LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.029	25	43	57	rBV	2793040	3305277	100.00%	17.557%
2	1.112	57	69	97	rBV	890623	2458204	74.37%	13.058%
3	1.228	99	105	124	rBV2	74757	252704	7.65%	1.342%
4	1.318	129	133	154	rVB2	202324	334576	10.12%	1.777%
5	1.479	176	183	210	rBV	1335029	2073175	62.72%	11.012%
6	1.582	211	215	265	rVB	143128	315840	9.56%	1.678%
7	2.054	353	362	376	rBV	202333	274666	8.31%	1.459%
8	2.132	377	386	397	rVB	215962	304558	9.21%	1.618%
9	2.209	400	410	414	rBV	101636	176429	5.34%	0.937%
10	2.321	438	445	451	rBV	28155	43524	1.32%	0.231%
11	2.466	483	490	504	rVB	114753	187915	5.69%	0.998%
12	2.688	550	559	578	rVB	188320	352026	10.65%	1.870%
13	2.791	582	591	606	rVB	120145	200320	6.06%	1.064%
14	3.964	940	956	974	rBV2	269527	666651	20.17%	3.541%
15	4.408	1076	1094	1113	rBV	135765	321124	9.72%	1.706%
16	5.099	1291	1309	1323	rBV2	341102	770349	23.31%	4.092%
17	5.173	1325	1332	1350	rVB4	28118	63196	1.91%	0.336%
18	5.668	1471	1486	1501	rBV	319142	699457	21.16%	3.715%
19	6.125	1618	1628	1650	rVB	190297	387091	11.71%	2.056%
20	7.035	1899	1911	1927	rVB	93693	160566	4.86%	0.853%
21	7.363	2000	2013	2027	rBV	398136	681449	20.62%	3.620%
22	7.569	2067	2077	2090	rBV	21374	35668	1.08%	0.189%
23	7.668	2098	2108	2124	rBV	55789	92963	2.81%	0.494%
24	8.141	2242	2255	2286	rBV	398631	672390	20.34%	3.572%
25	8.450	2334	2351	2400	rBV4	39910	223899	6.77%	1.189%
26	8.900	2472	2491	2525	rBV	419284	759094	22.97%	4.032%
27	9.353	2622	2632	2646	rBV	30019	44914	1.36%	0.239%
28	9.633	2711	2719	2738	rBV4	15034	38953	1.18%	0.207%
29	9.752	2750	2756	2771	rVB	21385	35096	1.06%	0.186%
30	10.266	2905	2916	2930	rBV	130661	201711	6.10%	1.071%
31	10.986	3121	3140	3164	rBV	114306	187155	5.66%	0.994%
32	11.105	3164	3177	3189	rBV2	40211	83267	2.52%	0.442%
33	11.298	3226	3237	3258	rBV	412703	640994	19.39%	3.405%
34	11.578	3313	3324	3336	rBV2	33185	58981	1.78%	0.313%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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	11.678	3343	3355	3373	rVB	359780	565178	17.10%	3.002%
36	12.285	3533	3544	3552	rBV	65166	106101	3.21%	0.564%
37	12.330	3552	3558	3573	rVB3	23575	50425	1.53%	0.268%
38	14.385	4186	4197	4219	rBV	108704	184297	5.58%	0.979%
39	16.372	4803	4815	4837	rBV	548375	815543	24.67%	4.332%

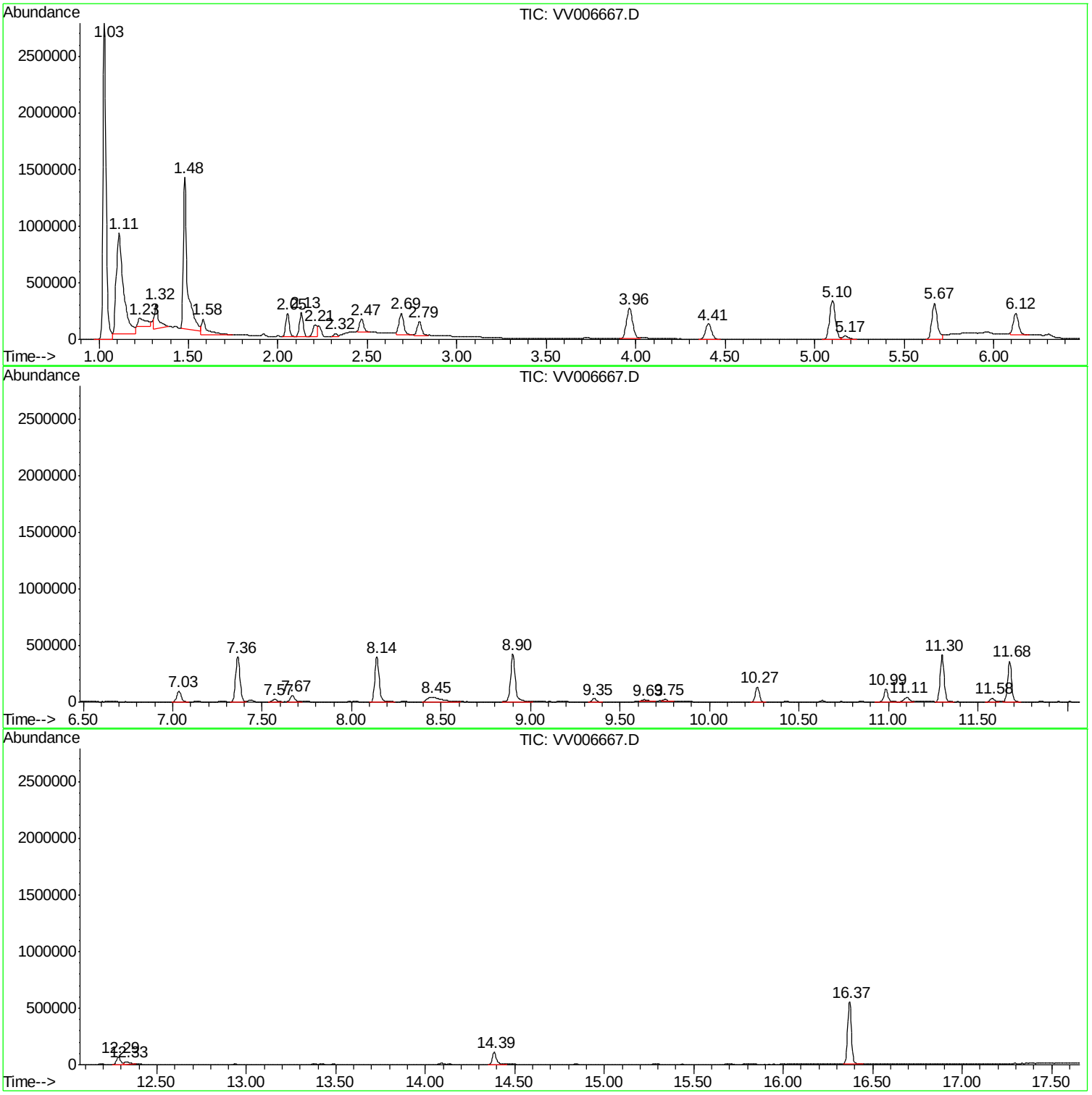
Sum of corrected areas: 18825726

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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 : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

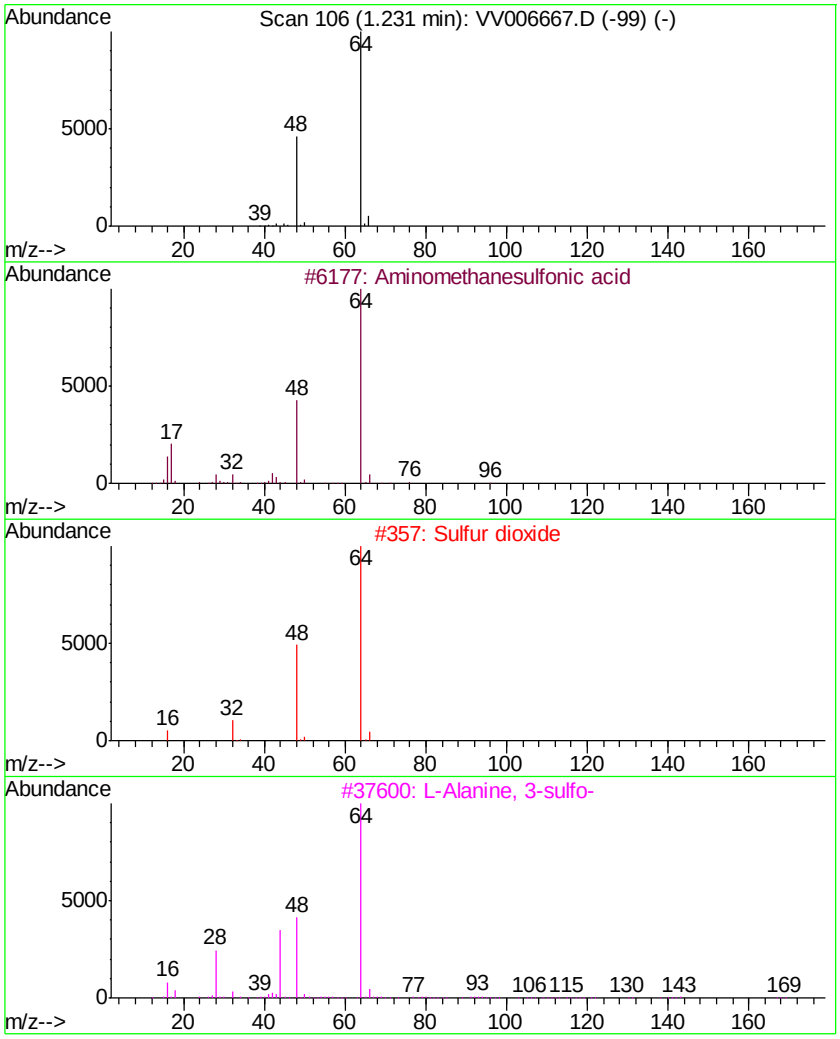
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

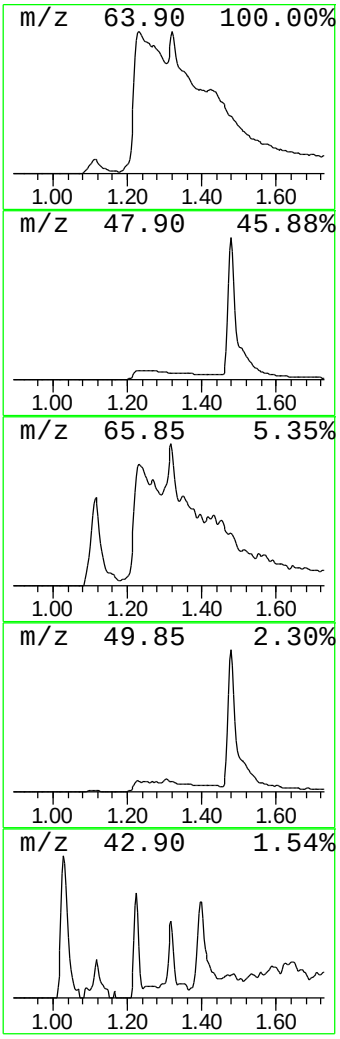
****

Peak Number 3 Aminomethanesulfonic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.23	1.81 ug/L	252704	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	83
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 : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

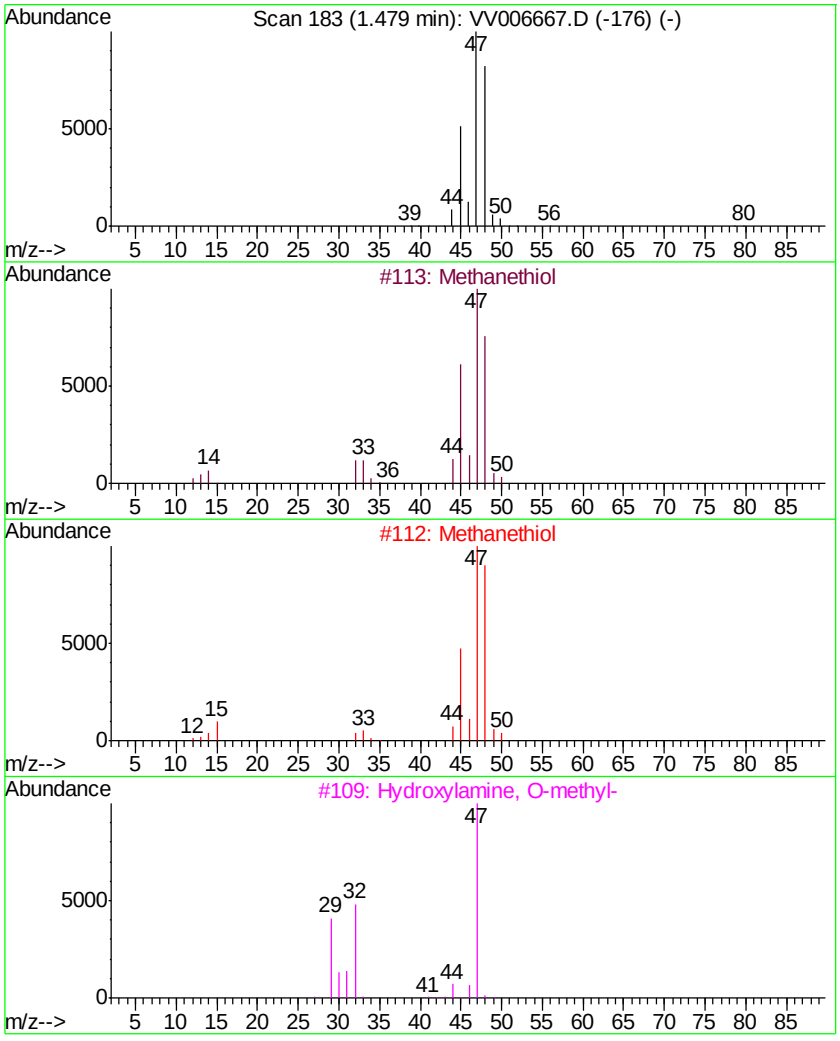
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

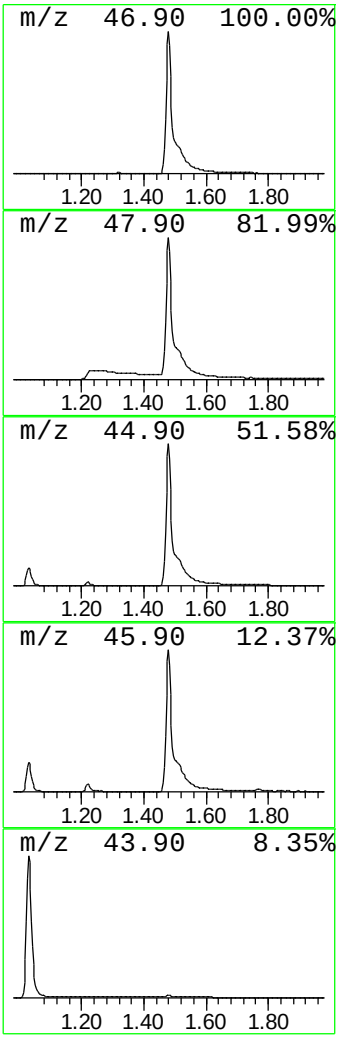
****

Peak Number 4 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	14.82 ug/L	2073180	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 : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

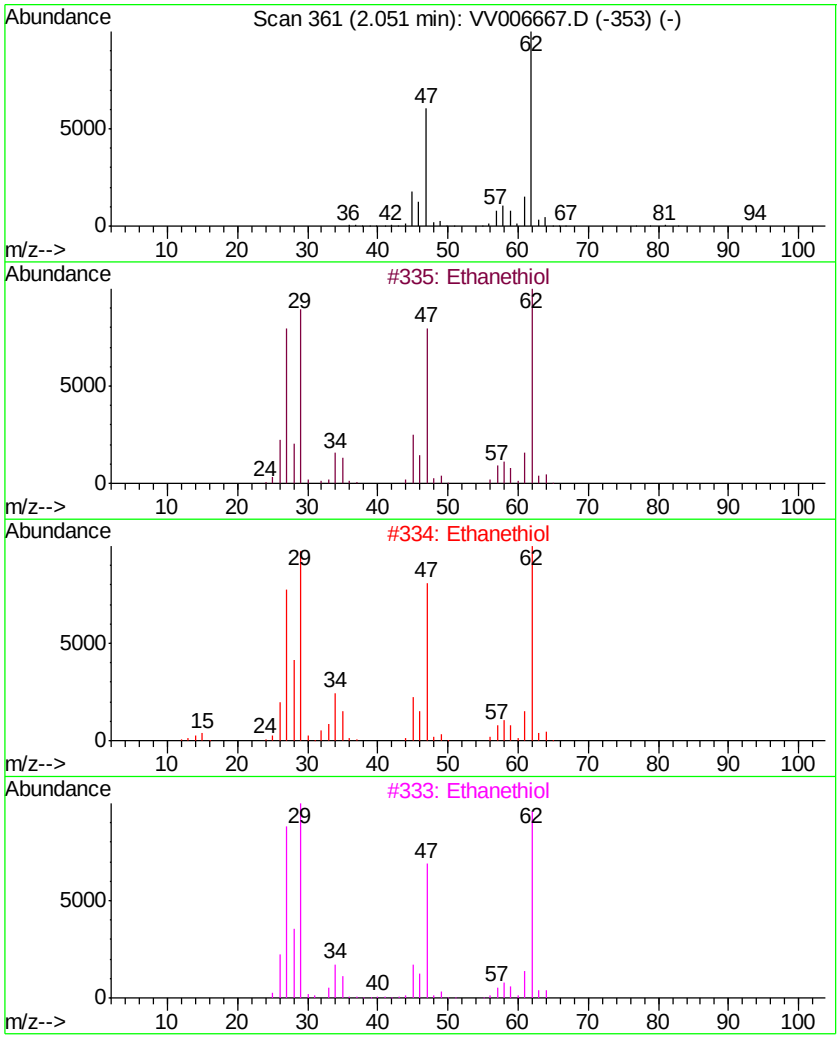
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

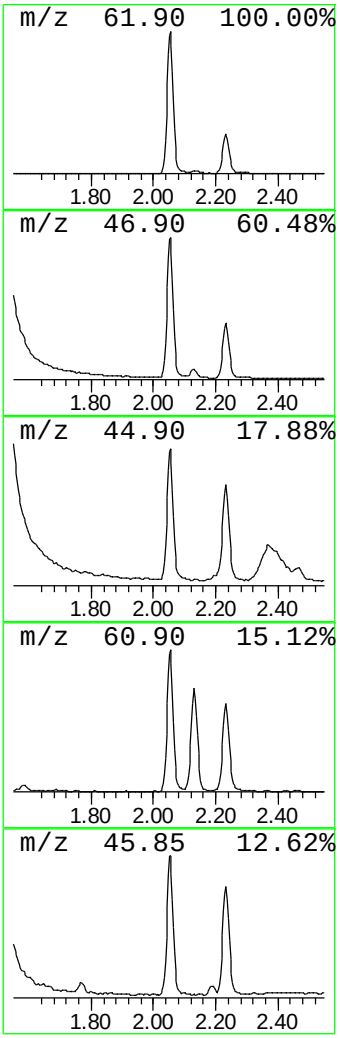
****

Peak Number 5 Ethanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	1.96 ug/L	274666	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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

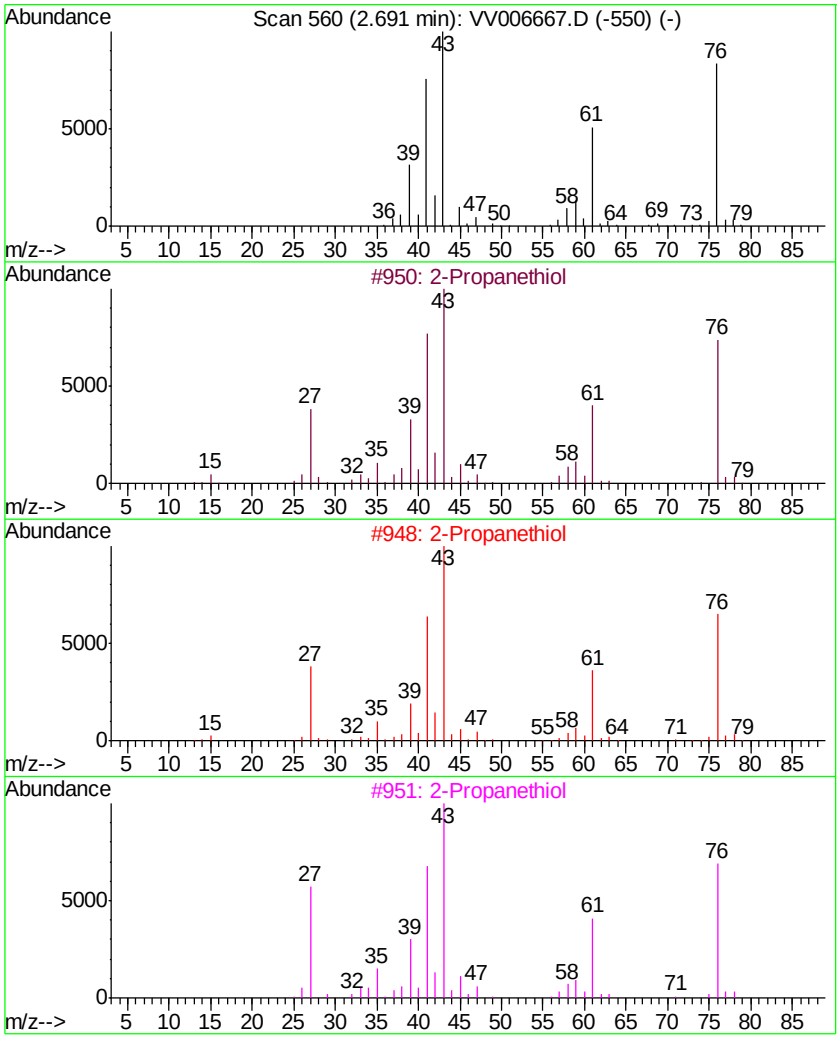
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

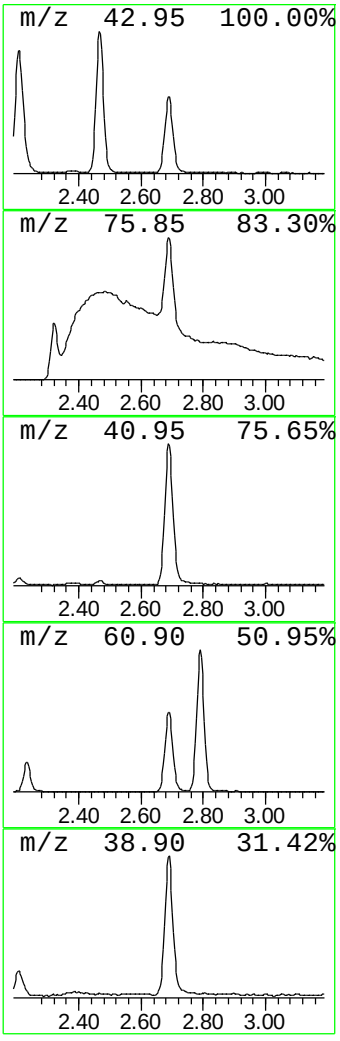
****

Peak Number 6 2-Propanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.69	2.52 ug/L	352026	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol	76	C3H8S	000075-33-2	91
2	2-Propanethiol	76	C3H8S	000075-33-2	91
3	2-Propanethiol	76	C3H8S	000075-33-2	91
4	2-Propanethiol	76	C3H8S	000075-33-2	90
5	Thiourea	76	CH4N2S	000062-56-6	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

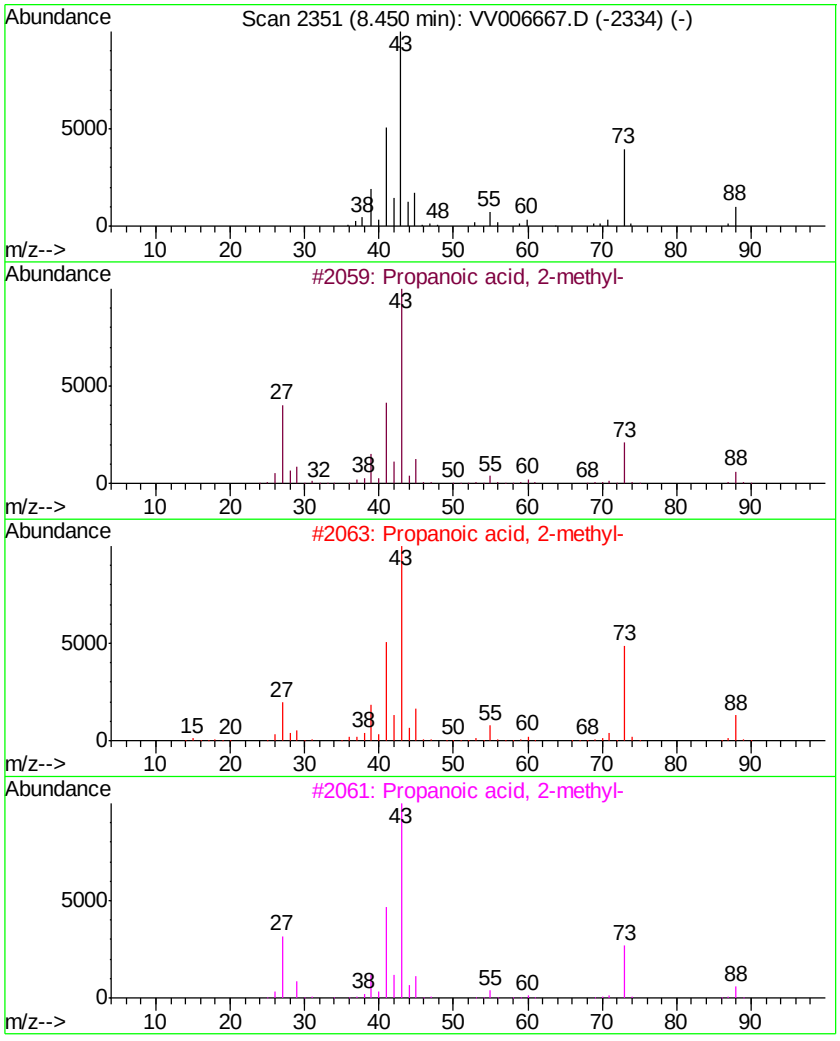
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

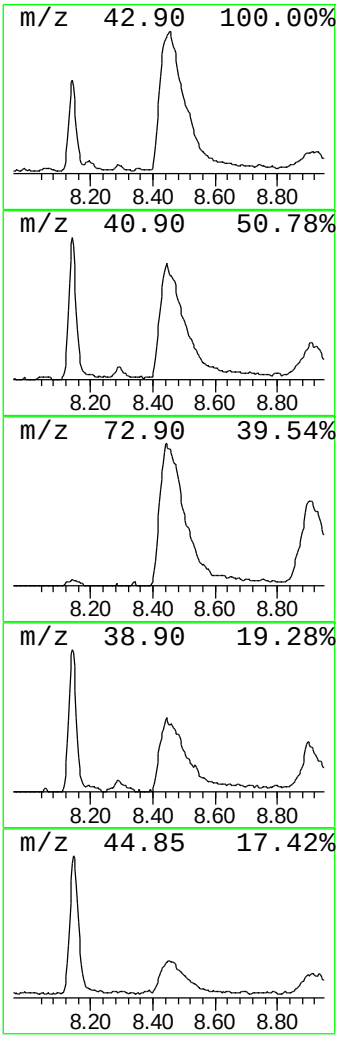
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	1.47 ug/L	223899	Chlorobenzene-d5	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	87
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	86
4	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	78
5	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

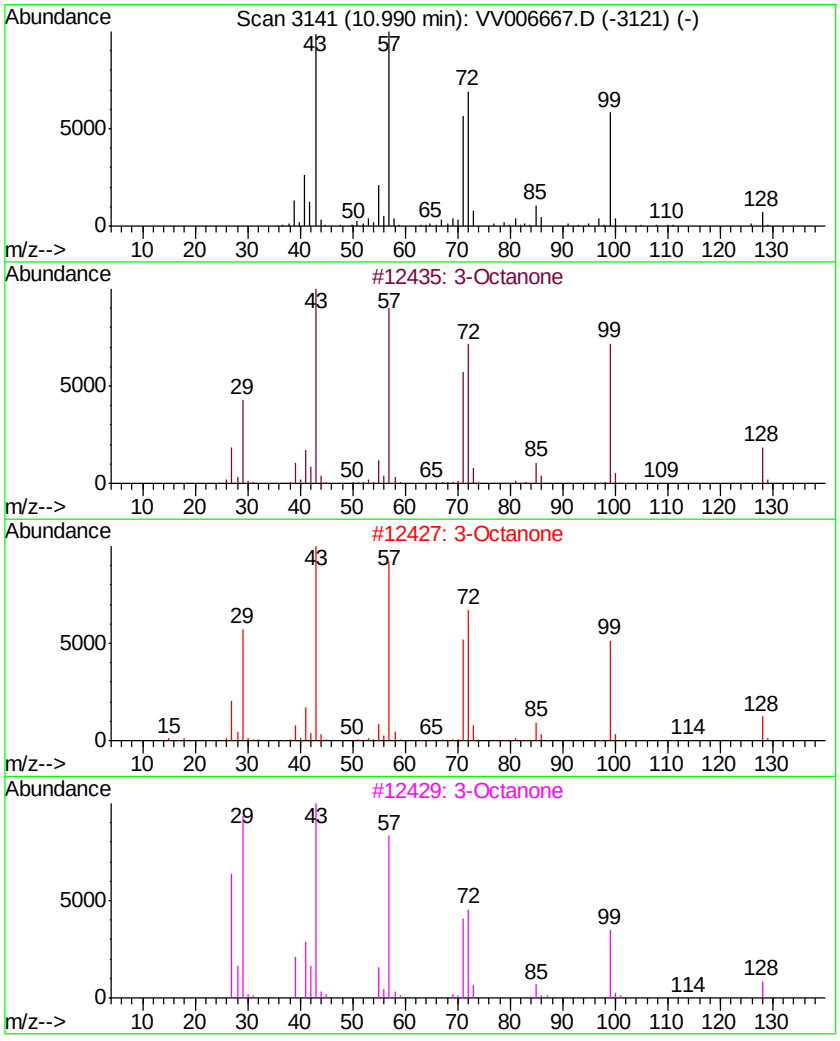
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

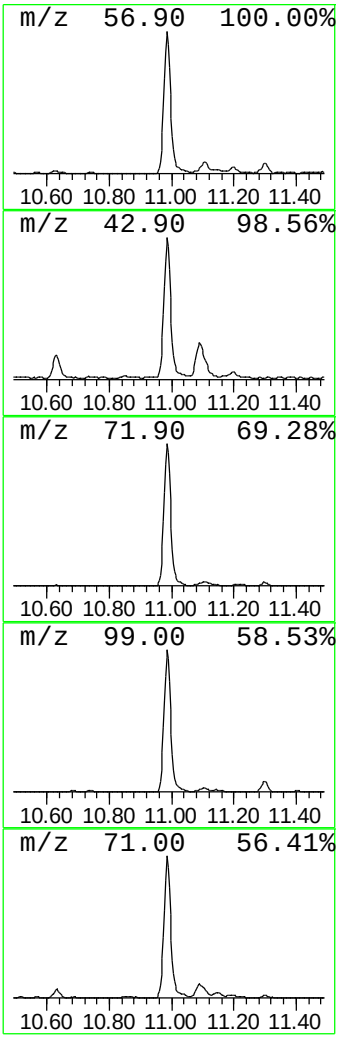
****

Peak Number 9 3-Octanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	1.46 ug/L	187155	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	94
2	3-Octanone	128	C8H16O	000106-68-3	91
3	3-Octanone	128	C8H16O	000106-68-3	90
4	3-Octanone	128	C8H16O	000106-68-3	64
5	4-Methylthiazole	99	C4H5NS	000693-95-8	49





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

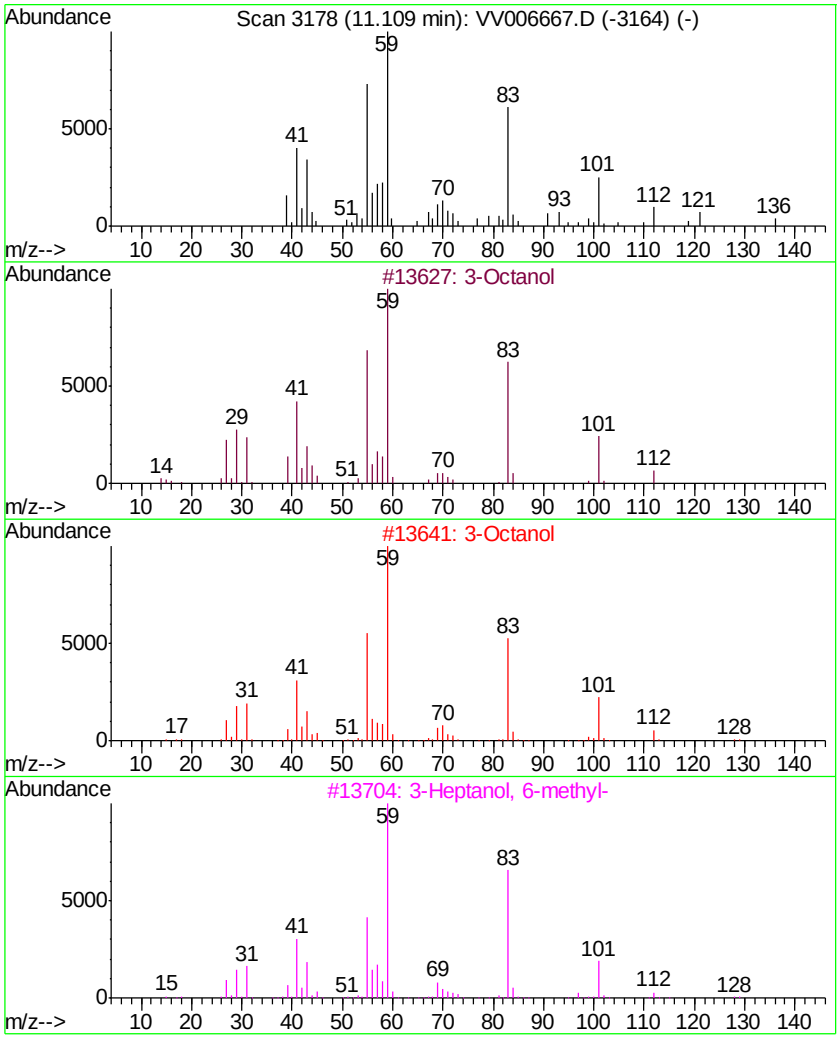
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

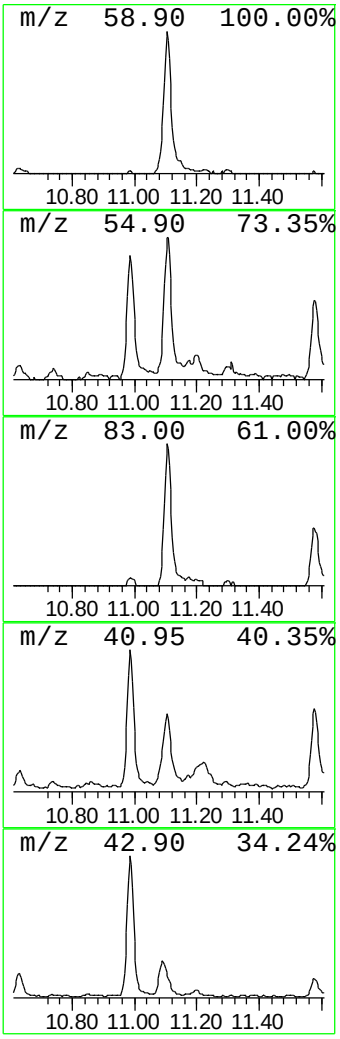
****

Peak Number 10 3-Octanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.11	0.65 ug/L	83267	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanol	130	C8H18O	000589-98-0	80
2	3-Octanol	130	C8H18O	000589-98-0	64
3	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	53
4	Oxetane, 2,2,3-trimethyl-	100	C6H12O	023120-43-6	27
5	Cyclobutanecarboxylic acid, cycl...	154	C9H14O2	042392-30-3	22





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

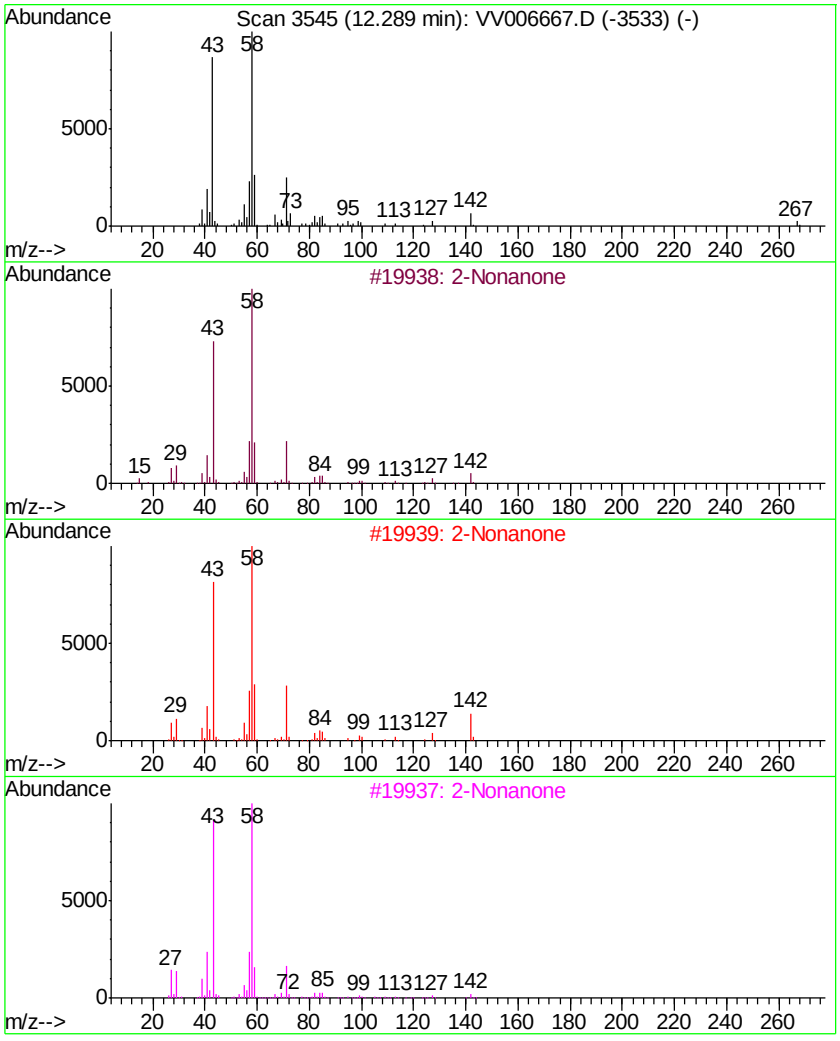
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

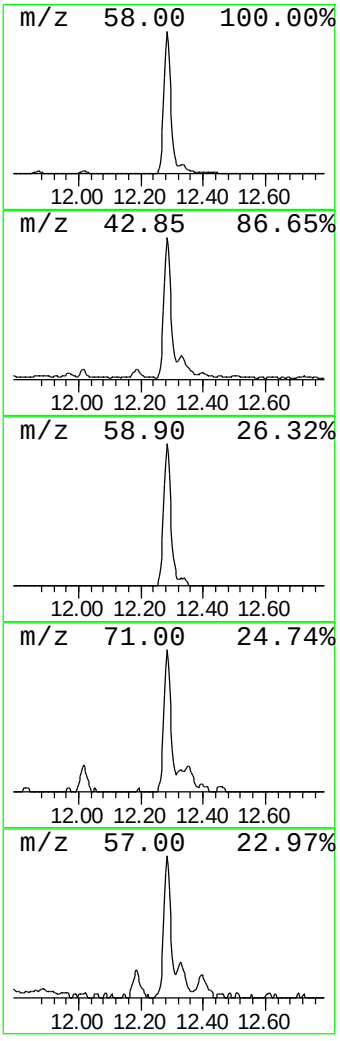
****

Peak Number 11 2-Nonanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	0.83 ug/L	106101	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	95
2	2-Nonanone	142	C9H18O	000821-55-6	91
3	2-Nonanone	142	C9H18O	000821-55-6	90
4	2-Nonanone	142	C9H18O	000821-55-6	87
5	2-Decanone	156	C10H20O	000693-54-9	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

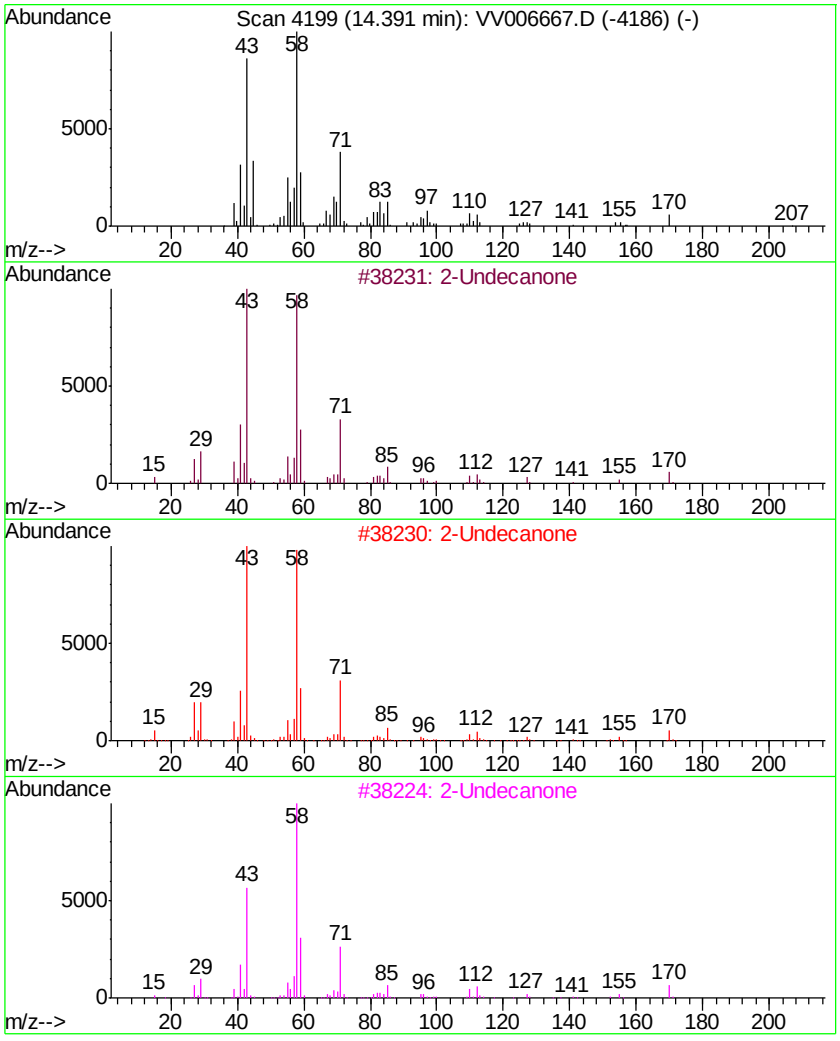
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

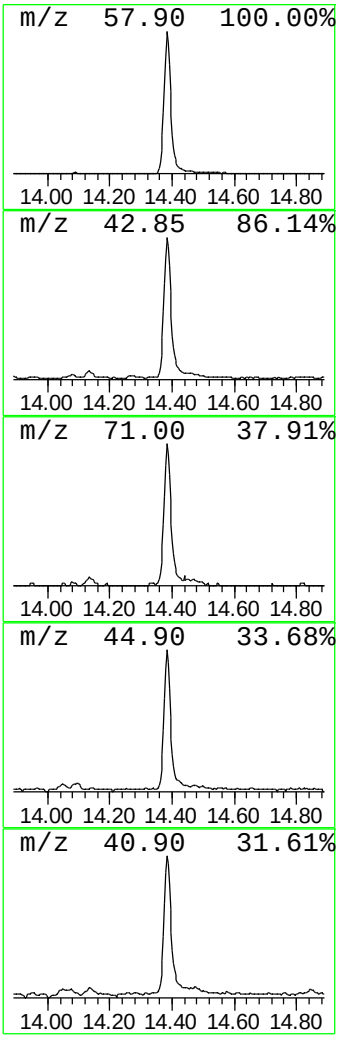
****

Peak Number 12 2-Undecanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	1.44 ug/L	184297	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecanone	170	C11H22O	000112-12-9	93
2	2-Undecanone	170	C11H22O	000112-12-9	87
3	2-Undecanone	170	C11H22O	000112-12-9	72
4	2-Tridecanone	198	C13H26O	000593-08-8	64
5	2-Tetradecanone	212	C14H28O	002345-27-9	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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

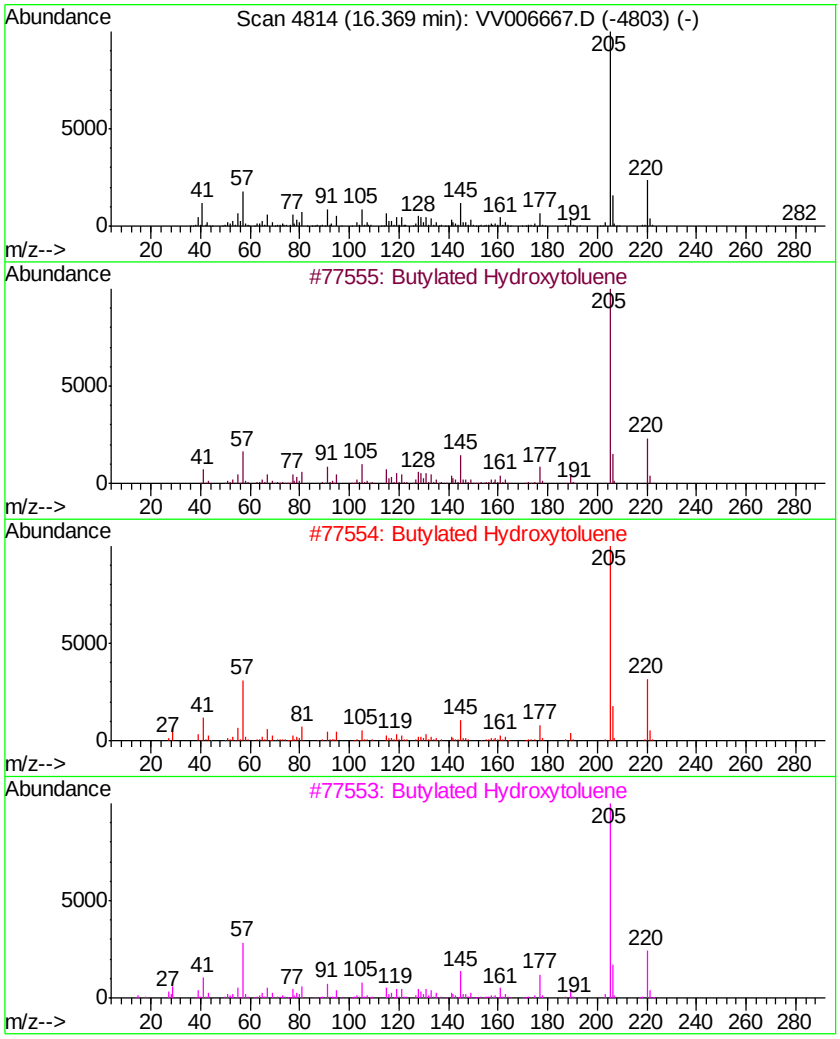
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

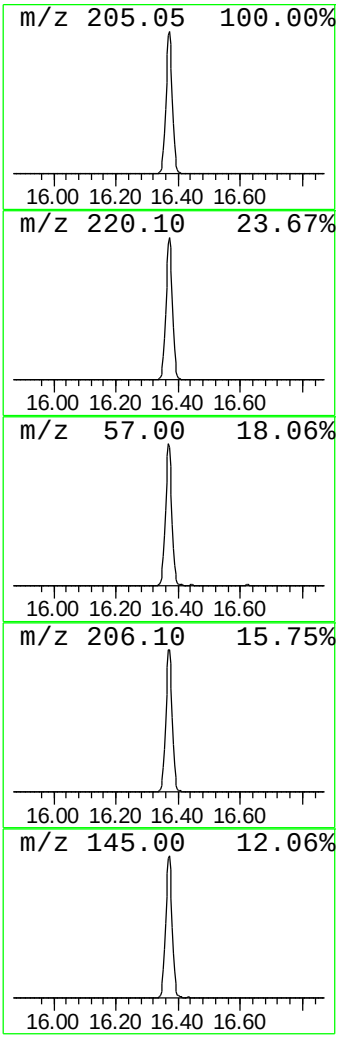
****

Peak Number 13 Butylated Hydroxytoluene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	6.36 ug/L	815543	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072018\
Data File : VV006667.D
Acq On : 20 Jul 2018 15:05
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB171

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
Aminomethanesulfo...	1.23	1.8	ug/L	252704	1	5.67	699457	5.0
Methanethiol	1.48	14.8	ug/L	2073180	1	5.67	699457	5.0
Ethanethiol	2.05	2.0	ug/L	274666	1	5.67	699457	5.0
2-Propanethiol	2.69	2.5	ug/L	352026	1	5.67	699457	5.0
Propanoic acid, 2...	8.45	1.5	ug/L	223899	2	8.90	759094	5.0
3-Octanone	10.99	1.5	ug/L	187155	3	11.30	640994	5.0
3-Octanol	11.11	0.7	ug/L	83267	3	11.30	640994	5.0
2-Nonanone	12.29	0.8	ug/L	106101	3	11.30	640994	5.0
2-Undecanone	14.39	1.4	ug/L	184297	3	11.30	640994	5.0
Butylated Hydroxy...	16.37	6.4	ug/L	815543	3	11.30	640994	5.0