LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

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\SOMVTR122319WMA.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	1.116	5	8	20	rVB2	513953	510519	37.15%	3.640%
2	1.319	62	71	80	rBV2	329676	455573	33.15%	3.248%
3	1.480	114	121	139	rBV	216163	266466	19.39%	1.900%
4	1.582	146	153	165	rVB	196900	234777	17.09%	1.674%
5	1.785	211	216	222	rVB2	35156	39002	2.84%	0.278%
6	1.827	223	229	237	rBV4	33312	46753	3.40%	0.333%
7	1.997	279	282	290	rVB6	15846	19474	1.42%	0.139%
8	2.055	292	300	311	rVV	85351	121133	8.82%	0.864%
9	2.132	314	324	334	rVV	326557	476253	34.66%	3.396%
10	2.184	335	340	353	rVB	26818	42169	3.07%	0.301%
11	2.319	372	382	395	rBV	171151	252835	18.40%	1.803%
12	3.737	805	823	837	rBV9	16930	51557	3.75%	0.368%
13	3.923	871	881	909	rBV2	147910	399735	29.09%	2.850%
14	4.396	1010	1028	1056	rBV	270106	668576	48.65%	4.767%
15	5.094	1228	1245	1272	rBV2	552230	1374136	100.00%	9.798%
16	5.405	1327	1342	1352	rBV8	10650	27679	2.01%	0.197%
17	5.659	1406	1421	1442	rBV	467879	938248	68.28%	6.690%
18	6.113	1545	1562	1582	rBV	309292	647763	47.14%	4.619%
19	6.341	1625	1633	1643	rVB2	10483	19566	1.42%	0.140%
20	7.026	1830	1846	1863	rBV	134266	246444	17.93%	1.757%
21	7.357	1933	1949	1964	rBV	636687	1109384	80.73%	7.910%
22	7.431	1964	1972	1983	rVB	20341	42917	3.12%	0.306%
23	7.563	2002	2013	2025	rBV	80014	140428	10.22%	1.001%
24	7.659	2034	2043	2055	rBV	80574	135487	9.86%	0.966%
25	8.129	2176	2189	2222	rBV	512752	1114276	81.09%	7.945%
26	8.280	2227	2236	2256	rVB3	134049	241554	17.58%	1.722%
27	8.891	2412	2426	2451	rBV	689117	1133256	82.47%	8.080%
28	9.145	2495	2505	2517	rBV2	18359	35954	2.62%	0.256%
29	9.852	2716	2725	2737	rBV6	26571	46678	3.40%	0.333%
30	10.257	2830	2851	2865	rBV2	204057	354305	25.78%	2.526%
31	10.759	2998	3007	3013	rBV3	9733	15398	1.12%	0.110%
32	11.193	3131	3142	3154	rBV2	64718	110918	8.07%	0.791%
33	11.289	3159	3172	3194	rVV	683026	1091067	79.40%	7.779%
34	11.392	3195	3204	3215	rVB	16341	32450	2.36%	0.231%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

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\SOMVTR122319WMA.M
Title : TRACE VOA SOM01.0

35	11.666	3276	3289	3312	rBV	588467	942381	68.58%	6.719%
36	11.804	3324	3332	3344	rVB	39162	63165	4.60%	0.450%
37	12.389	3502	3514	3532	rBV	322948	517695	37.67%	3.691%
38	12.920	3670	3679	3686	rBV	28381	40851	2.97%	0.291%
39	13.206	3758	3768	3776	rBV	10239	18353	1.34%	0.131%

Sum of corrected areas: 14025175

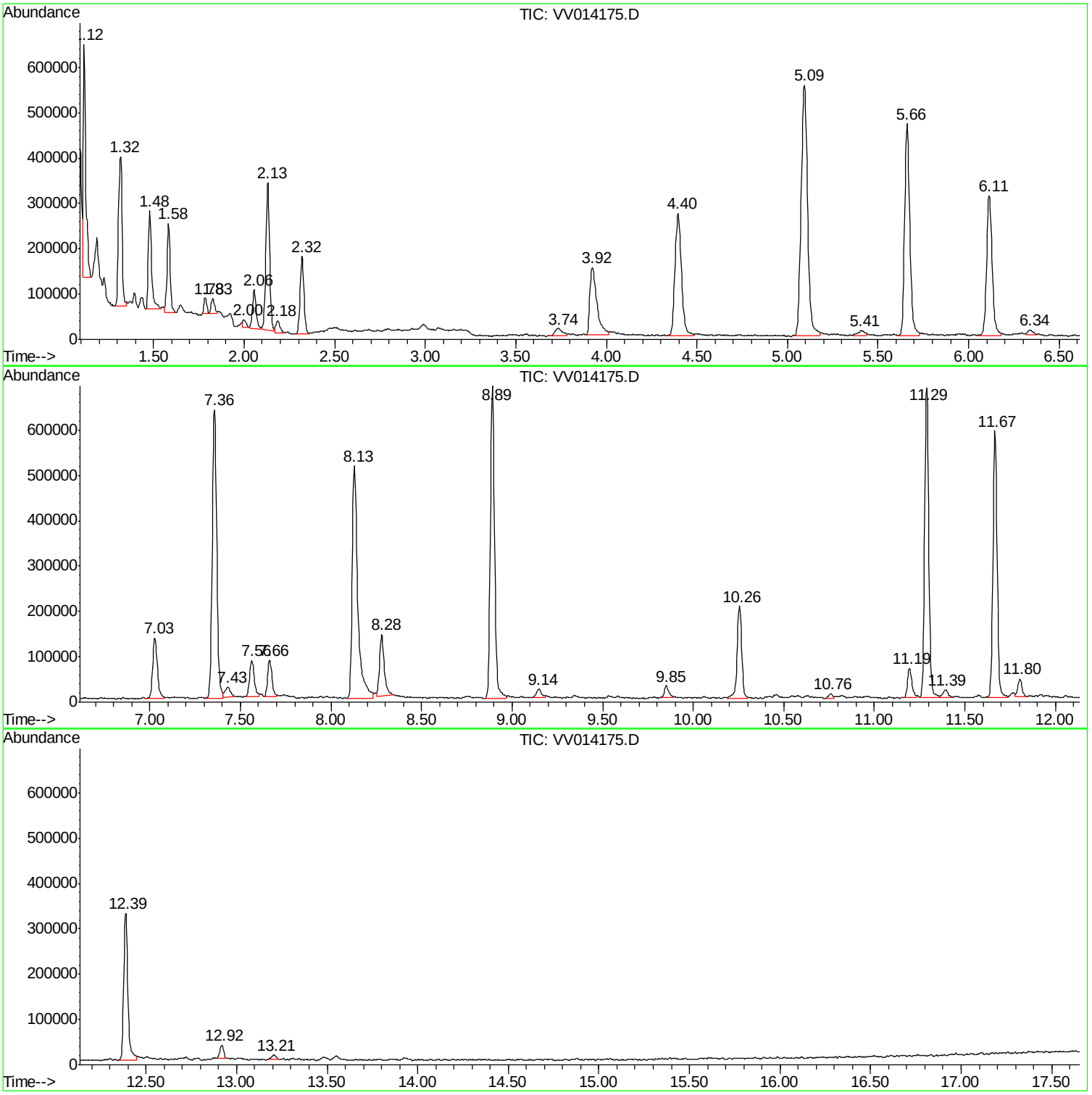
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.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\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

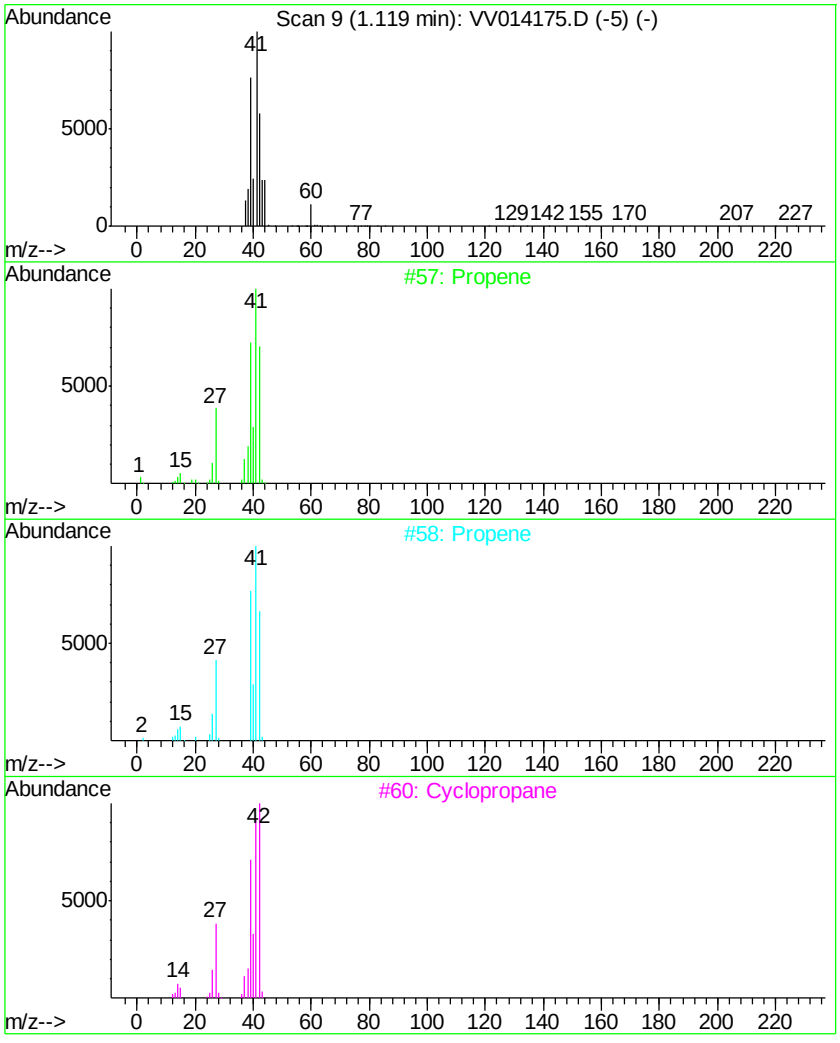
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

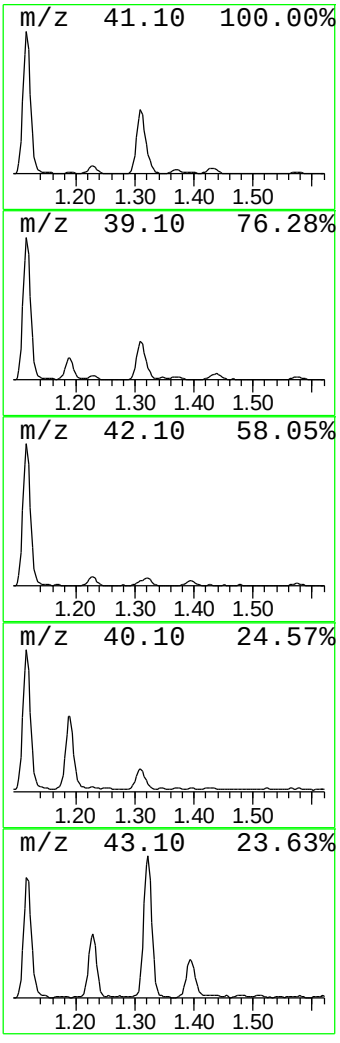
****

Peak Number 1 (DEL) Alkane: Cyclic1.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	2.72 ug/L	510519	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropene	40	C3H4	002781-85-3	9
5	Cyclopropane	42	C3H6	000075-19-4	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

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

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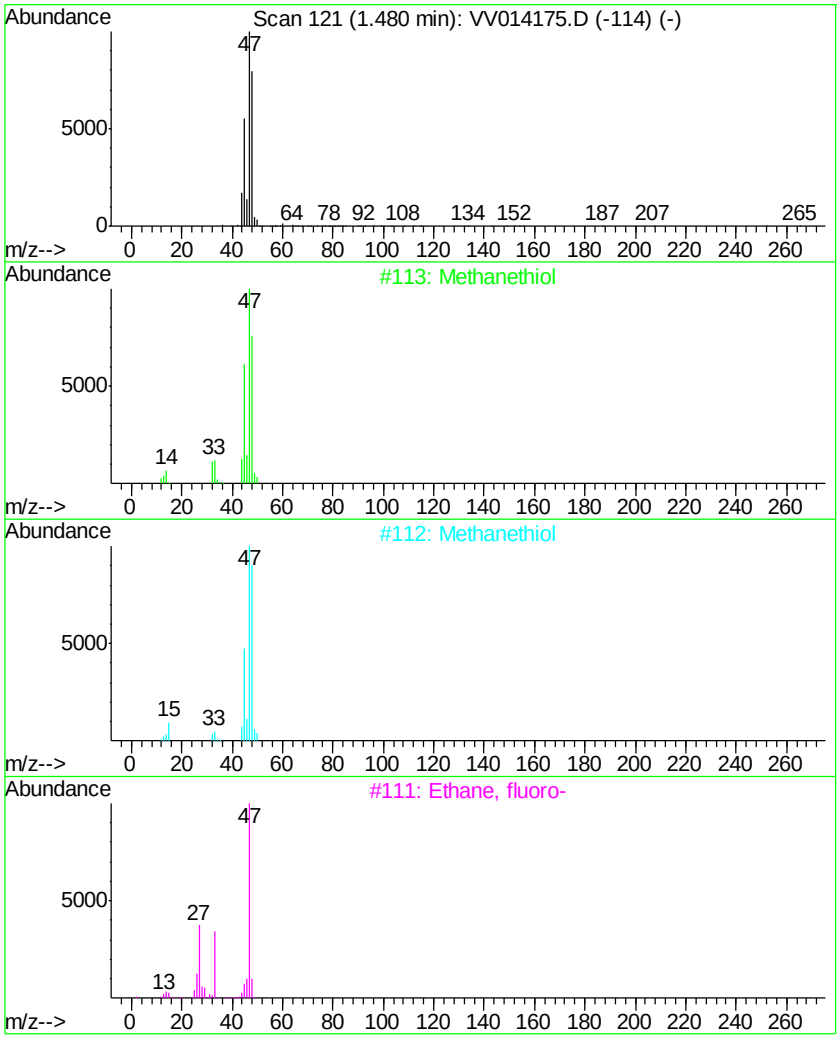
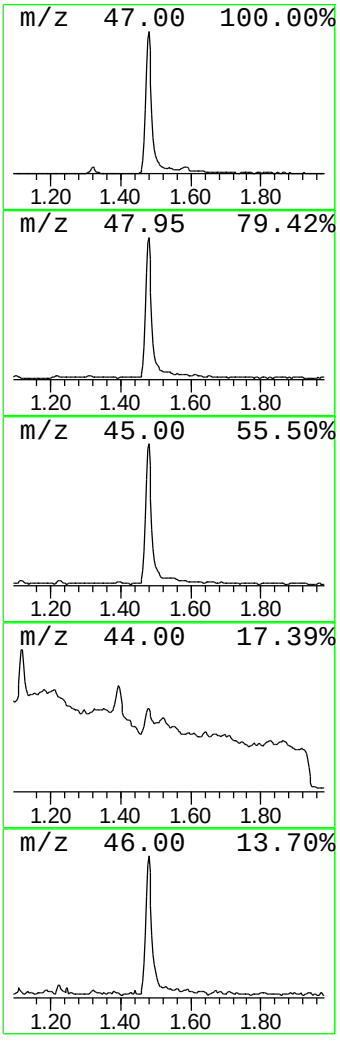
Peak Number 2 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	1.42 ug/L	266466	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Methanethiol	48	CH4S	000074-93-1	72
3	Ethane, fluoro-	48	C2H5F	000353-36-6	5
4	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	4
5	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

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

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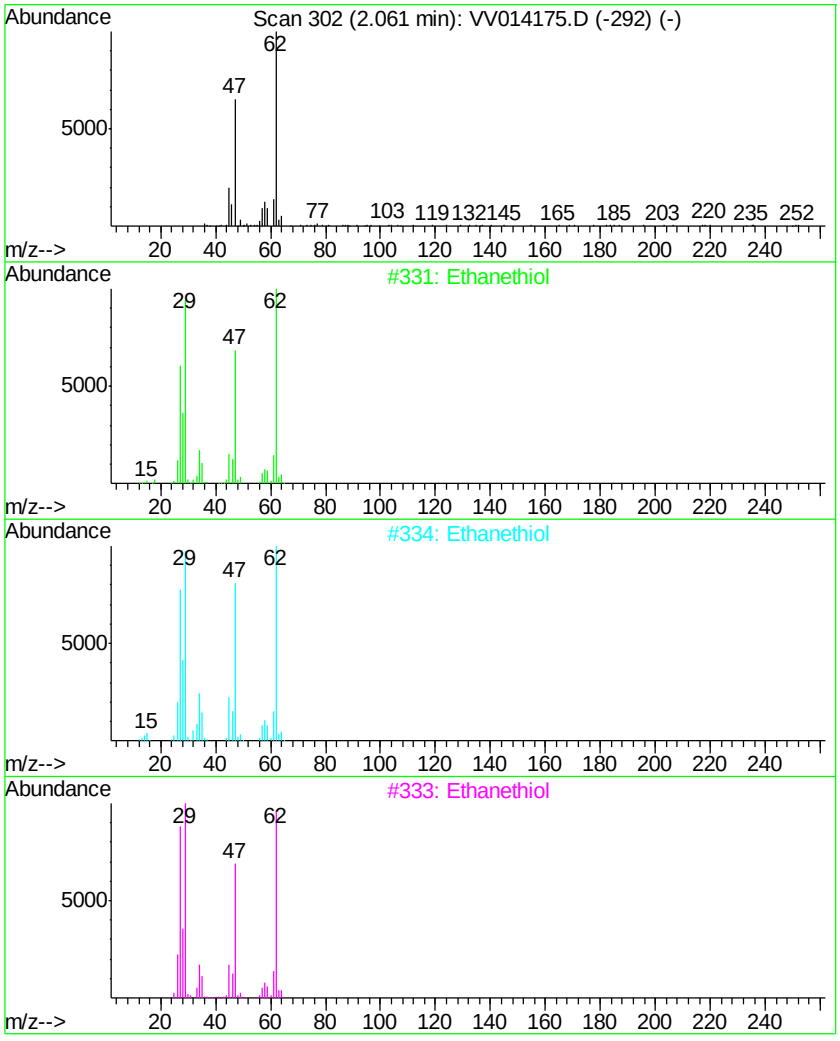
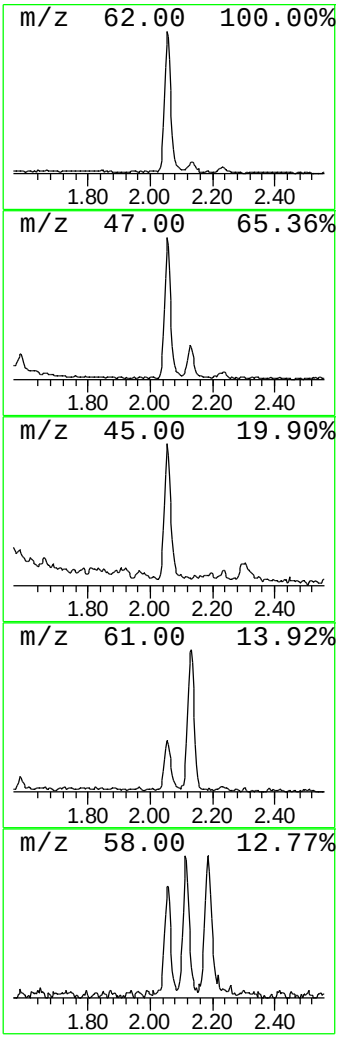
Peak Number 3 Ethanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	0.65 ug/L	121133	1,4-Difluorobenzene	5.66

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	90





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

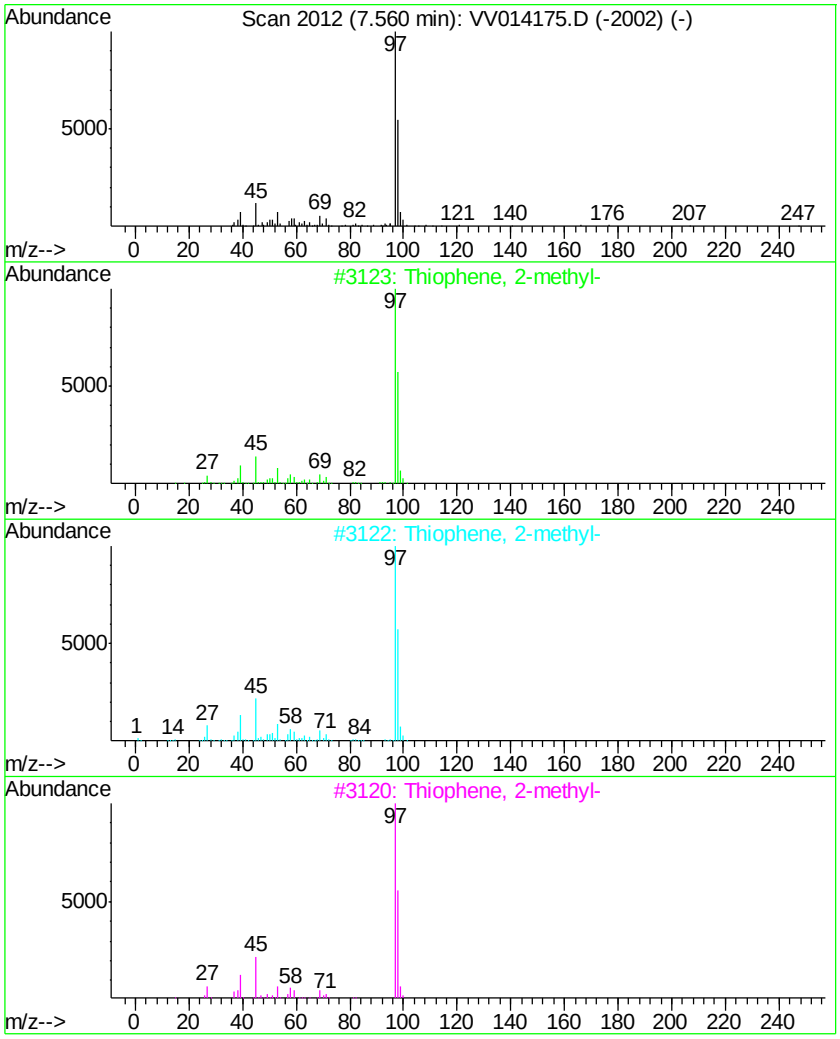
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

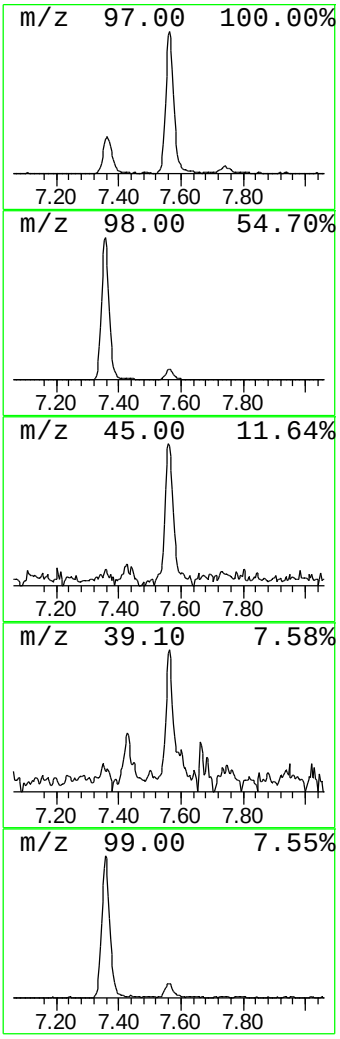
****

Peak Number 5 Thiophene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	0.62 ug/L	140428	Chlorobenzene-d5	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-methyl-	98	C5H6S	000554-14-3	94
2	Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
3	Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
4	Thiophene, 3-methyl-	98	C5H6S	000616-44-4	90
5	Thiophene, 3-methyl-	98	C5H6S	000616-44-4	90





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

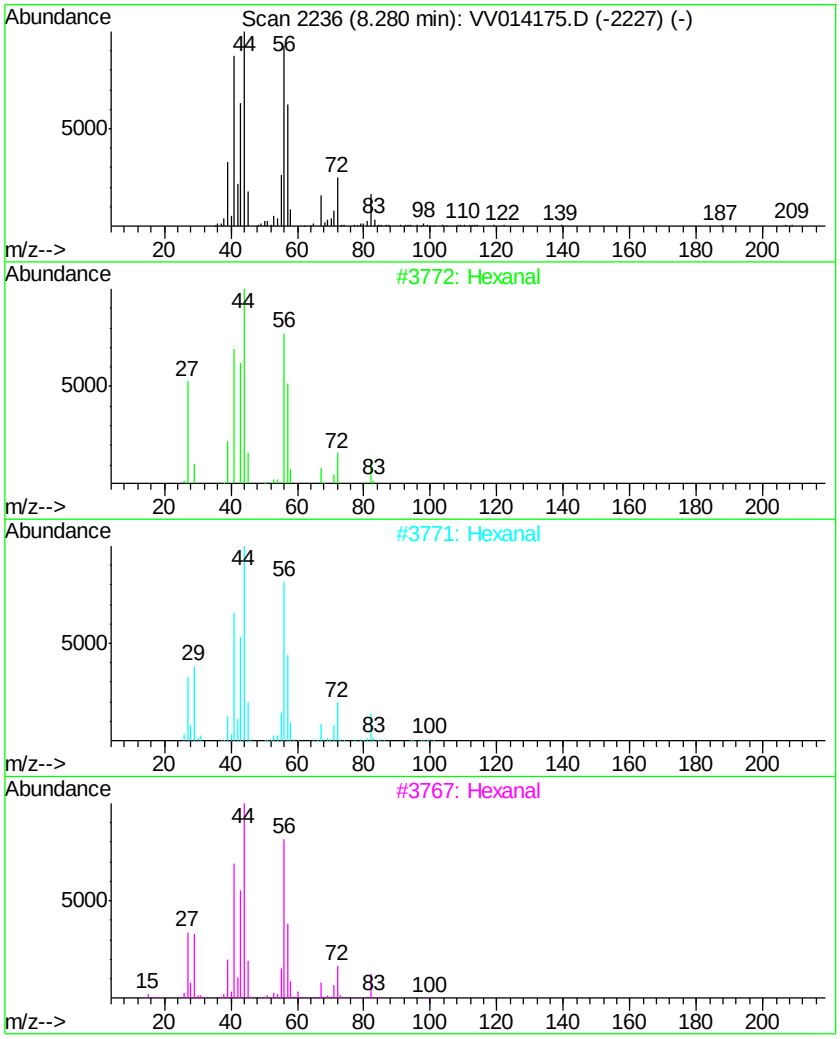
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

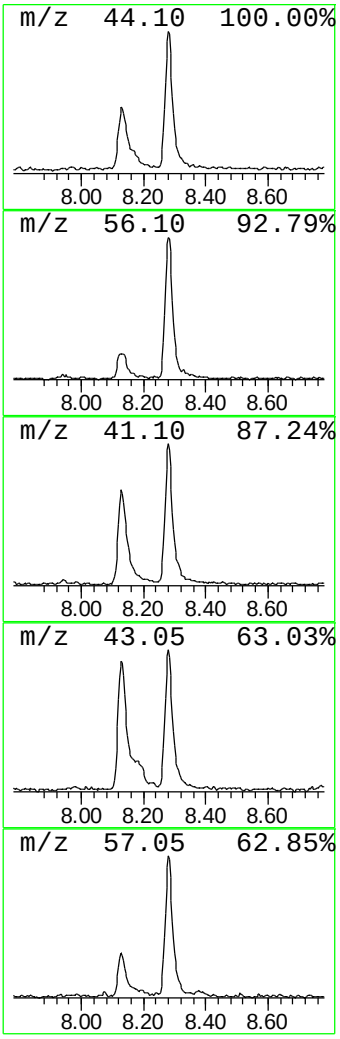
****

Peak Number 6 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	1.07 ug/L	241554	Chlorobenzene-d5	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	80
2	Hexanal	100	C6H12O	000066-25-1	78
3	Hexanal	100	C6H12O	000066-25-1	72
4	Hexanal	100	C6H12O	000066-25-1	42
5	Butanal, 3-methyl-	86	C5H10O	000590-86-3	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

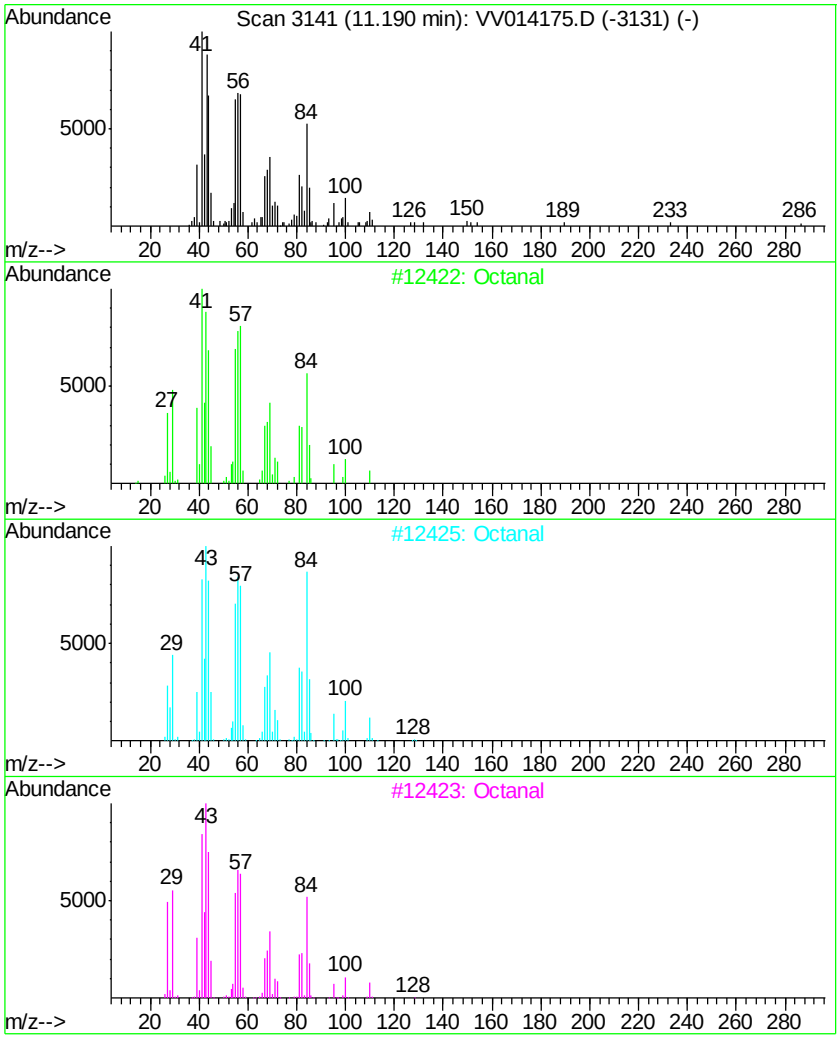
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

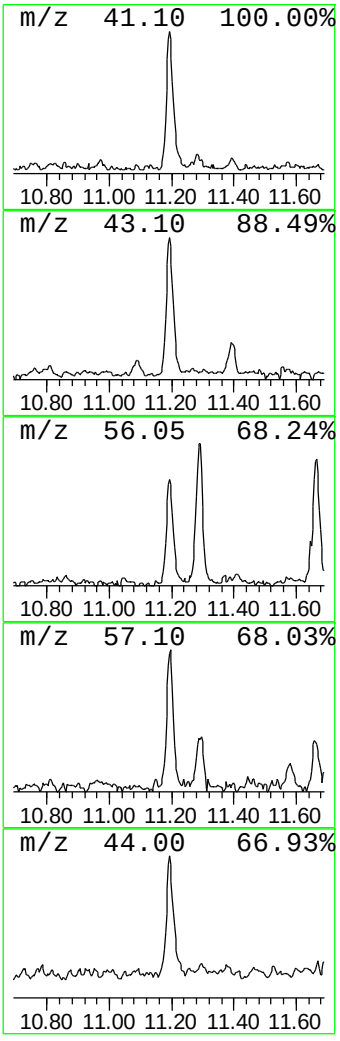
****

Peak Number 7 Octanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	0.51 ug/L	110918	1,4-Dichlorobenzene-d4	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	91
2	Octanal	128	C8H16O	000124-13-0	90
3	Octanal	128	C8H16O	000124-13-0	87
4	Octanal	128	C8H16O	000124-13-0	80
5	2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFE04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

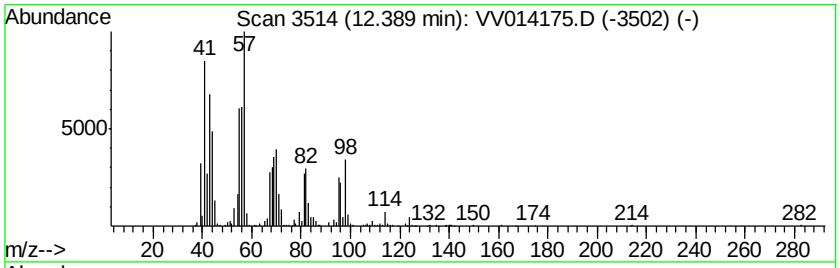
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

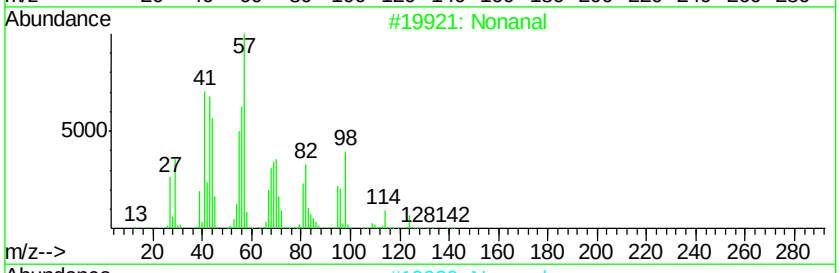
****

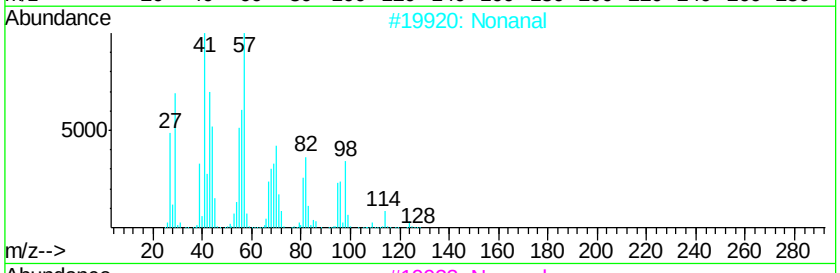
Peak Number 8 Nonanal Concentration Rank 2

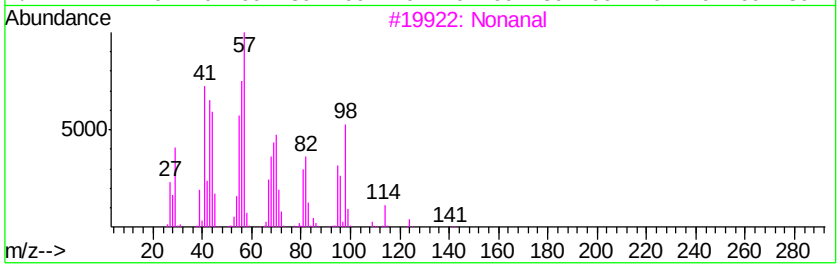
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	2.37 ug/L	517695	1,4-Dichlorobenzene-d4	11.29

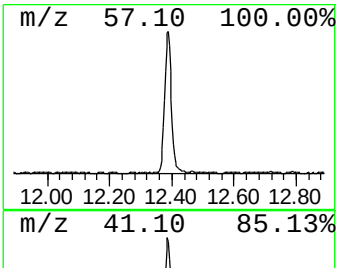
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	96
2	Nonanal	142	C9H18O	000124-19-6	91
3	Nonanal	142	C9H18O	000124-19-6	90
4	Nonanal	142	C9H18O	000124-19-6	64
5	2-Nonen-1-ol	142	C9H18O	022104-79-6	41

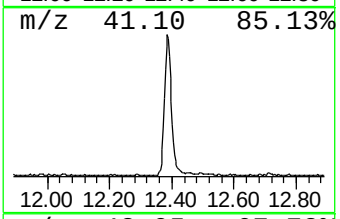


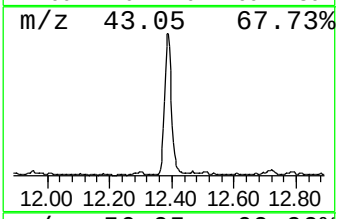


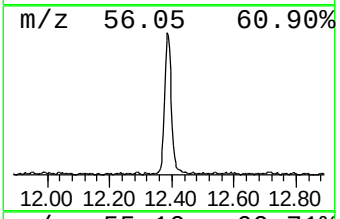


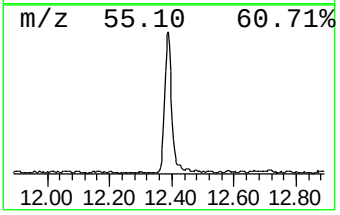












Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014175.D
Acq On : 23 Dec 2019 22:19
Operator : SY/MD
Sample : K6404-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_V
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.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
(DEL) Alkane: Cyc...	1.12	2.7	ug/L	510519	1	5.66	938248	5.0
Methanethiol	1.48	1.4	ug/L	266466	1	5.66	938248	5.0
Ethanethiol	2.06	0.7	ug/L	121133	1	5.66	938248	5.0
Thiophene, 2-methyl-	7.56	0.6	ug/L	140428	2	8.89	1133260	5.0
Hexanal	8.28	1.1	ug/L	241554	2	8.89	1133260	5.0
Octanal	11.19	0.5	ug/L	110918	3	11.29	1091070	5.0
Nonanal	12.39	2.4	ug/L	517695	3	11.29	1091070	5.0