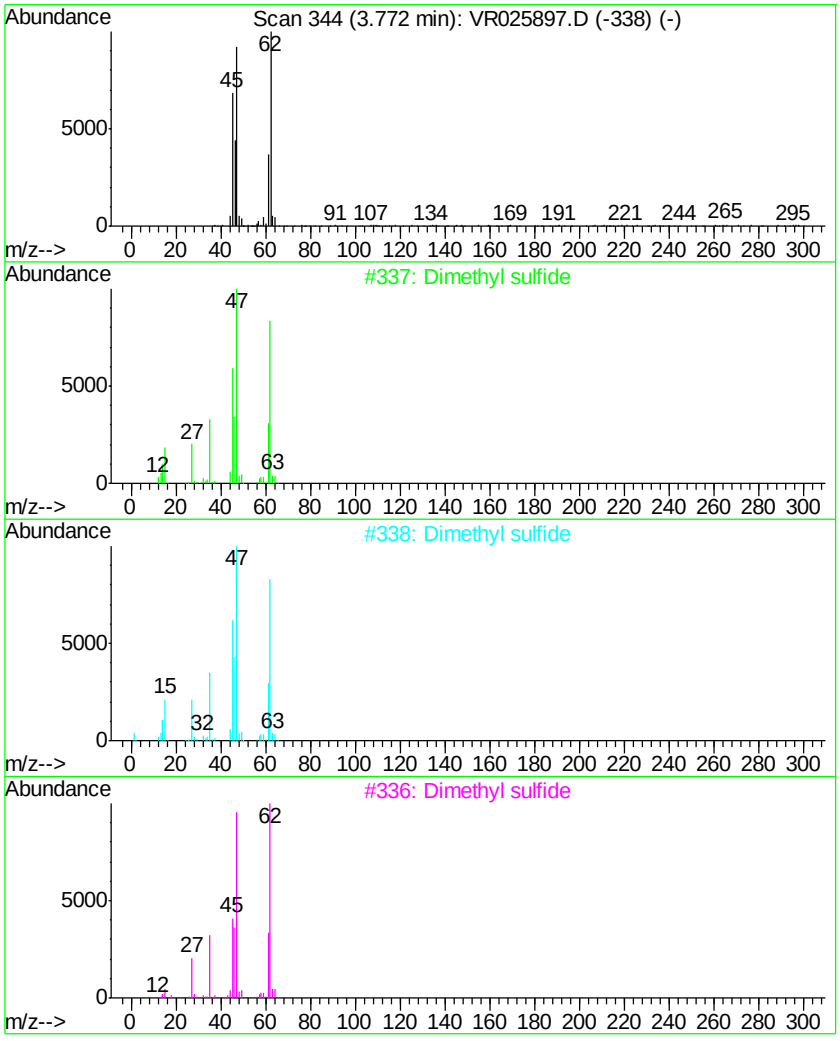
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

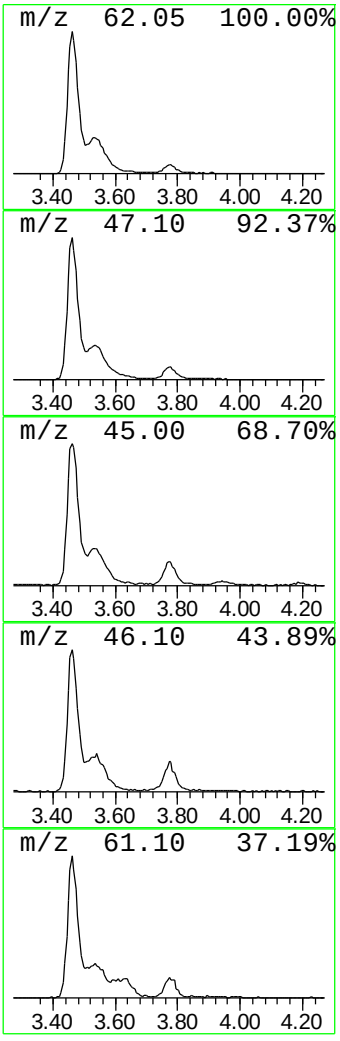
****

Peak Number 4 Dimethyl sulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.77	1.30 ug/L	347354	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Dimethyl sulfide	62	C2H6S	000075-18-3	91
3	Dimethyl sulfide	62	C2H6S	000075-18-3	91
4	Dimethyl sulfide	62	C2H6S	000075-18-3	90
5	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

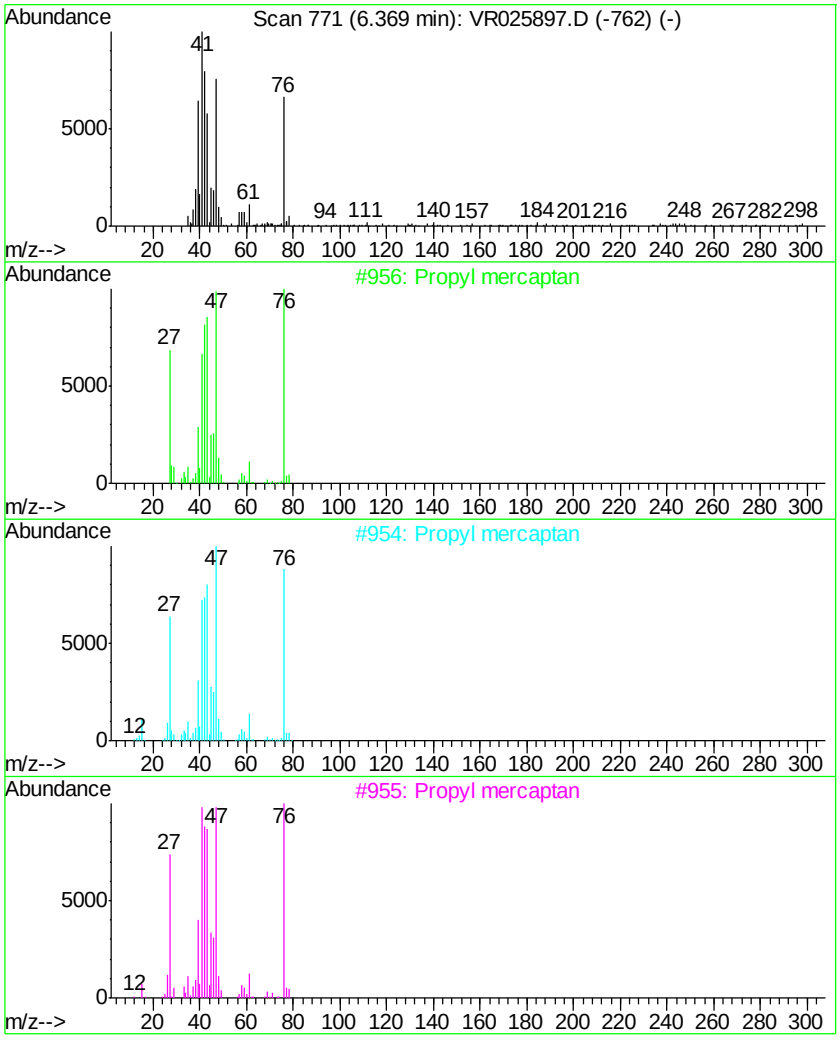
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

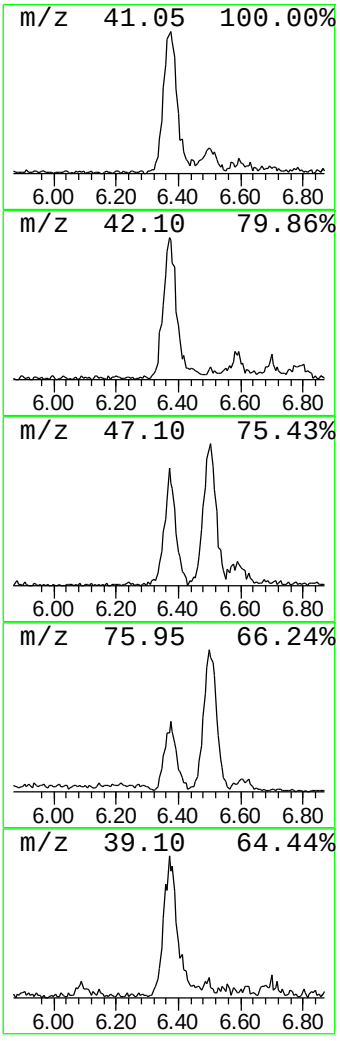
****

Peak Number 5 Propyl mercaptan Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	1.00 ug/L	268428	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	92
2	Propyl mercaptan	76	C3H8S	000107-03-9	91
3	Propyl mercaptan	76	C3H8S	000107-03-9	64
4	Propyl mercaptan	76	C3H8S	000107-03-9	60
5	Propyl mercaptan	76	C3H8S	000107-03-9	60





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

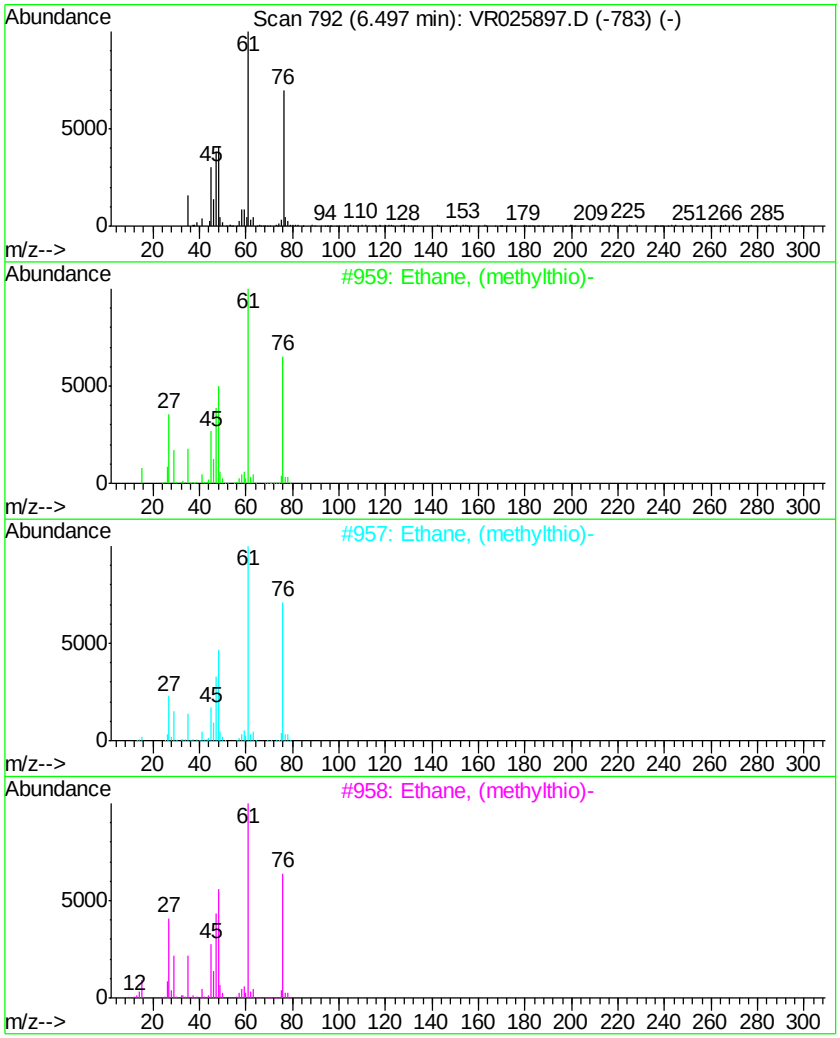
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

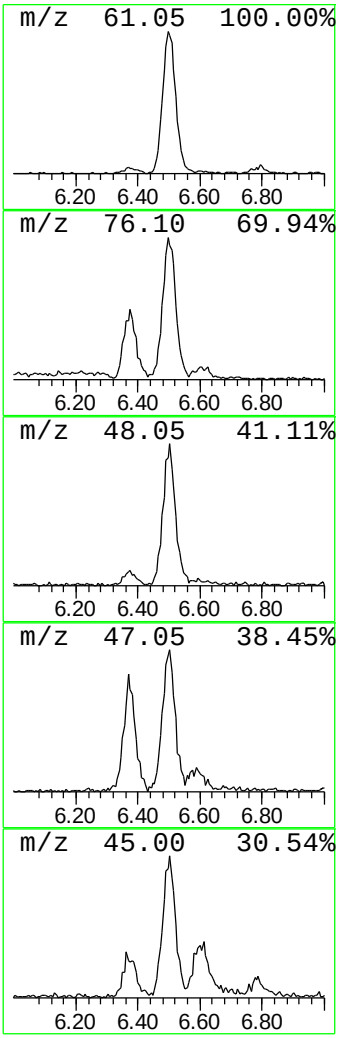
****

Peak Number 6 Ethane, (methylthio)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	1.36 ug/L	364267	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, (methylthio)-	76	C3H8S	000624-89-5	96
2	Ethane, (methylthio)-	76	C3H8S	000624-89-5	95
3	Ethane, (methylthio)-	76	C3H8S	000624-89-5	94
4	Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	53
5	Trimethylphosphine	76	C3H9P	000594-09-2	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

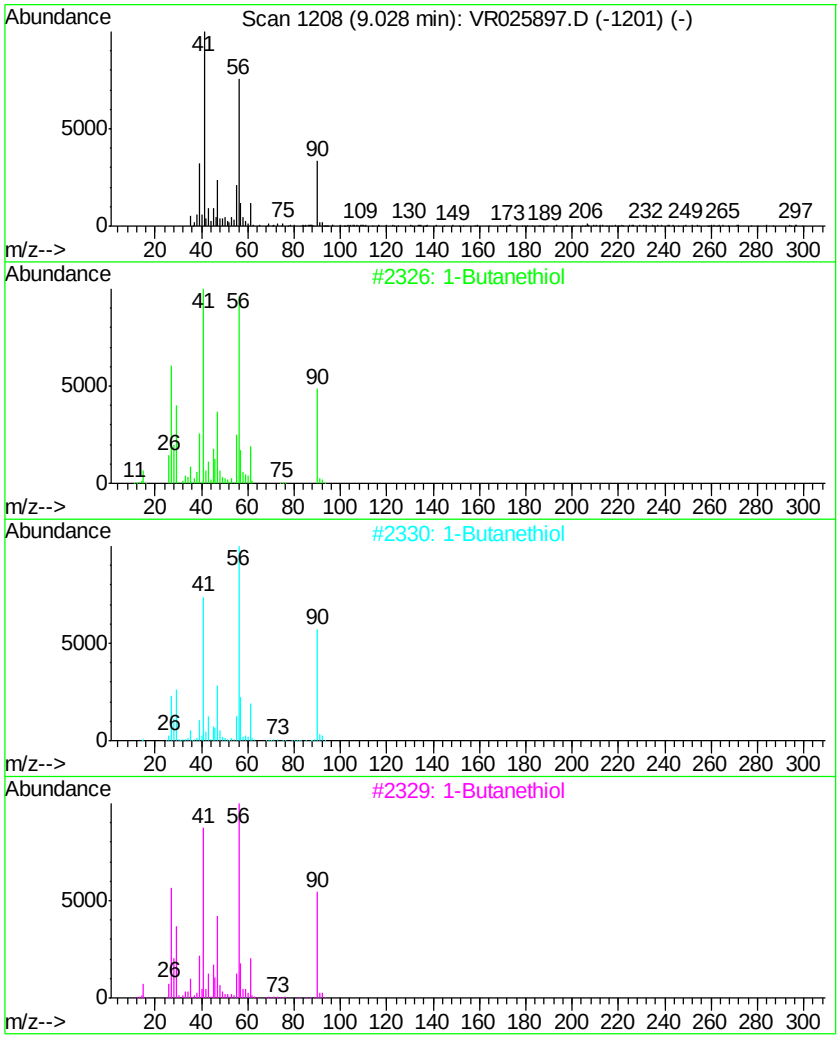
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

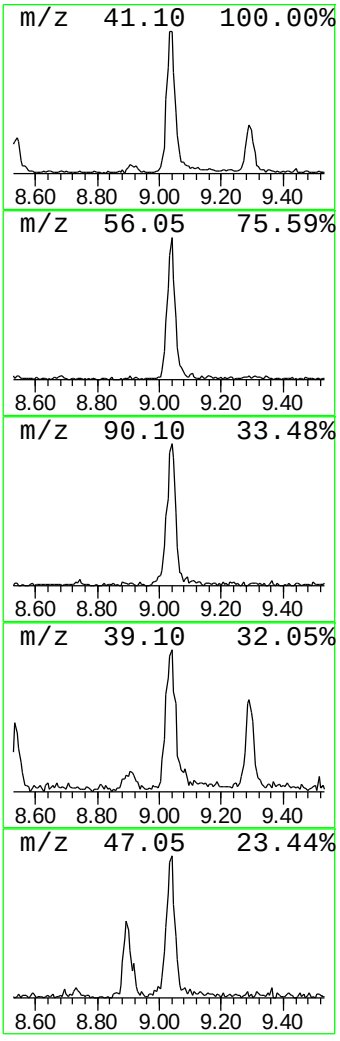
****

Peak Number 7 1-Butanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.03	1.02 ug/L	272471	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanethiol	90	C4H10S	000109-79-5	91
2	1-Butanethiol	90	C4H10S	000109-79-5	90
3	1-Butanethiol	90	C4H10S	000109-79-5	86
4	Oxetane, 2,3,4-trimethyl-	100	C6H12O	053778-61-3	37
5	Cyclobutane	56	C4H8	000287-23-0	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

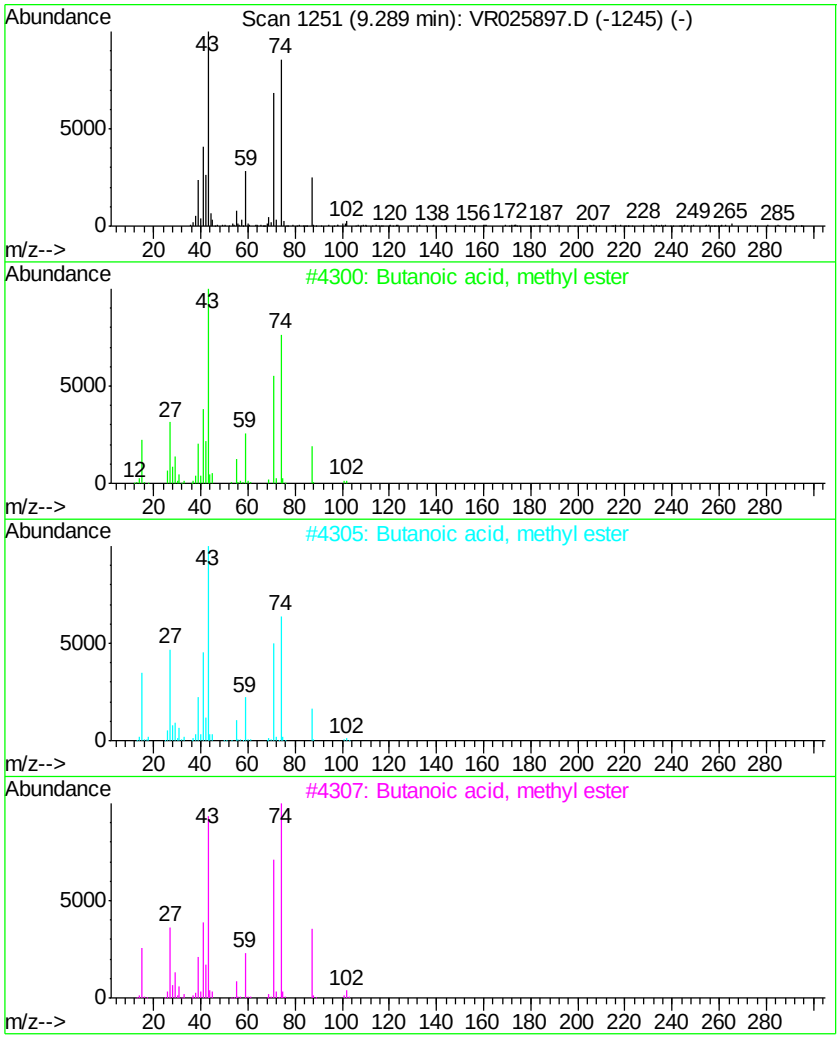
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

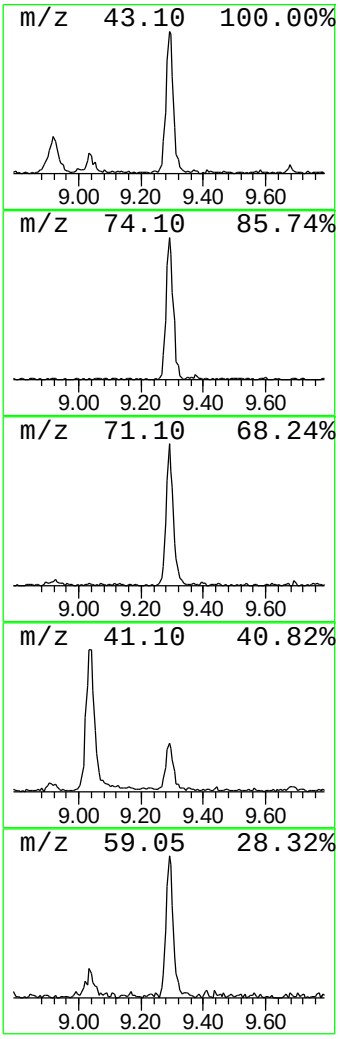
****

Peak Number 8 Butanoic acid, methyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	0.78 ug/L	207708	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
4	Propanoic acid, 2-methyl-, methy...	102	C5H10O2	000547-63-7	43
5	2,3,4-Trimethylpentanoic acid	144	C8H16O2	090435-18-0	42





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

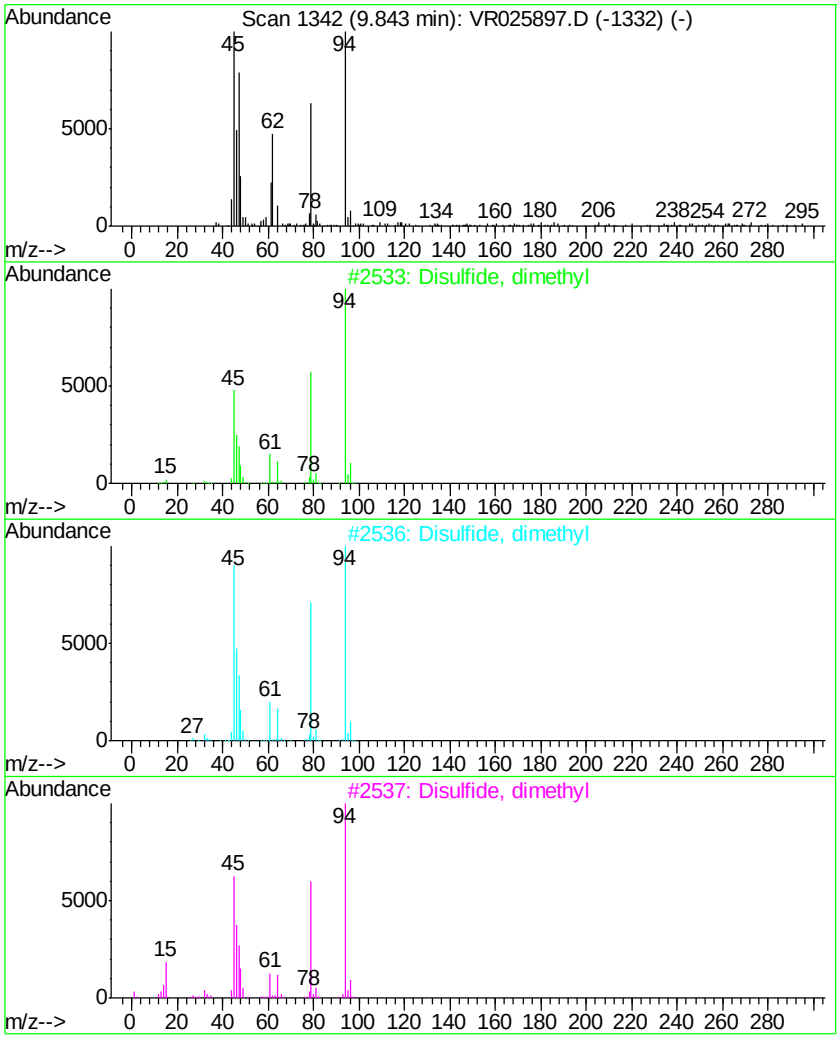
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

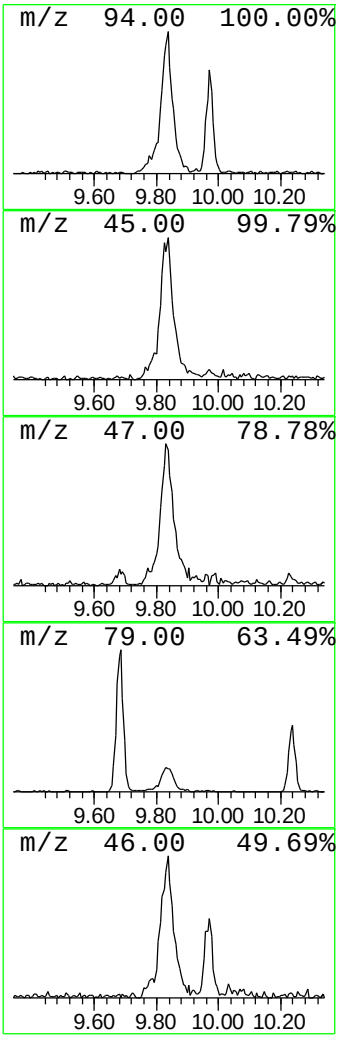
****

Peak Number 10 Disulfide, dimethyl Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	0.84 ug/L	224883	1,4-Difluorobenzene	8.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	70
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	58
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	47
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	43
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	37





Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

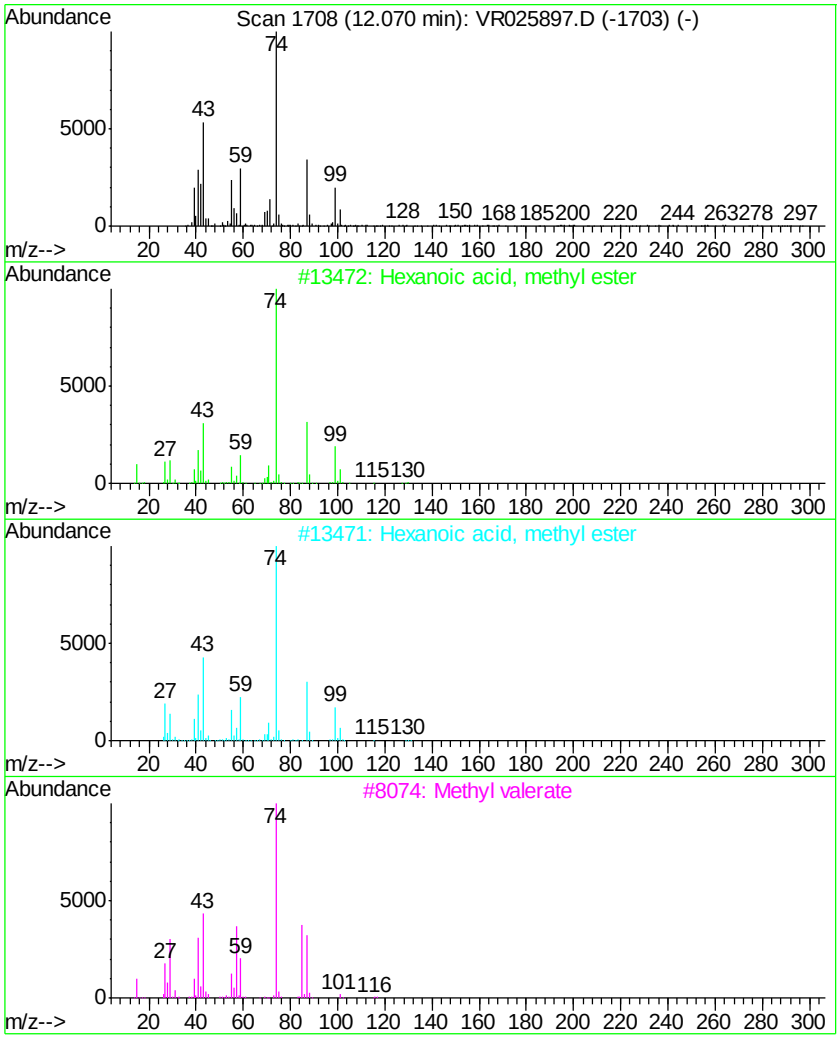
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

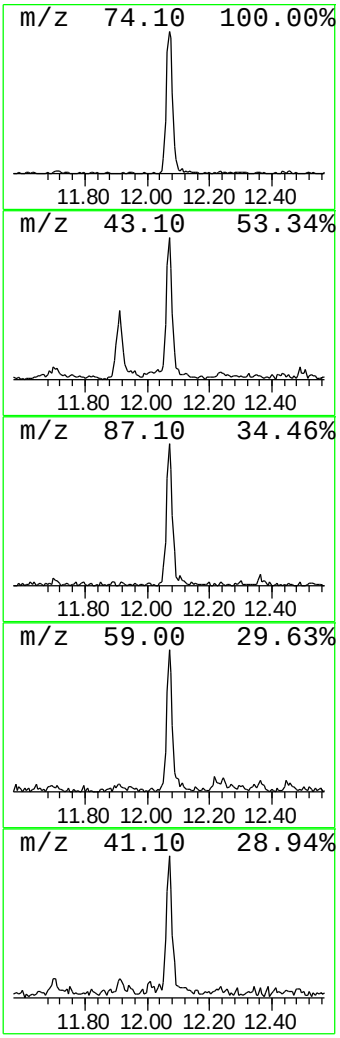
****

Peak Number 11 Hexanoic acid, methyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	0.60 ug/L	167897	Chlorobenzene-d5	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	59
2	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	59
3	Methyl valerate	116	C6H12O2	000624-24-8	53
4	Methyl valerate	116	C6H12O2	000624-24-8	53
5	Pentanoic acid, 3-methyl-, methy...	130	C7H14O2	002177-78-8	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

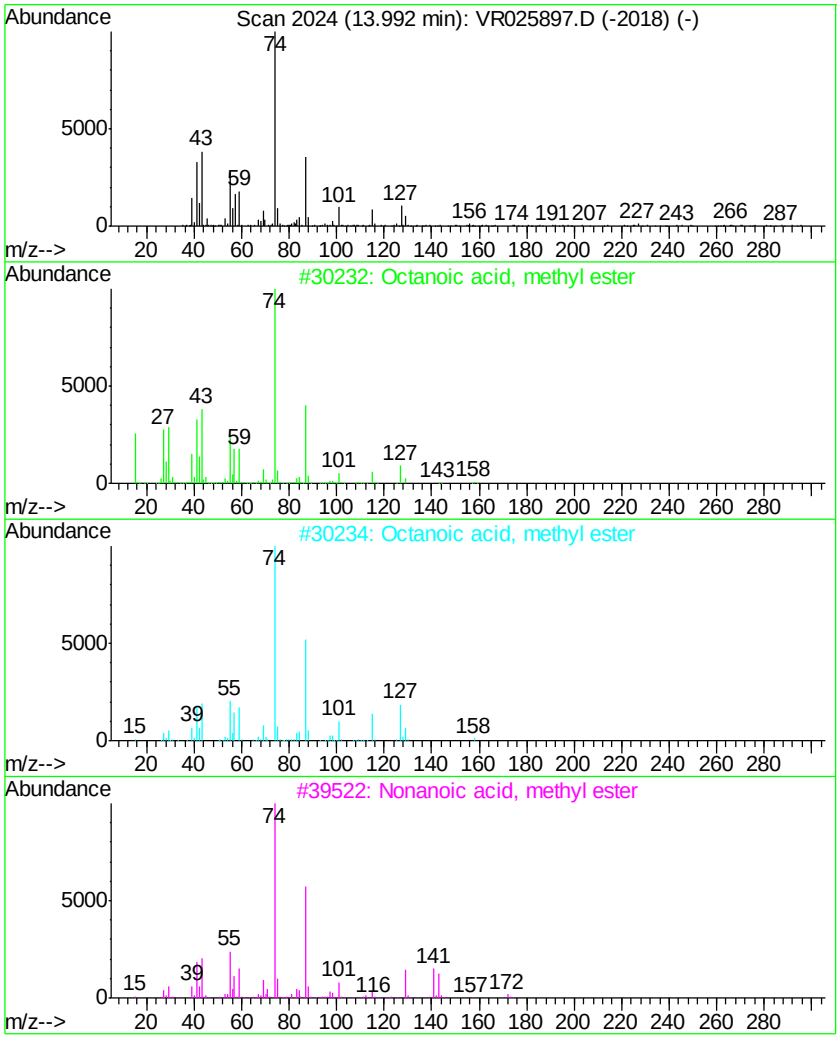
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

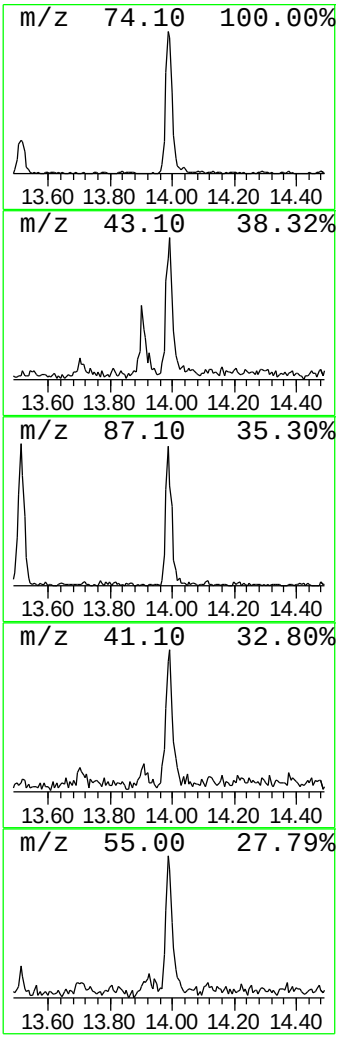
****

Peak Number 12 Octanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	0.72 ug/L	158509	1,4-Dichlorobenzene-d4	13.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	90
2	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	78
3	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	72
4	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	72
5	Methyl 6-methyl heptanoate	158	C9H18O2	002519-37-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_R\DATA\VR092818\
Data File : VR025897.D
Acq On : 28 Sep 2018 13:03
Operator : SY/MD
Sample : J5062-14
Misc : 25mL/MSVOA_R/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_R
ClientSampleId : GAC14

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.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
Methanethiol	2.43	32.8	ug/L	8765970	1	8.46	1335670	5.0
Ethanethiol	3.46	17.0	ug/L	4535820	1	8.46	1335670	5.0
Dimethyl sulfide	3.77	1.3	ug/L	347354	1	8.46	1335670	5.0
Propyl mercaptan	6.37	1.0	ug/L	268428	1	8.46	1335670	5.0
Ethane, (methylth...	6.50	1.4	ug/L	364267	1	8.46	1335670	5.0
1-Butanethiol	9.03	1.0	ug/L	272471	1	8.46	1335670	5.0
Butanoic acid, me...	9.29	0.8	ug/L	207708	1	8.46	1335670	5.0
Disulfide, dimethyl	9.84	0.8	ug/L	224883	1	8.46	1335670	5.0
Hexanoic acid, me...	12.07	0.6	ug/L	167897	2	11.29	1400270	5.0
Octanoic acid, me...	13.99	0.7	ug/L	158509	3	13.22	1094010	5.0