LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

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\SOMVTR112219WMA.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	6	8	24	rVB2	105913	128405	3.71%	0.533%
2	1.203	29	35	62	rBV	1259331	2075136	59.92%	8.620%
3	1.315	65	70	80	rVB	186994	213728	6.17%	0.888%
4	1.476	115	120	128	rVB	66698	71005	2.05%	0.295%
5	1.582	147	153	174	rVB	145797	209644	6.05%	0.871%
6	2.138	314	326	333	rBV	2387421	3463016	100.00%	14.385%
7	2.183	333	340	366	rVB	1329507	2003948	57.87%	8.324%
8	2.299	367	376	395	rVB	194218	347502	10.03%	1.443%
9	2.534	439	449	464	rVB	42633	72971	2.11%	0.303%
10	2.987	577	590	607	rBV	80862	163490	4.72%	0.679%
11	3.225	647	664	690	rBV	1261191	2603073	75.17%	10.813%
12	3.720	804	818	847	rBV	223634	564122	16.29%	2.343%
13	3.926	870	882	886	rBV2	192115	369992	10.68%	1.537%
14	4.399	1008	1029	1048	rBV2	207661	516810	14.92%	2.147%
15	5.093	1225	1245	1265	rBV2	447487	1108611	32.01%	4.605%
16	5.659	1406	1421	1447	rBV	348426	691300	19.96%	2.872%
17	5.955	1496	1513	1538	rBV	1541459	2960243	85.48%	12.296%
18	6.113	1549	1562	1580	rBV	256293	517359	14.94%	2.149%
19	6.219	1585	1595	1613	rVB3	61874	124001	3.58%	0.515%
20	6.608	1704	1716	1732	rBV5	15695	39335	1.14%	0.163%
21	7.026	1836	1846	1864	rVB2	123733	217240	6.27%	0.902%
22	7.177	1881	1893	1905	rBV2	133984	262699	7.59%	1.091%
23	7.357	1936	1949	1965	rBV	524265	902556	26.06%	3.749%
24	7.659	2032	2043	2056	rBV2	75043	128743	3.72%	0.535%
25	8.129	2177	2189	2218	rBV	636636	1273356	36.77%	5.289%
26	8.280	2227	2236	2260	rVB	117621	230423	6.65%	0.957%
27	8.891	2415	2426	2453	rBV	520850	856428	24.73%	3.557%
28	9.852	2709	2725	2734	rBV5	31460	63099	1.82%	0.262%
29	10.254	2840	2850	2867	rVB	219744	354466	10.24%	1.472%
30	11.289	3159	3172	3188	rBV	449661	712179	20.57%	2.958%
31	11.669	3278	3290	3311	rBV	464776	750939	21.68%	3.119%
32	12.392	3507	3515	3529	rBV4	45209	78489	2.27%	0.326%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

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\SOMVTR112219WMA.M
Title : TRACE VOA SOM01.0

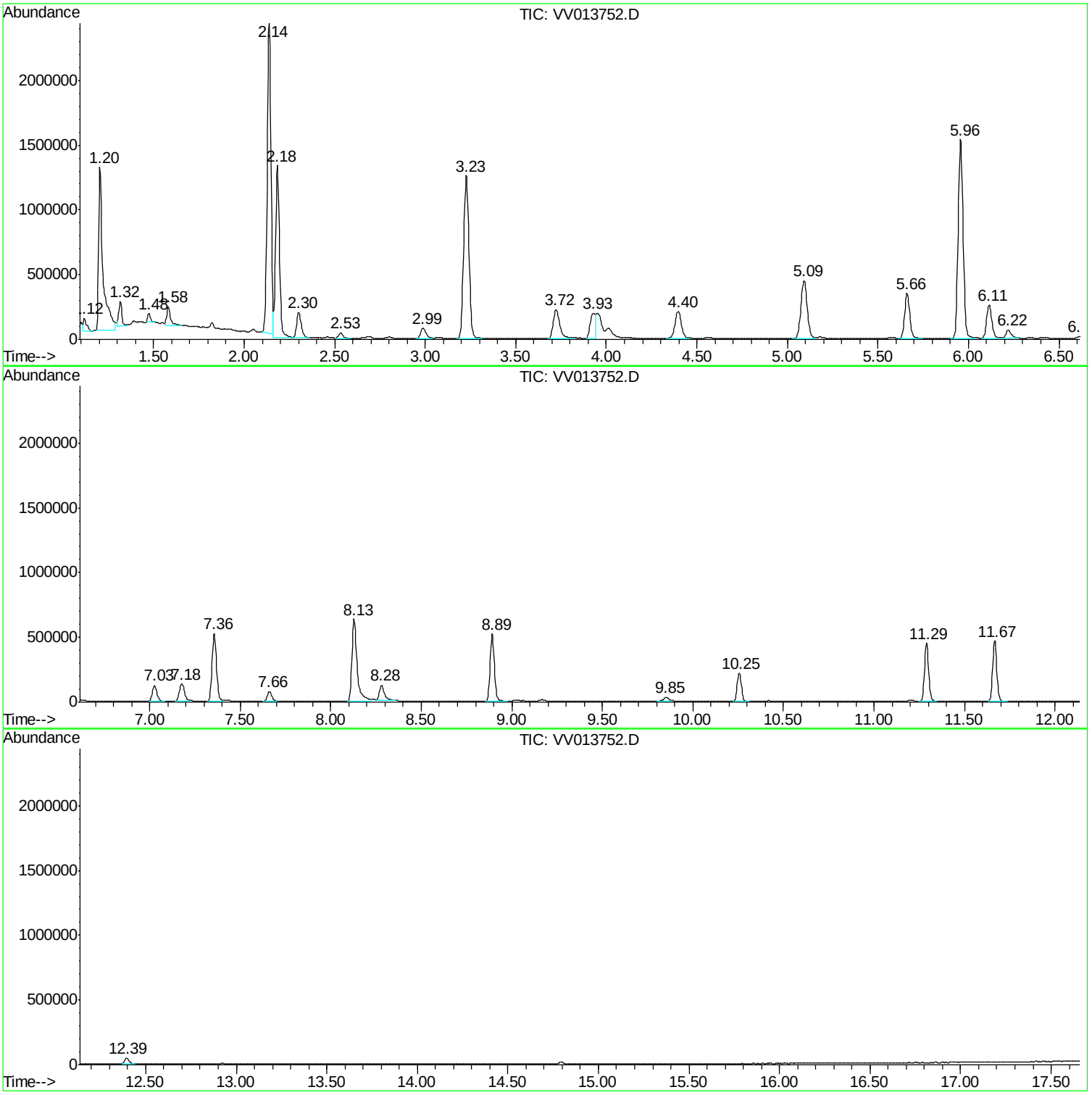
Sum of corrected areas: 24074308

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.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\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

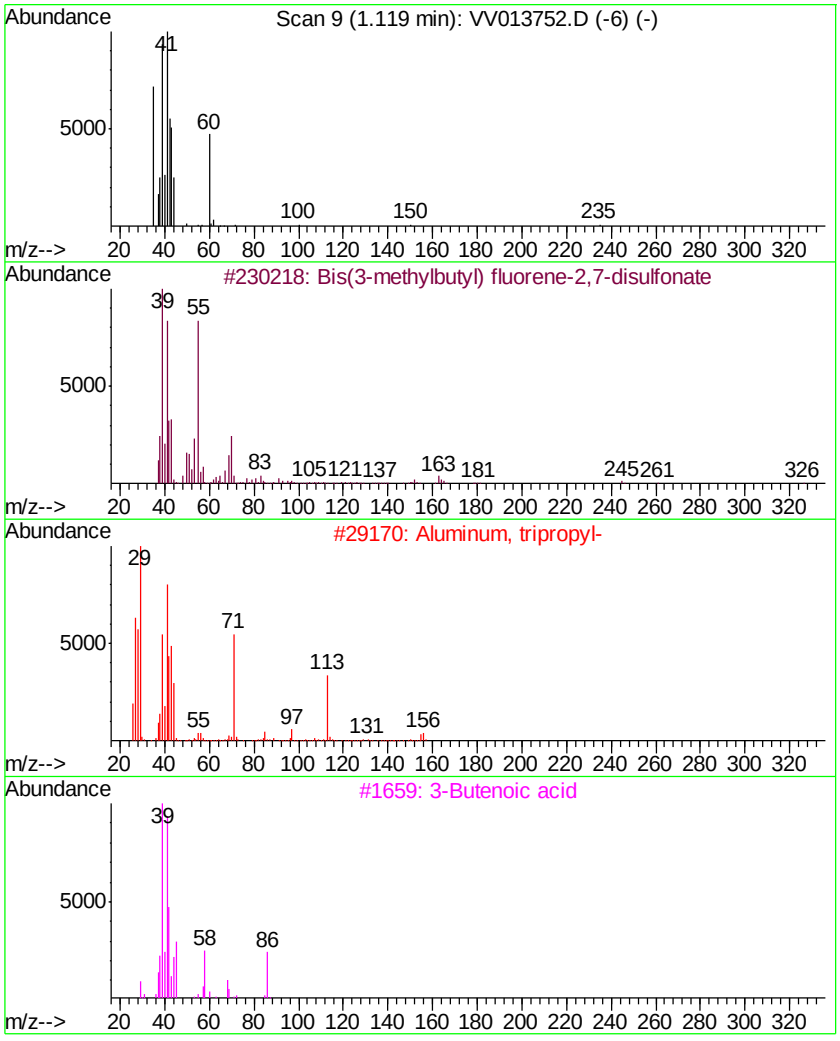
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

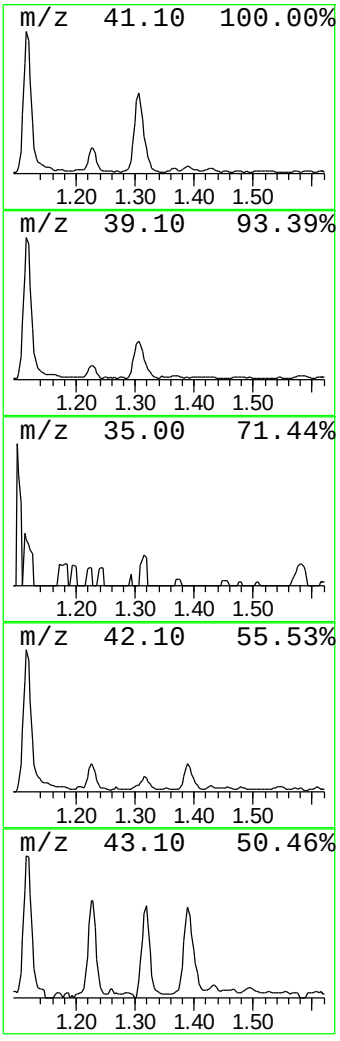
****

Peak Number 1 Bis(3-methylbutyl) fluorene... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	0.93 ug/L	128405	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	72
2	Aluminum, tripropyl-	156	C9H21Al	000102-67-0	59
3	3-Butenoic acid	86	C4H6O2	000625-38-7	50
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	50
5	Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

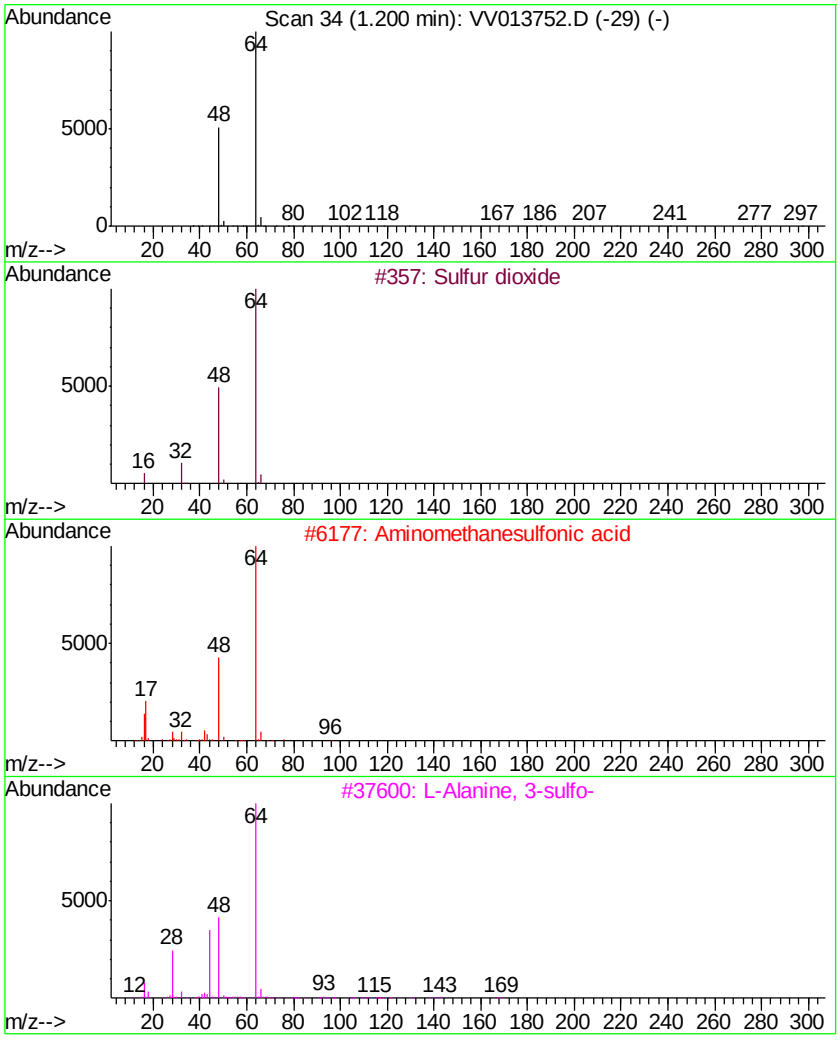
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

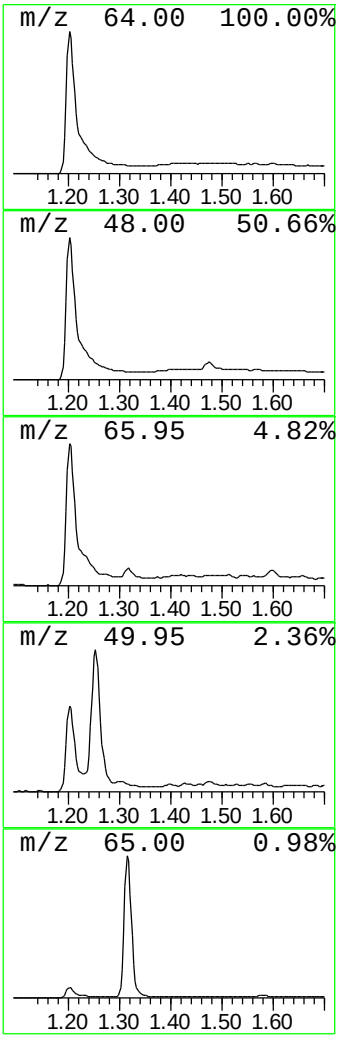
****

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.20	15.01 ug/L	2075140	1,4-Difluorobenzene	5.66

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	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

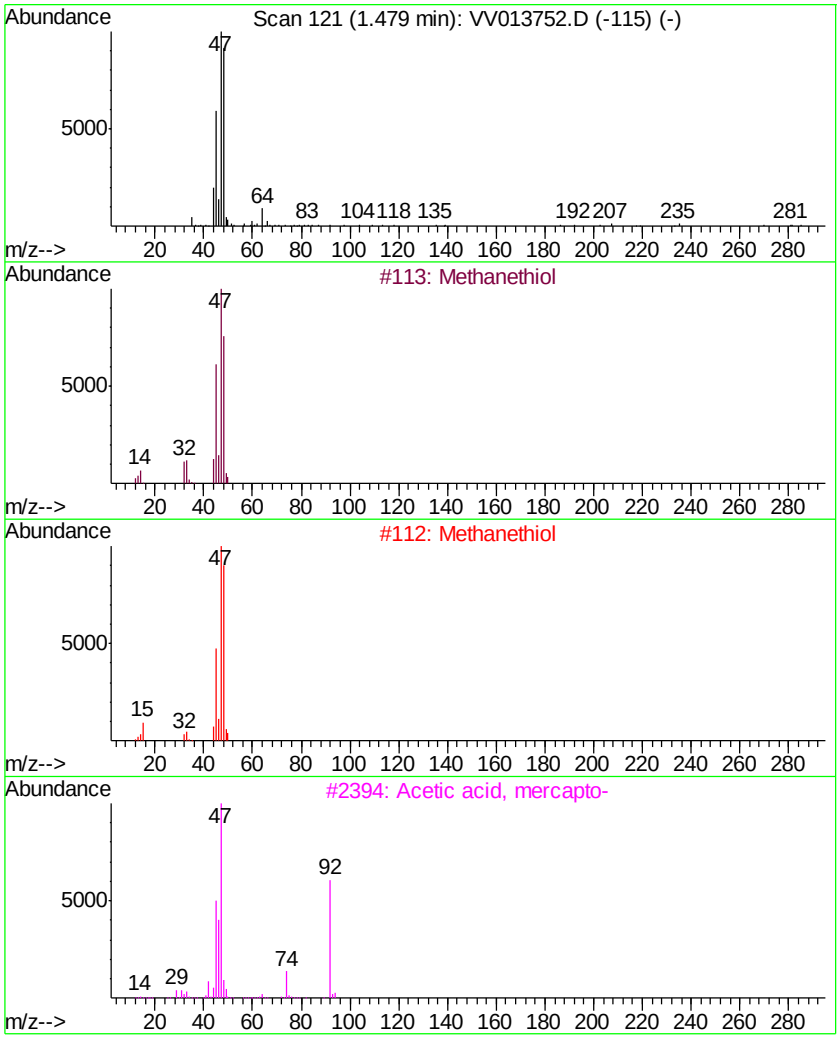
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

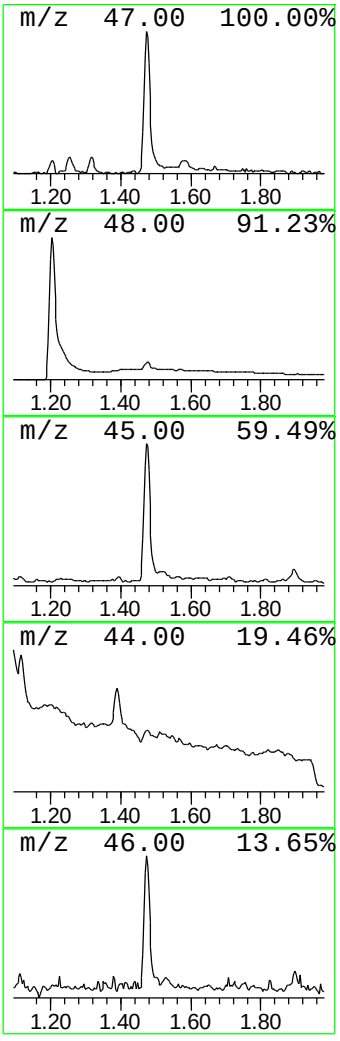
****

Peak Number 3 Methanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	0.51 ug/L	71005	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Methanethiol	48	CH4S	000074-93-1	86
3	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
4	Methional	104	C4H8OS	003268-49-3	9
5	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

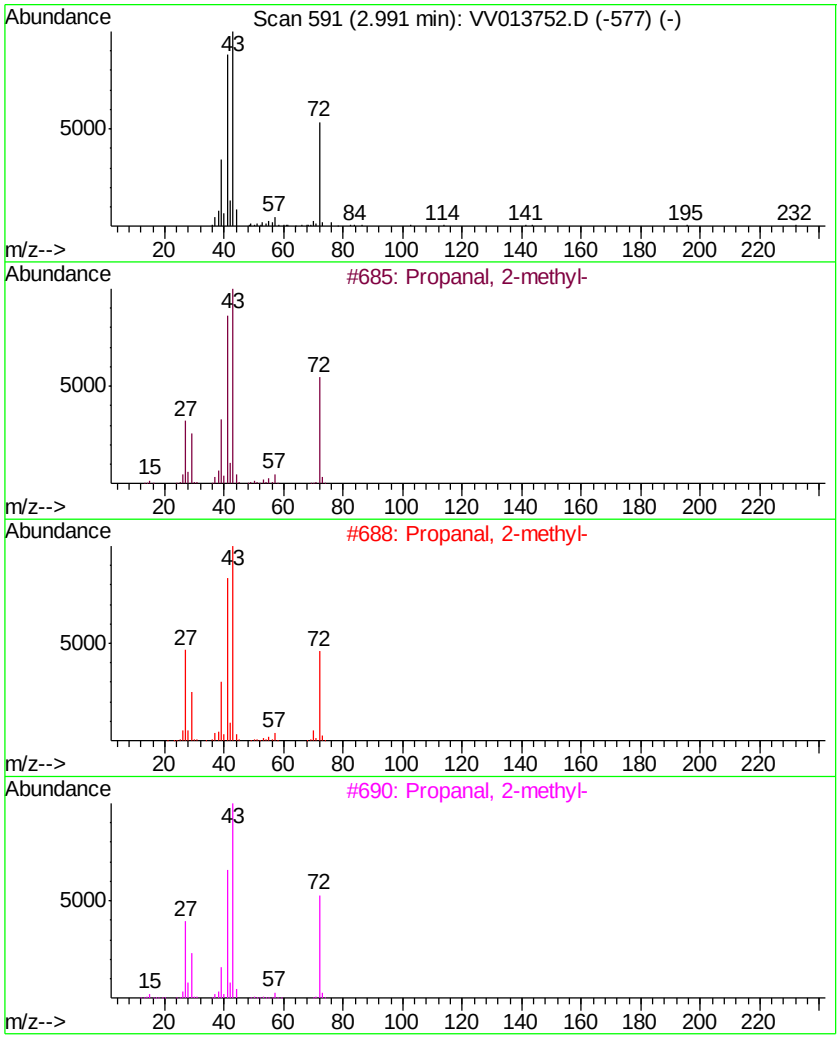
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

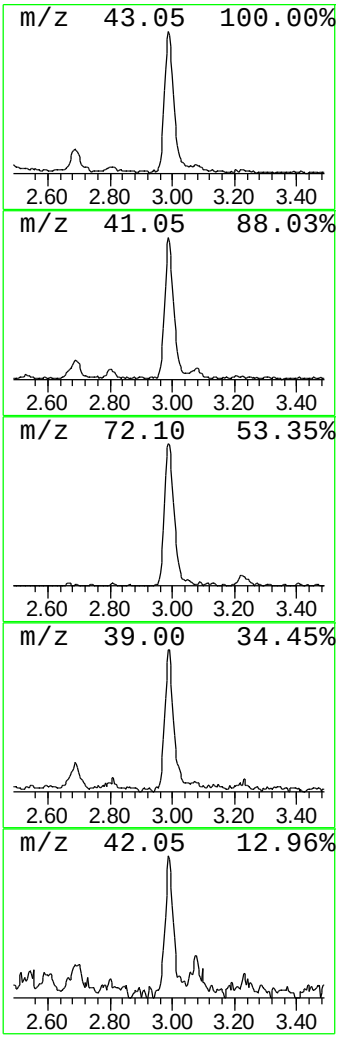
****

Peak Number 4 Propanal, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	1.18 ug/L	163490	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	90
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	90
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	72
4	Butanal	72	C4H8O	000123-72-8	58
5	Isobutylene epoxide	72	C4H8O	000558-30-5	42





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

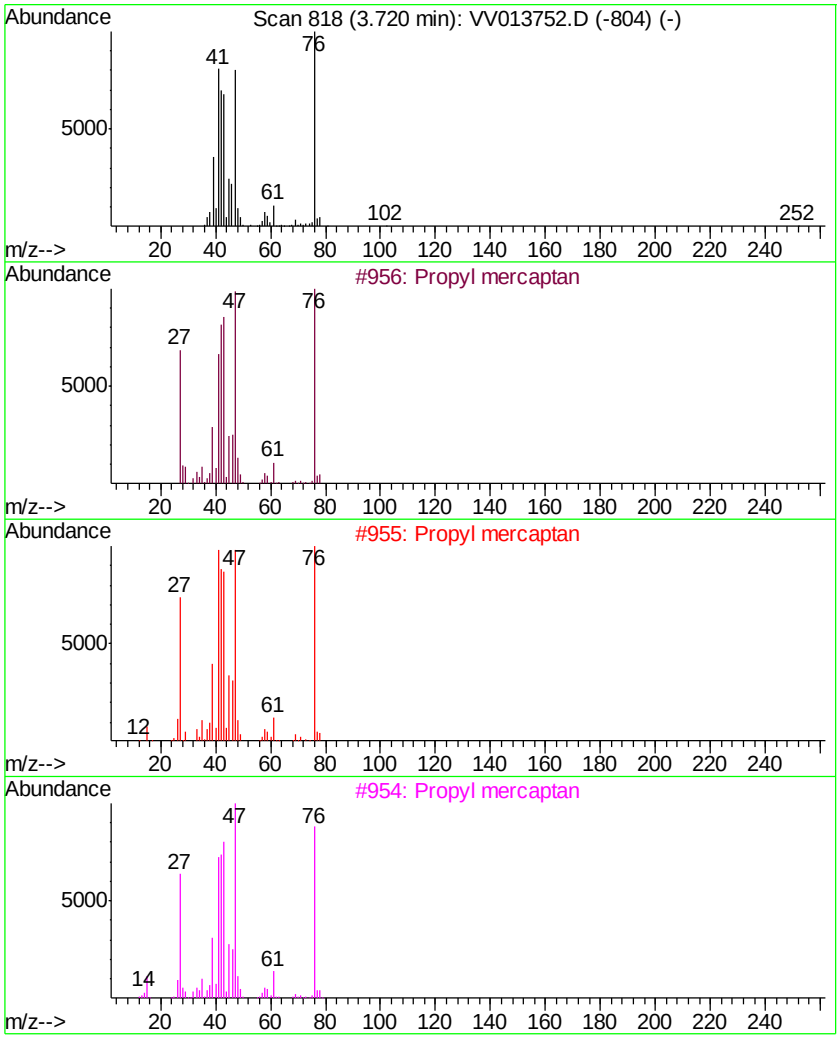
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

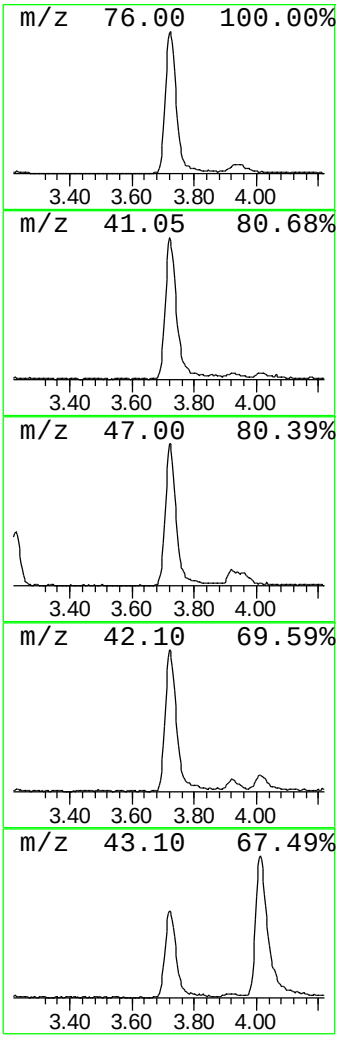
****

Peak Number 5 Propyl mercaptan Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	4.08 ug/L	564122	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	97
2	Propyl mercaptan	76	C3H8S	000107-03-9	96
3	Propyl mercaptan	76	C3H8S	000107-03-9	96
4	Propyl mercaptan	76	C3H8S	000107-03-9	95
5	Propyl mercaptan	76	C3H8S	000107-03-9	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

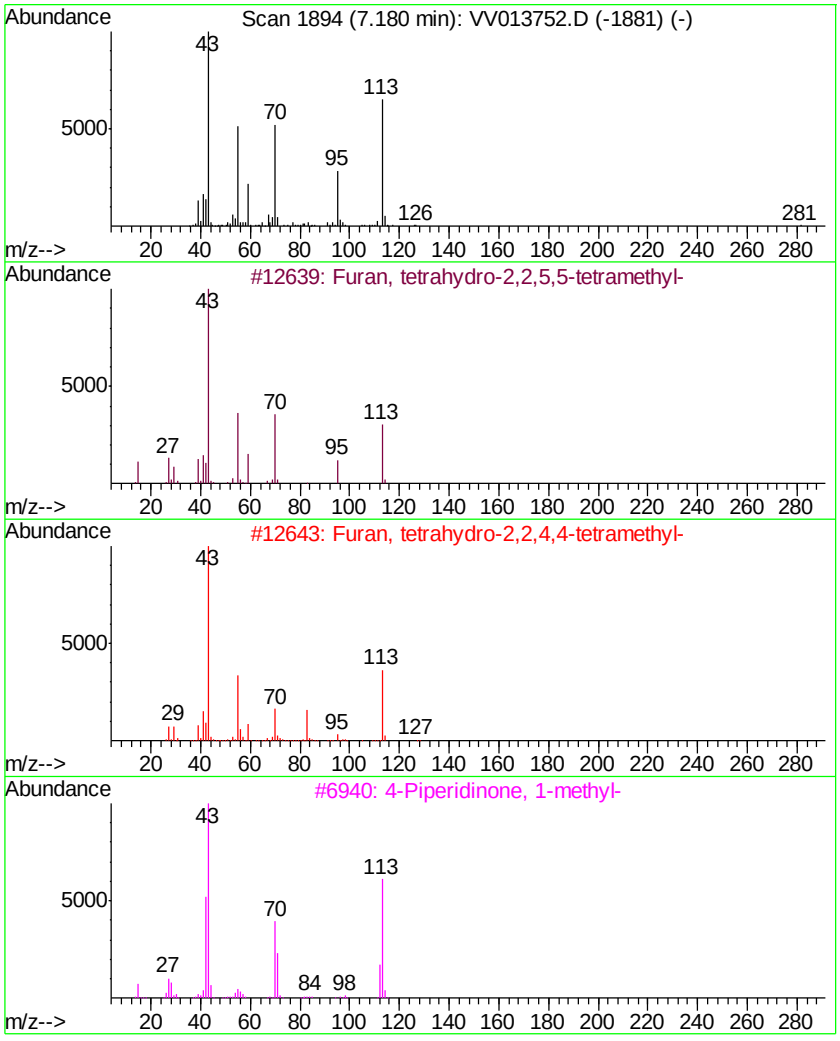
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

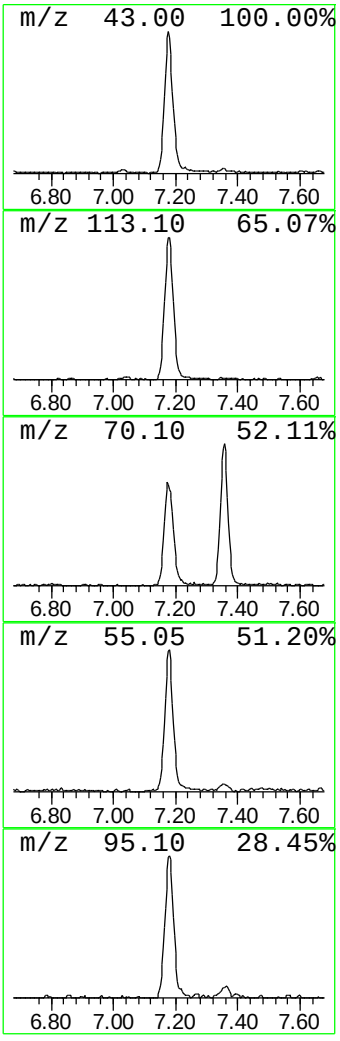
****

Peak Number 7 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	1.90 ug/L	262699	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	52
4	1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	43
5	1-[2-(3,4-Dichlorophenyl)ethyl]-...	272	C13H18Cl2N2	150208-28-9	43





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

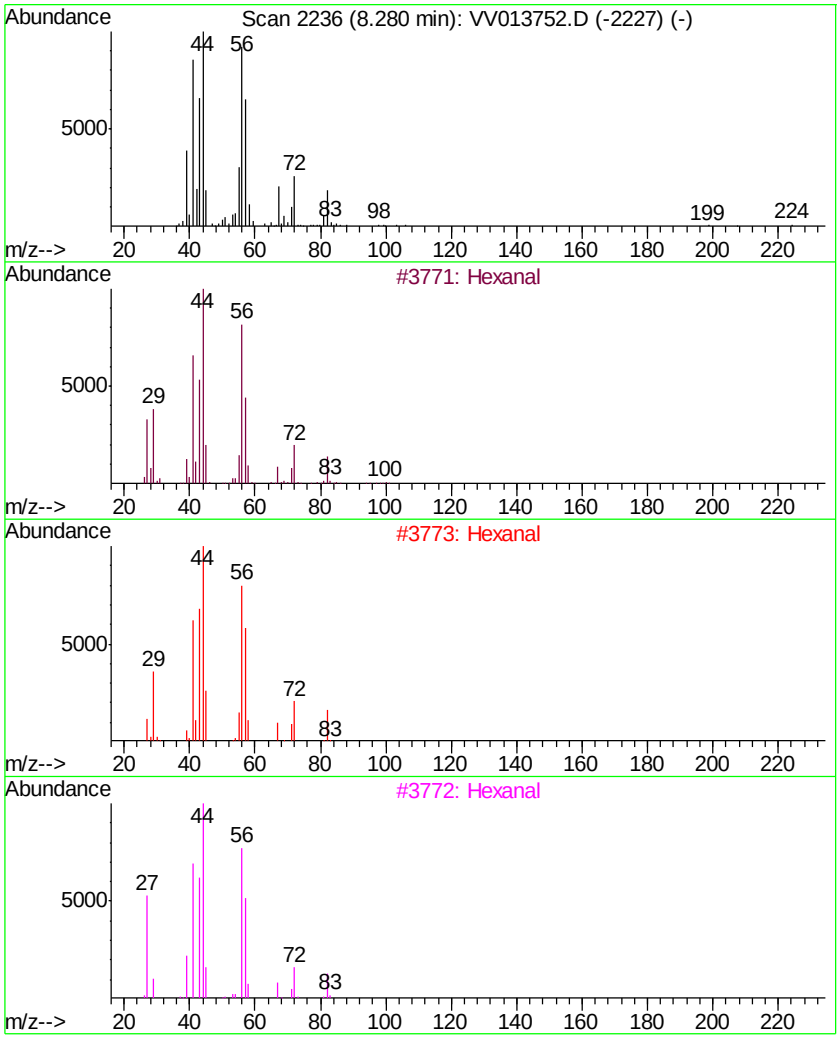
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

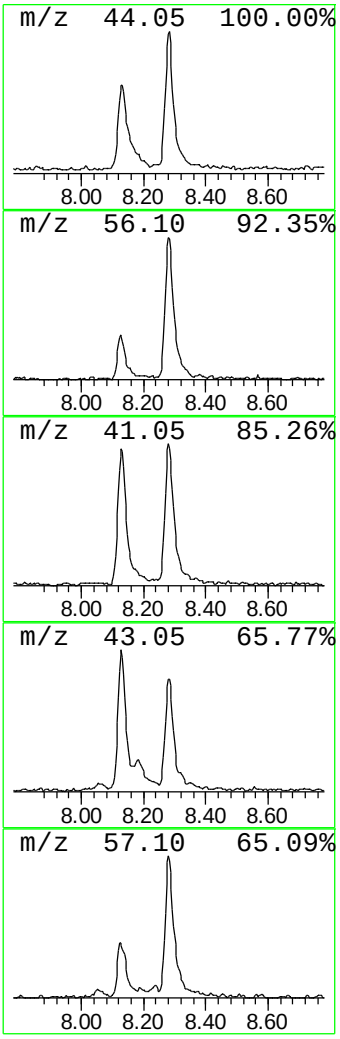
****

Peak Number 8 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	1.35 ug/L	230423	Chlorobenzene-d5	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	64
2	Hexanal	100	C6H12O	000066-25-1	64
3	Hexanal	100	C6H12O	000066-25-1	64
4	Hexanal	100	C6H12O	000066-25-1	58
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35





Library Search Compound Report

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ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.M
Quant Title : TRACE VOA SOM01.0

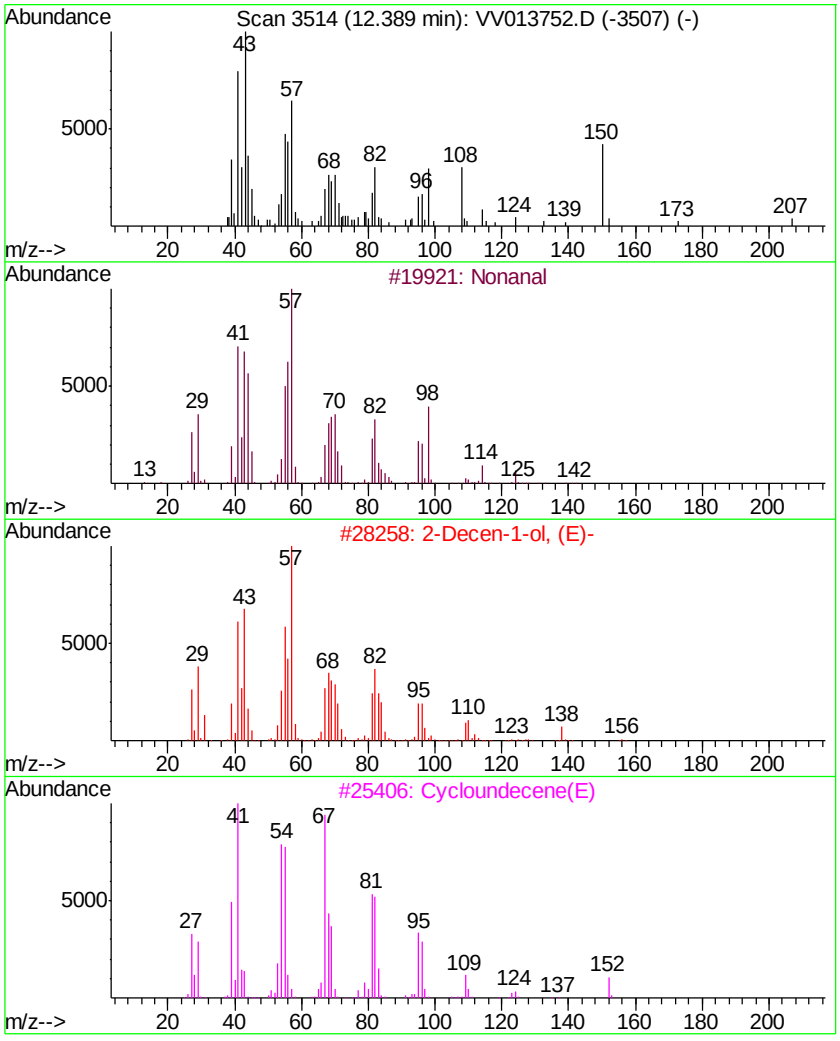
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

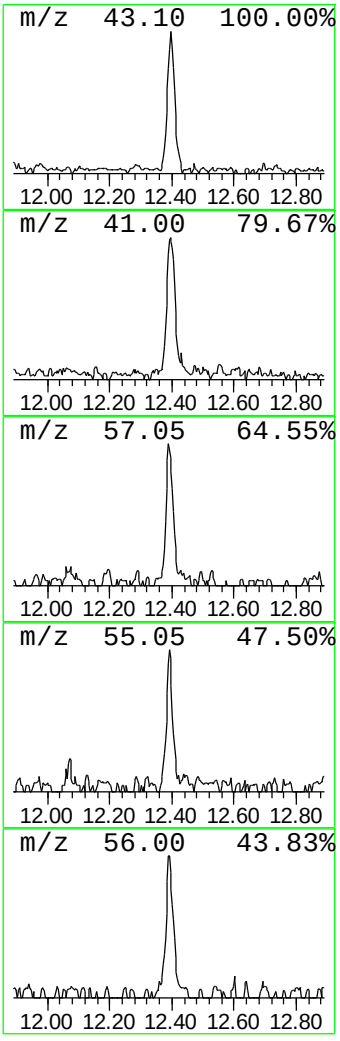
****

Peak Number 9 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	0.55 ug/L	78489	1,4-Dichlorobenzene-d4	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	49
2	2-Decen-1-ol, (E)-	156	C10H20O	018409-18-2	35
3	Cycloundecene(E)	152	C11H20	013151-60-5	25
4	Dodecanal	184	C12H24O	000112-54-9	25
5	Disulfide, dipropyl	150	C6H14S2	000629-19-6	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV112219\
Data File : VV013752.D
Acq On : 22 Nov 2019 22:36
Operator : SY/MD
Sample : K5941-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : B0AD7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR112219WMA.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
Bis(3-methylbutyl...	1.12	0.9	ug/L	128405	1	5.66	691300	5.0
Sulfur dioxide	1.20	15.0	ug/L	2075140	1	5.66	691300	5.0
Methanethiol	1.48	0.5	ug/L	71005	1	5.66	691300	5.0
Propanal, 2-methyl-	2.99	1.2	ug/L	163490	1	5.66	691300	5.0
Propyl mercaptan	3.72	4.1	ug/L	564122	1	5.66	691300	5.0
Furan, tetrahydro...	7.18	1.9	ug/L	262699	1	5.66	691300	5.0
Hexanal	8.28	1.4	ug/L	230423	2	8.89	856428	5.0
unknown-01	12.39	0.6	ug/L	78489	3	11.29	712179	5.0