LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

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_X\METHOD\82X071320W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	40	47	54	rBV	50895	61145	4.05%	0.444%
2	1.569	74	79	88	rBV	54607	87670	5.81%	0.637%
3	2.416	212	218	222	rBV	210430	346193	22.94%	2.514%
4	2.459	222	225	235	rVB	228708	370346	24.54%	2.690%
5	2.575	235	244	251	rBV	104106	240844	15.96%	1.749%
6	2.837	284	287	296	rVB5	11440	24069	1.59%	0.175%
7	3.007	309	315	326	rVB3	18390	43373	2.87%	0.315%
8	4.635	571	582	596	rBV	49731	145756	9.66%	1.059%
9	5.092	651	657	665	rBV3	5970	18270	1.21%	0.133%
10	5.470	706	719	730	rBV2	174567	519049	34.39%	3.770%
11	5.629	734	745	759	rVV	253724	720383	47.73%	5.232%
12	6.031	802	811	827	rBV2	178048	465859	30.87%	3.384%
13	6.830	932	942	956	rBV	419923	1002237	66.40%	7.279%
14	7.049	961	978	981	rBV4	17429	90765	6.01%	0.659%
15	7.165	991	997	1013	rVB2	32473	108187	7.17%	0.786%
16	7.519	1050	1055	1060	rVB	9716	17942	1.19%	0.130%
17	7.696	1079	1084	1091	rBV2	10599	20316	1.35%	0.148%
18	7.952	1121	1126	1133	rBV6	7163	15126	1.00%	0.110%
19	8.464	1204	1210	1218	rBV	56798	109706	7.27%	0.797%
20	8.622	1231	1236	1241	rBV	13498	21700	1.44%	0.158%
21	8.695	1241	1248	1255	rBV	954336	1455419	96.43%	10.571%
22	8.762	1255	1259	1267	rVB2	12768	23851	1.58%	0.173%
23	10.098	1469	1478	1488	rBV	1014385	1353339	89.67%	9.829%
24	10.232	1495	1500	1507	rBV2	13714	24543	1.63%	0.178%
25	10.341	1510	1518	1524	rVB	20928	37398	2.48%	0.272%
26	11.122	1641	1646	1656	rVV	897225	1098517	72.78%	7.978%
27	11.414	1687	1694	1697	rBV7	7300	15728	1.04%	0.114%
28	11.658	1729	1734	1736	rBV3	14636	21358	1.42%	0.155%
29	11.701	1738	1741	1745	rVB2	16002	23484	1.56%	0.171%
30	11.792	1750	1756	1762	rVV	43670	58579	3.88%	0.425%
31	11.878	1766	1770	1775	rVV3	28783	41459	2.75%	0.301%
32	11.939	1775	1780	1788	rVV3	12136	22325	1.48%	0.162%
33	12.061	1794	1800	1807	rBV	1230788	1509312	100.00%	10.962%
34	12.140	1807	1813	1817	rBV5	11811	23726	1.57%	0.172%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

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_X\METHOD\82X071320W.M
Title : SW846 8260

35	12.256	1827	1832	1841	rBV	266561	395003	26.17%	2.869%
36	12.506	1869	1873	1878	rVB8	8318	16013	1.06%	0.116%
37	12.835	1924	1927	1933	rVB7	9510	16336	1.08%	0.119%
38	13.006	1950	1955	1966	rBV	579366	862166	57.12%	6.262%
39	13.109	1966	1972	1974	rVV	545329	761863	50.48%	5.533%
40	13.134	1974	1976	2001	rVB	738591	1138947	75.46%	8.272%
41	13.463	2027	2030	2040	rVB8	18099	29471	1.95%	0.214%
42	13.548	2040	2044	2052	rVV5	18200	29495	1.95%	0.214%
43	13.634	2053	2058	2063	rVB7	12884	24615	1.63%	0.179%
44	13.768	2075	2080	2081	rBV4	35477	49250	3.26%	0.358%
45	13.786	2081	2083	2095	rVB3	55885	87806	5.82%	0.638%
46	13.896	2098	2101	2104	rBV2	37304	50209	3.33%	0.365%
47	14.524	2201	2204	2211	rVB7	16963	25905	1.72%	0.188%
48	14.658	2221	2226	2231	rVV9	12654	23369	1.55%	0.170%
49	14.713	2231	2235	2241	rVB9	11969	16946	1.12%	0.123%
50	15.255	2317	2324	2328	rBV5	15850	30452	2.02%	0.221%
51	15.420	2347	2351	2360	rBV5	9085	19173	1.27%	0.139%
52	15.652	2385	2389	2396	rVB10	8297	16569	1.10%	0.120%
53	16.151	2465	2471	2477	rBV8	19324	36912	2.45%	0.268%

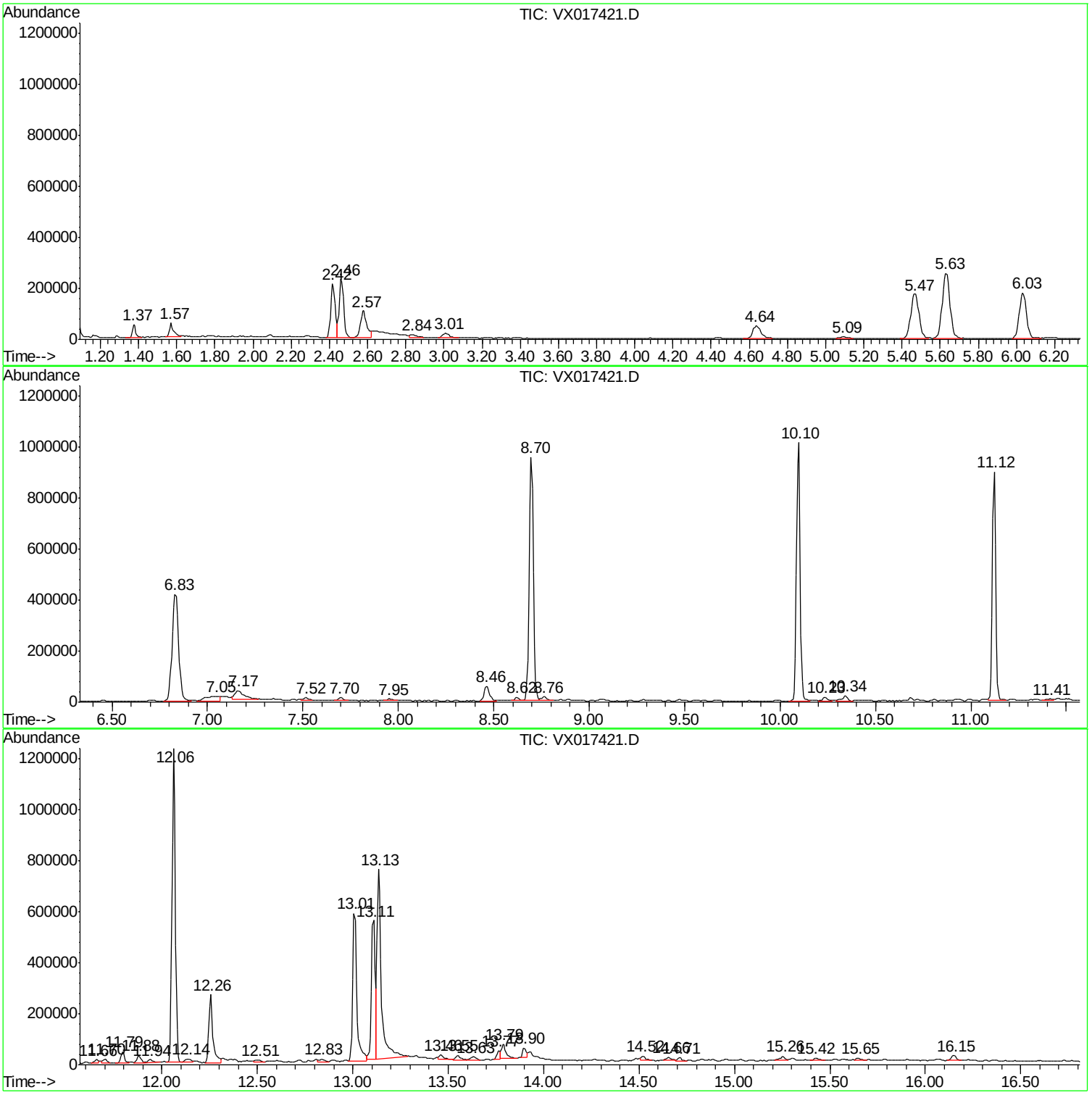
Sum of corrected areas: 13768474

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

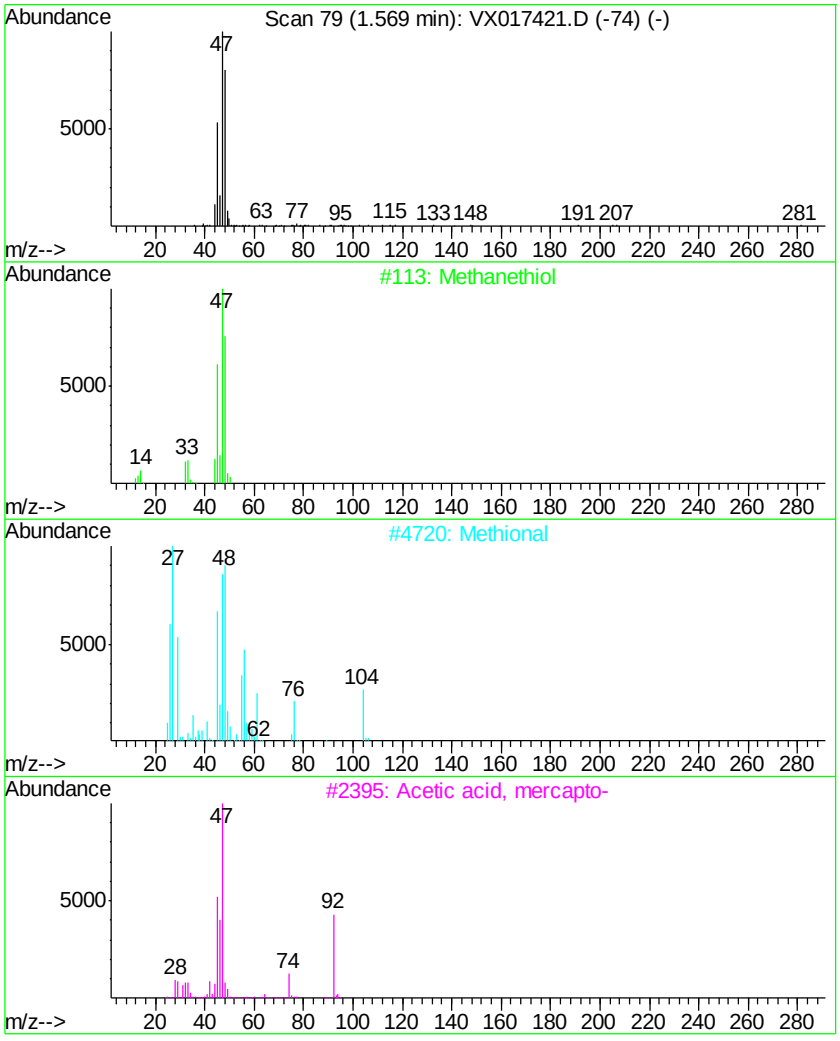
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

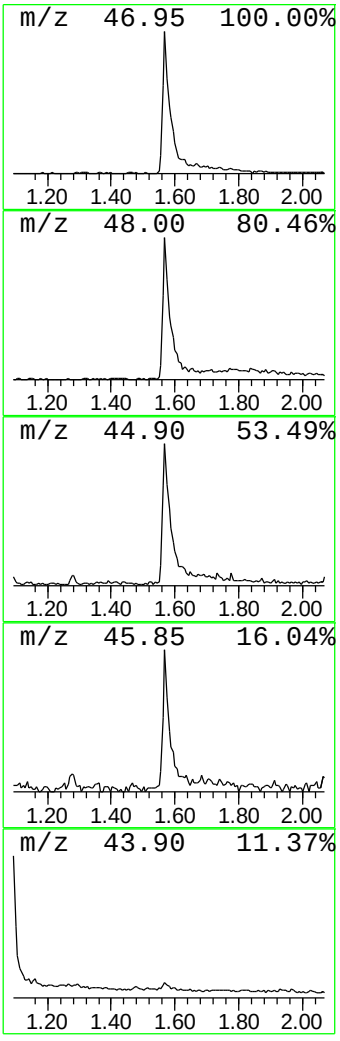
****

Peak Number 1 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.57	6.08 ug/l	87670	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Methional	104	C4H8OS	003268-49-3	56
3	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	7
5	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

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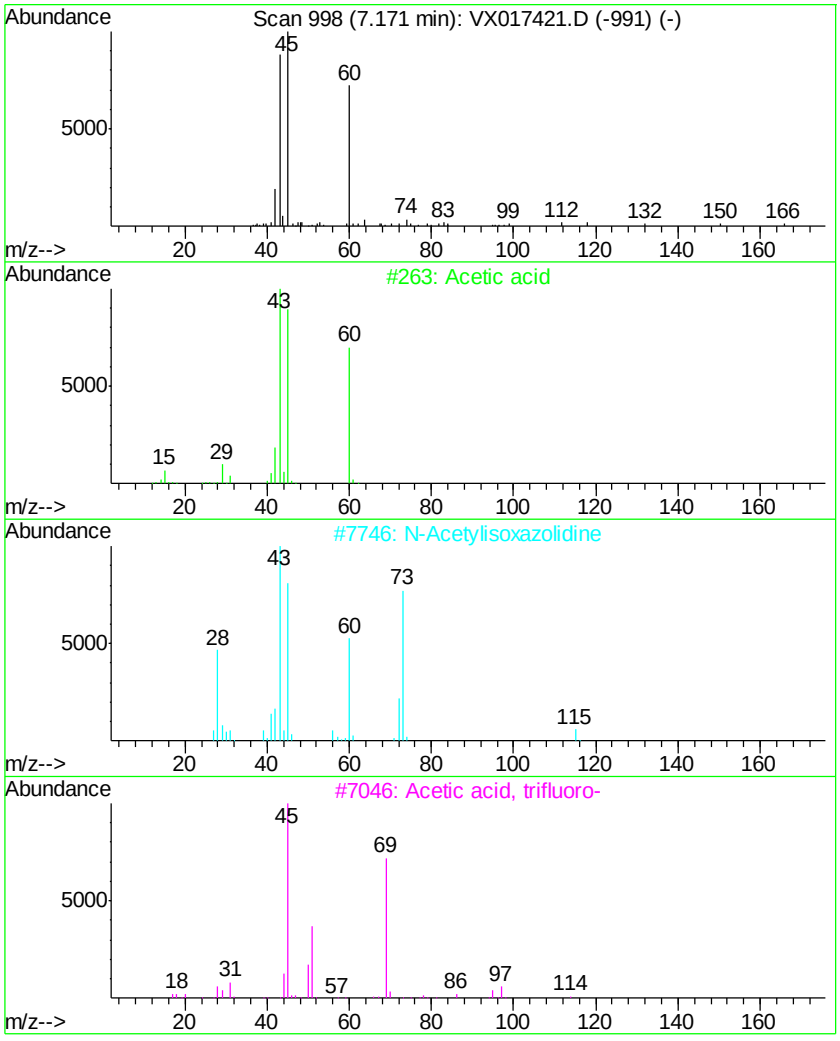
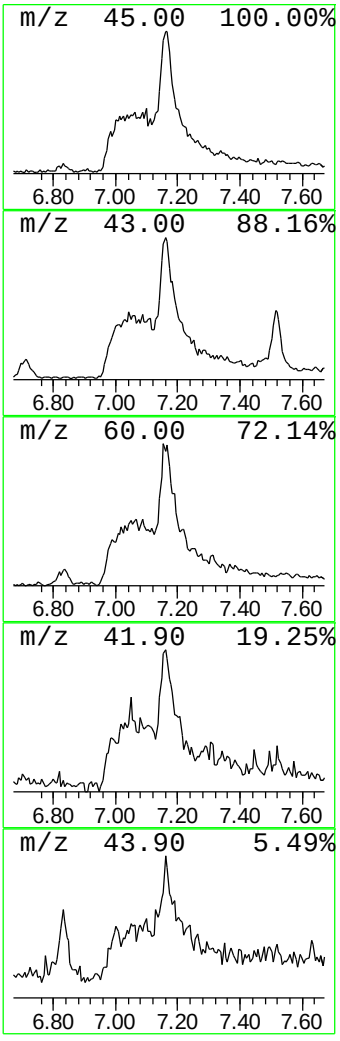
Peak Number 2 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	5.40 ug/l	108187	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	N-Acetylisoxazolidine	115	C5H9NO2	115615-36-6	43
3	Acetic acid, trifluoro-	114	C2HF3O2	000076-05-1	37
4	1,3-Oxathiolane, 2,2-dimethyl-	118	C5H10OS	005684-31-1	10
5	Carbonyl sulfide	60	COS	000463-58-1	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

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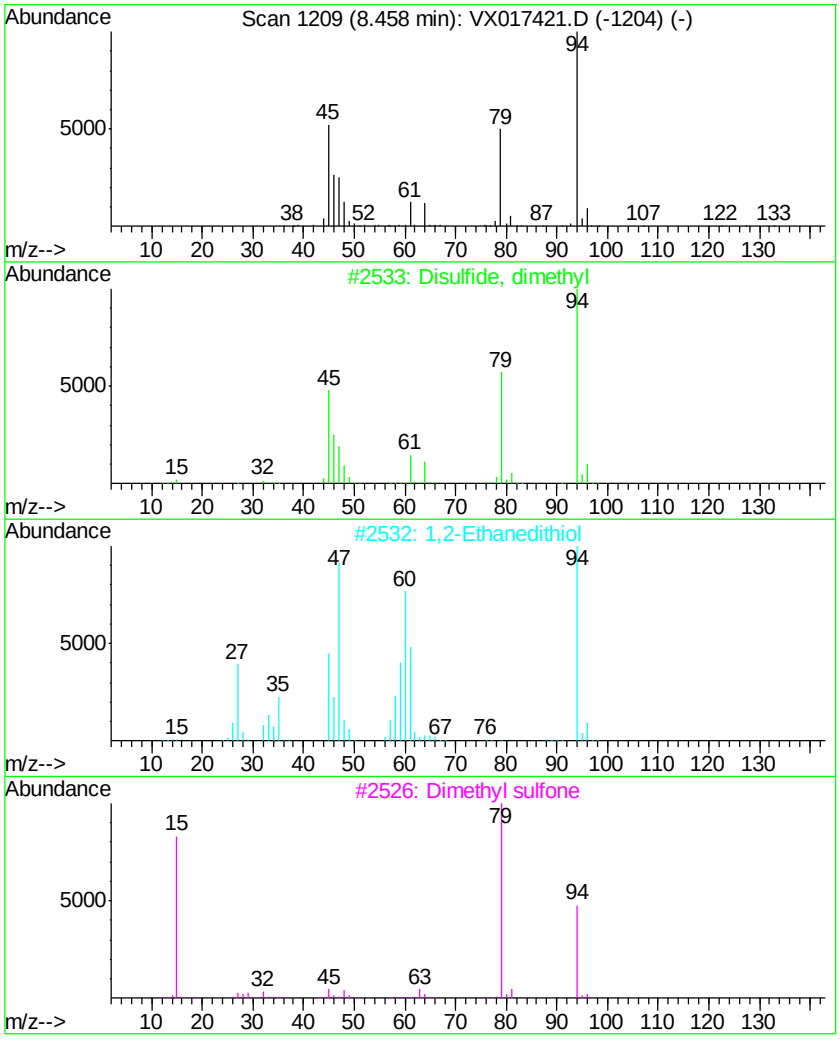
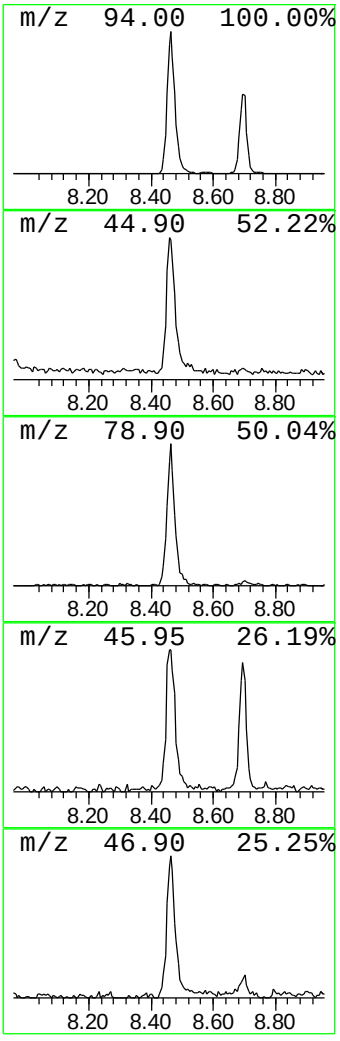
Peak Number 3 Disulfide, dimethyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	5.47 ug/l	109706	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	52
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	46
4	Phosphonic acid, (3-methyl-2-oxo...	206	C8H15O4P	054543-04-3	39
5	Ethyne, dichloro-	94	C2Cl2	007572-29-4	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

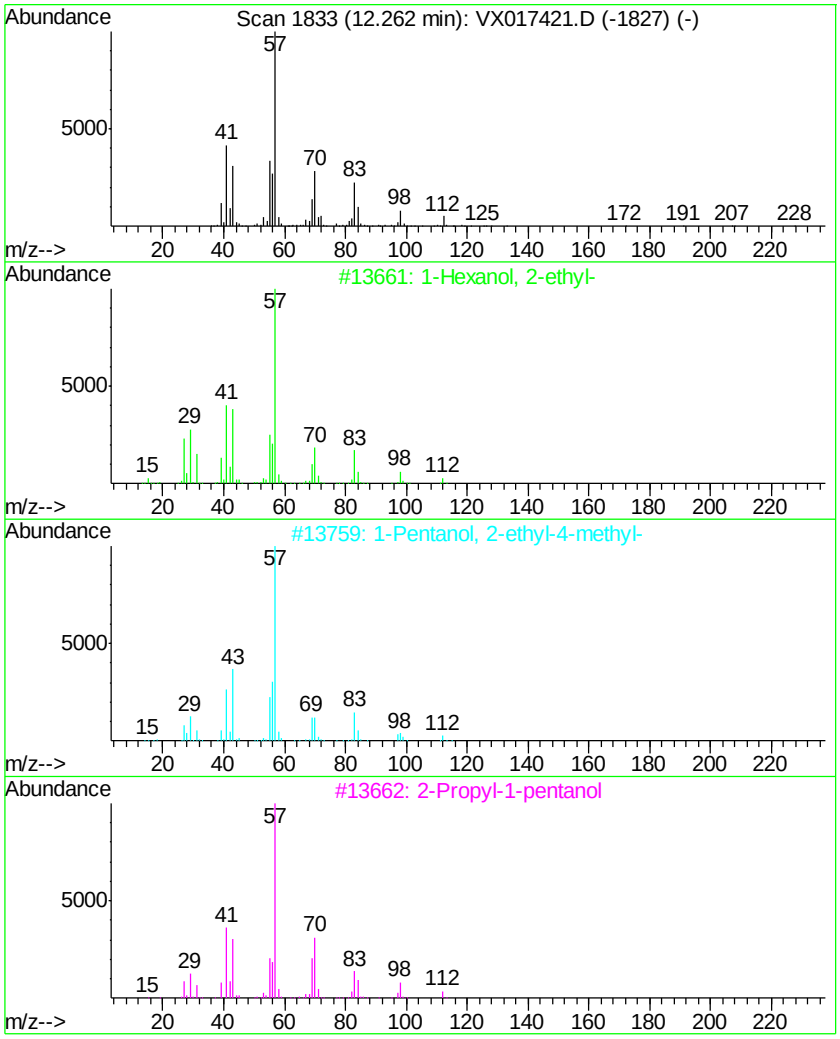
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

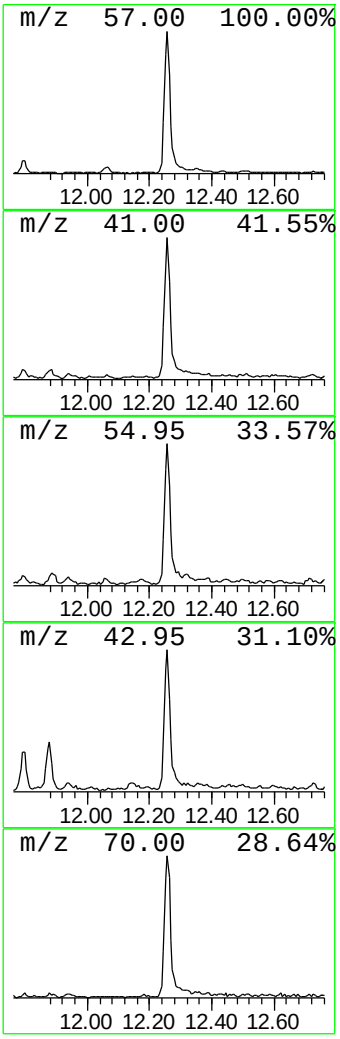
****

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	13.09 ug/l	395003	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
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Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

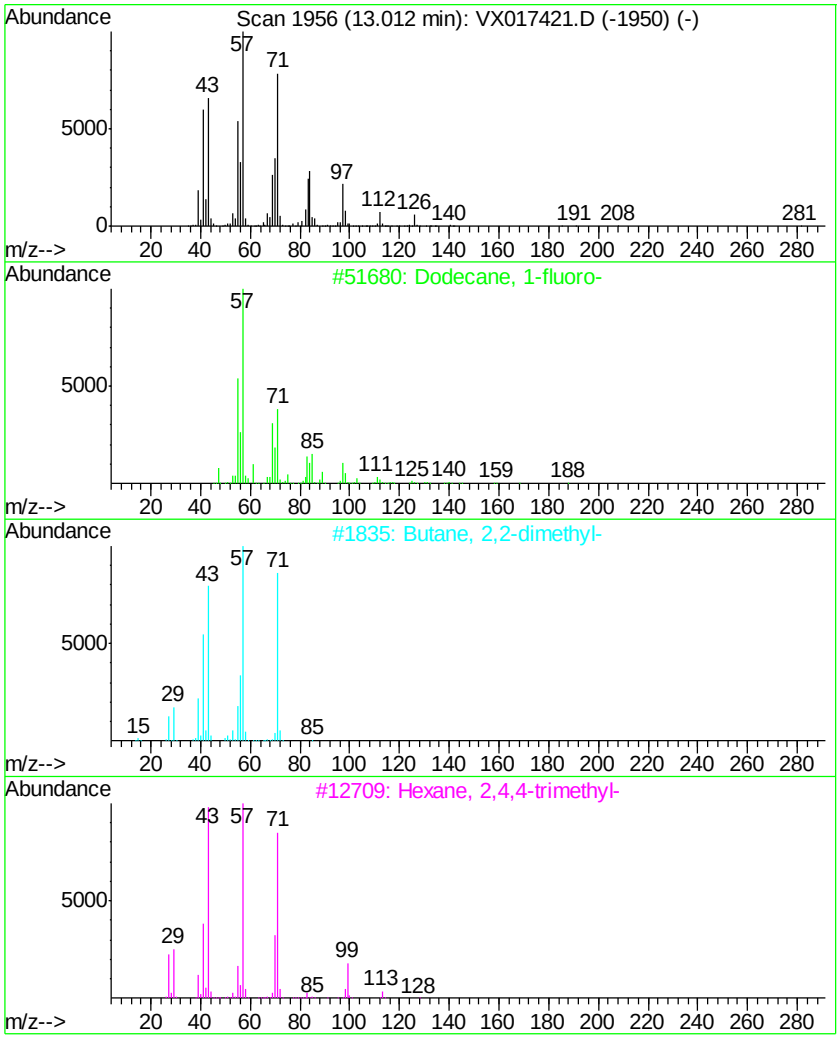
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

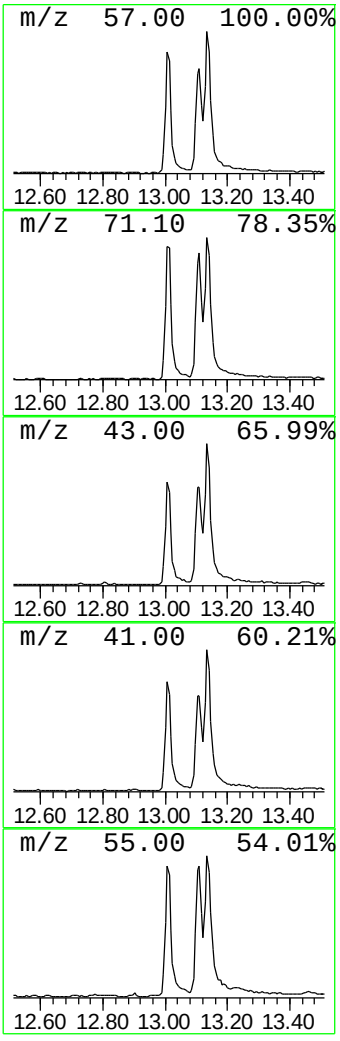
****

Peak Number 5 Dodecane, 1-fluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	28.56 ug/l	862166	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	53
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
3	Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	47
4	1-Decene, 4-methyl-	154	C11H22	013151-29-6	47
5	4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
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Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

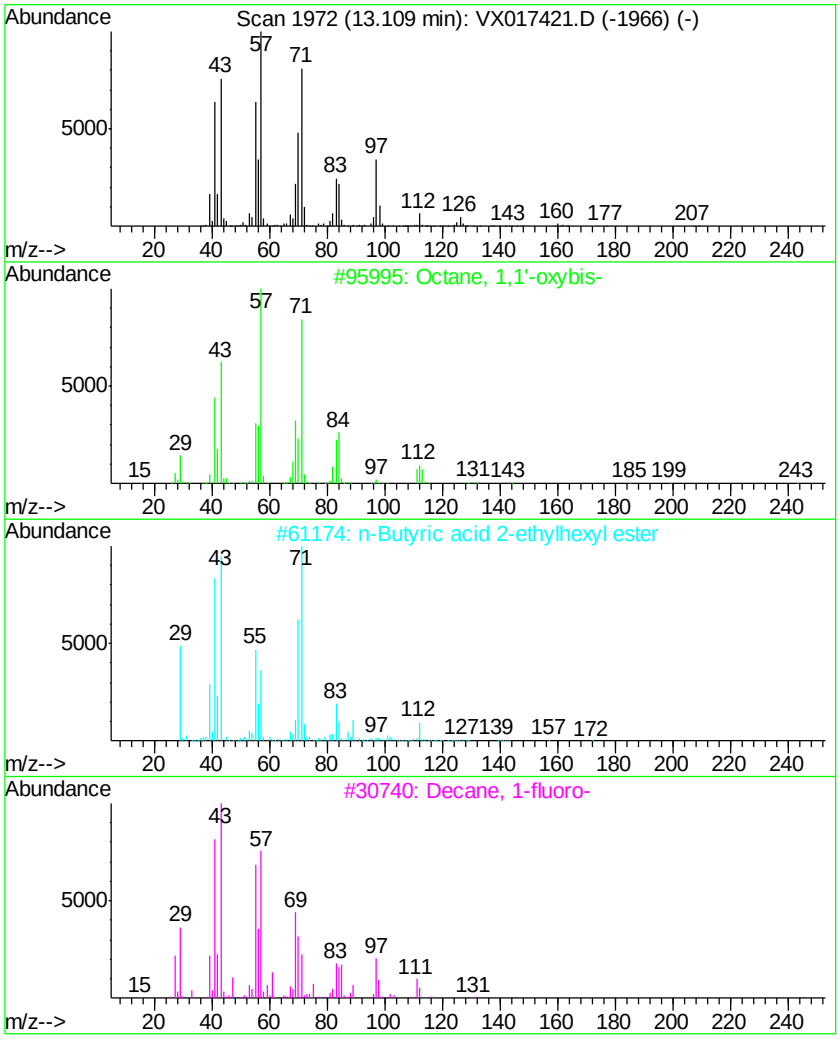
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

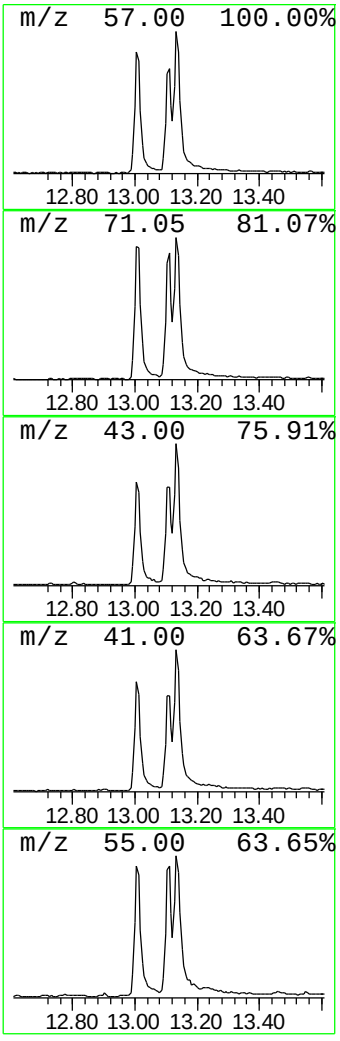
****

Peak Number 6 Octane, 1,1'-oxybis- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	25.24 ug/l	761863	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50
2	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	47
3	Decane, 1-fluoro-	160	C10H21F	000334-56-5	43
4	1-Undecene	154	C11H22	000821-95-4	43
5	Cyclopentanecarboxylic acid, 2-t...	198	C11H18O3	1000282-42-9	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

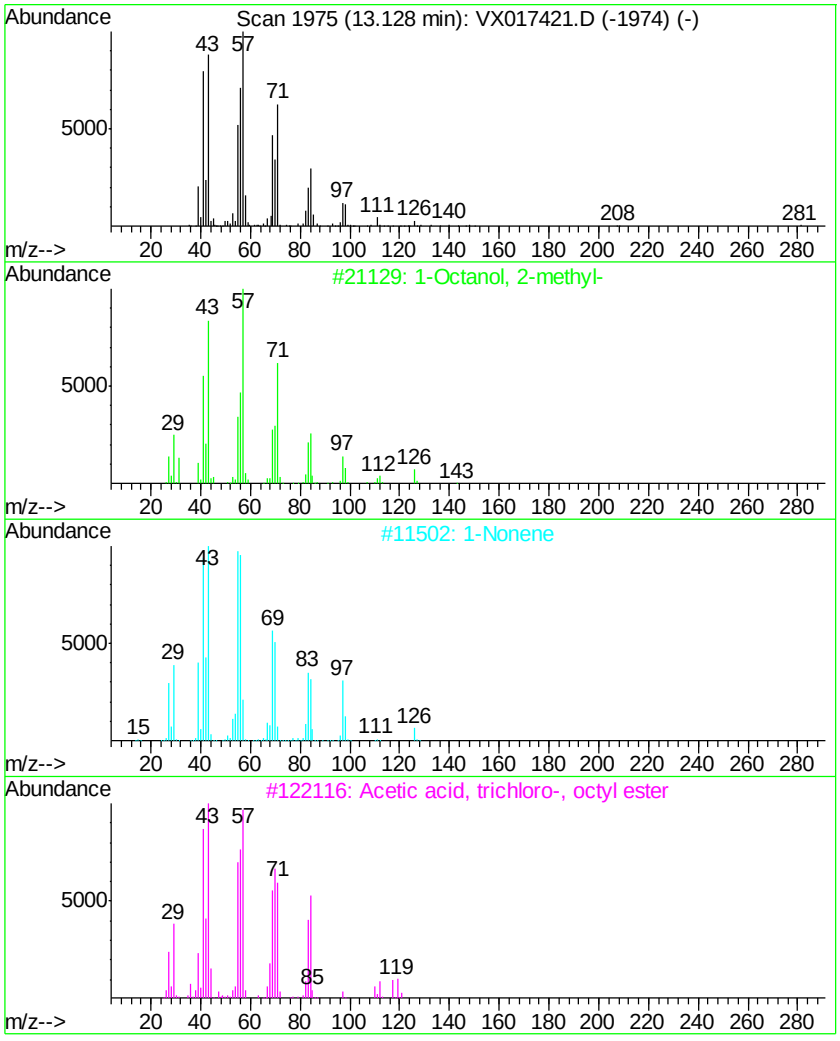
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

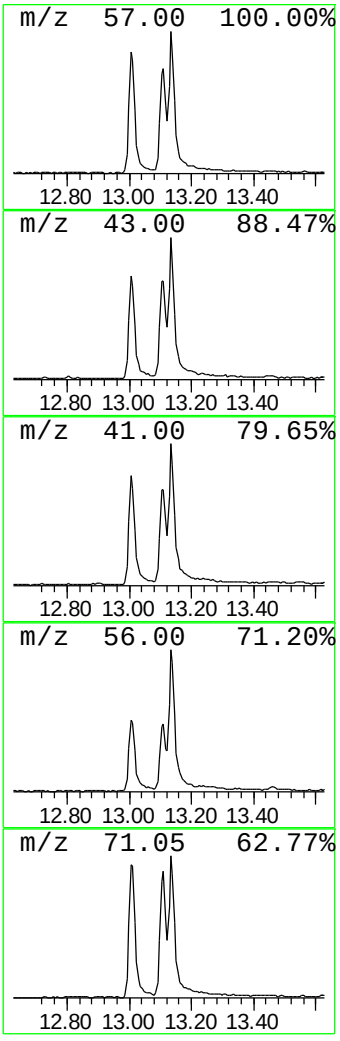
****

Peak Number 7 1-Octanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	37.73 ug/l	1138950	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	90
2	1-Nonene	126	C9H18	000124-11-8	53
3	Acetic acid, trichloro-, octyl e...	274	C10H17Cl3O2	016958-78-4	53
4	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	50
5	1-Octanol	130	C8H18O	000111-87-5	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071720\
Data File : VX017421.D
Acq On : 17 Jul 2020 15:48
Operator : JC/SP
Sample : L3324-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TOTE-50-DIAZ

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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	1.57	6.1	ug/l	87670	1	5.63	720383	50.0
Acetic acid	7.17	5.4	ug/l	108187	2	6.83	1002240	50.0
Disulfide, dimethyl	8.46	5.5	ug/l	109706	2	6.83	1002240	50.0
1-Hexanol, 2-ethyl-	12.26	13.1	ug/l	395003	4	12.06	1509310	50.0
Dodecane, 1-fluoro-	13.01	28.6	ug/l	862166	4	12.06	1509310	50.0
Octane, 1,1'-oxybis-	13.11	25.2	ug/l	761863	4	12.06	1509310	50.0
1-Octanol, 2-methyl-	13.13	37.7	ug/l	1138950	4	12.06	1509310	50.0