LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

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\82X032421W.M
Title : SW846 8260

Signal : TIC: VX021446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.158	9	12	21	rVB	73897	73783	12.30%	1.381%
2	1.387	46	51	56	rVB2	6519	9942	1.66%	0.186%
3	1.617	79	90	95	rBV6	5018	16454	2.74%	0.308%
4	2.099	168	172	183	rVB	5574	8353	1.39%	0.156%
5	2.329	206	211	219	rVB	5322	9103	1.52%	0.170%
6	2.423	219	227	235	rBV	27391	45601	7.60%	0.854%
7	2.587	249	255	266	rVB	8236	15185	2.53%	0.284%
8	3.017	320	328	336	rBV4	6047	14429	2.40%	0.270%
9	3.382	383	390	401	rVB3	2689	7214	1.20%	0.135%
10	3.752	440	453	466	rBV	27217	77987	13.00%	1.460%
11	4.299	534	546	564	rBV	121264	334196	55.70%	6.255%
12	5.464	733	744	755	rBV	49185	141849	23.64%	2.655%
13	5.629	761	772	784	rVB	74831	209994	35.00%	3.931%
14	6.029	829	840	852	rBV	55778	146038	24.34%	2.734%
15	6.829	966	976	989	rBV	126314	299105	49.85%	5.599%
16	7.270	1042	1051	1062	rBV2	21407	51639	8.61%	0.967%
17	7.629	1105	1112	1119	rBV	11608	22660	3.78%	0.424%
18	8.000	1167	1175	1183	rVB3	7371	13078	2.18%	0.245%
19	8.694	1286	1293	1301	rBV	265212	417453	69.57%	7.814%
20	8.765	1301	1305	1310	rVV	14957	24374	4.06%	0.456%
21	9.006	1339	1346	1351	rBV3	5486	9723	1.62%	0.182%
22	9.277	1387	1392	1397	rBV	34038	52479	8.75%	0.982%
23	10.094	1524	1531	1542	rBV	299707	413347	68.89%	7.737%
24	10.194	1543	1548	1566	rVV	67189	115654	19.27%	2.165%
25	10.341	1569	1573	1579	rVB	7912	12214	2.04%	0.229%
26	10.483	1593	1597	1603	rBV5	3840	6425	1.07%	0.120%
27	10.683	1625	1631	1636	rBV2	3905	6167	1.03%	0.115%
28	10.788	1644	1649	1661	rBV	30579	45079	7.51%	0.844%
29	11.118	1700	1705	1711	rBV	252127	326071	54.34%	6.103%
30	11.171	1711	1714	1718	rVB	19257	23371	3.89%	0.437%
31	11.318	1735	1739	1747	rVB2	6137	9636	1.61%	0.180%
32	11.459	1758	1763	1767	rBV	41394	50477	8.41%	0.945%
33	11.612	1782	1789	1792	rBV	23116	33708	5.62%	0.631%
34	11.642	1792	1794	1803	rVV2	17206	23544	3.92%	0.441%
35	11.718	1803	1807	1816	rVV	152853	182028	30.34%	3.407%
36	11.906	1834	1839	1849	rBV	103302	138308	23.05%	2.589%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

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\82X032421W.M
Title : SW846 8260

37	11.995	1849	1854	1856	rBV	31878	45164	7.53%	0.845%
38	12.024	1856	1859	1862	rVV2	54667	78726	13.12%	1.474%
39	12.059	1862	1865	1872	rVB	323719	388206	64.70%	7.266%
40	12.253	1893	1898	1909	rBV	437104	600040	100.00%	11.231%
41	12.342	1909	1913	1928	rVB5	22891	51946	8.66%	0.972%
42	12.630	1954	1962	1970	rVB5	8338	17023	2.84%	0.319%
43	12.824	1991	1995	2002	rVB7	6478	12758	2.13%	0.239%
44	12.942	2011	2015	2022	rBV5	4212	7228	1.20%	0.135%
45	13.448	2097	2101	2110	rVB5	5670	9102	1.52%	0.170%
46	13.648	2126	2135	2143	rBV	23279	37418	6.24%	0.700%
47	13.730	2143	2149	2155	rVB6	7775	13633	2.27%	0.255%
48	13.789	2155	2159	2161	rBV2	7559	10034	1.67%	0.188%
49	13.812	2161	2163	2169	rVB	7582	10309	1.72%	0.193%
50	13.883	2169	2175	2182	rBV	224388	311178	51.86%	5.825%
51	13.954	2182	2187	2198	rVB	229465	317293	52.88%	5.939%
52	14.265	2231	2240	2244	rVV6	3272	7511	1.25%	0.141%
53	14.465	2270	2274	2280	rVB	5631	7303	1.22%	0.137%
54	14.677	2303	2310	2320	rVB	10063	15866	2.64%	0.297%
55	14.818	2330	2334	2339	rBV	7269	8929	1.49%	0.167%
56	16.024	2535	2539	2546	rVB6	3510	6183	1.03%	0.116%

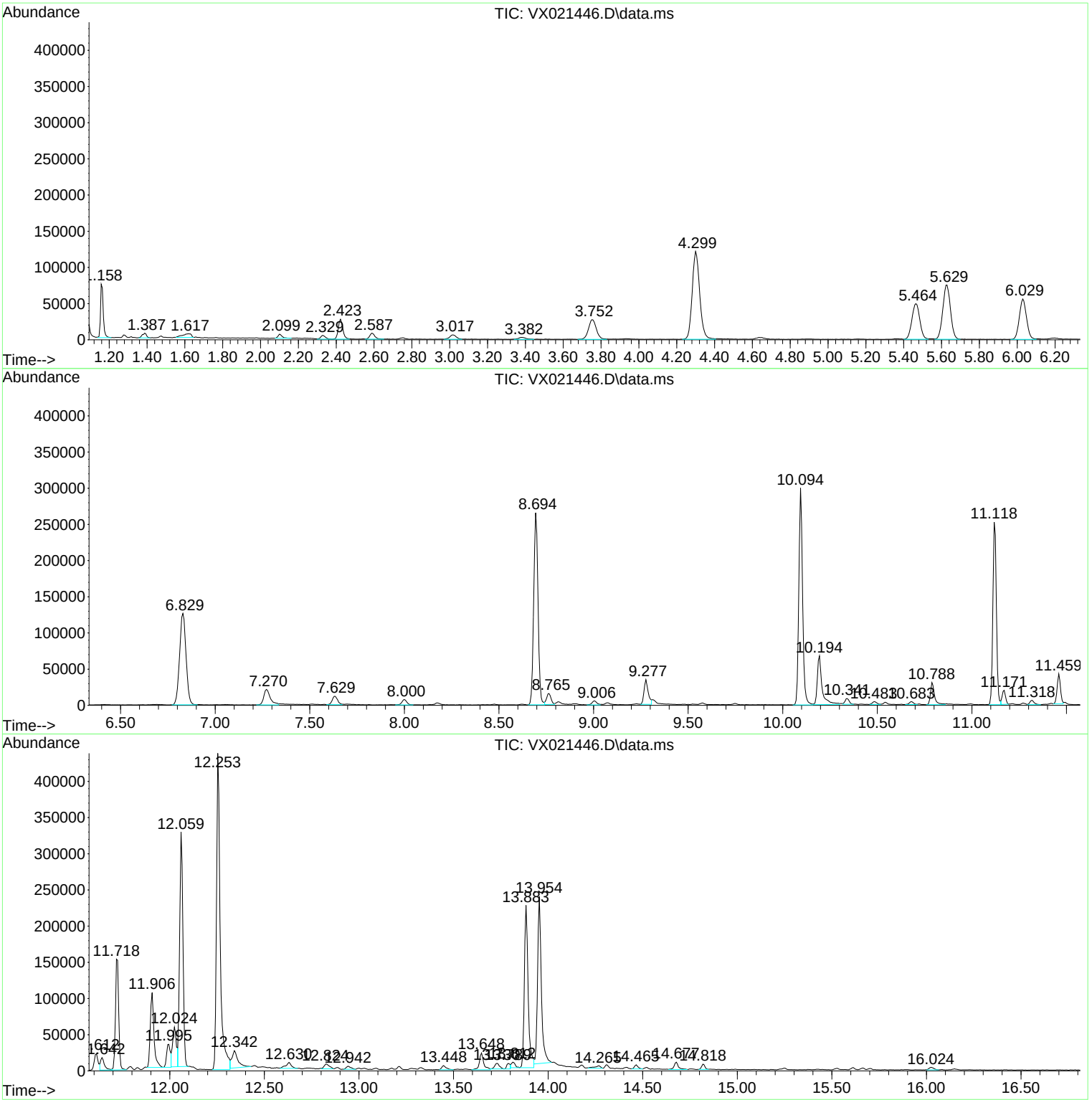
Sum of corrected areas: 5342518

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30807

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

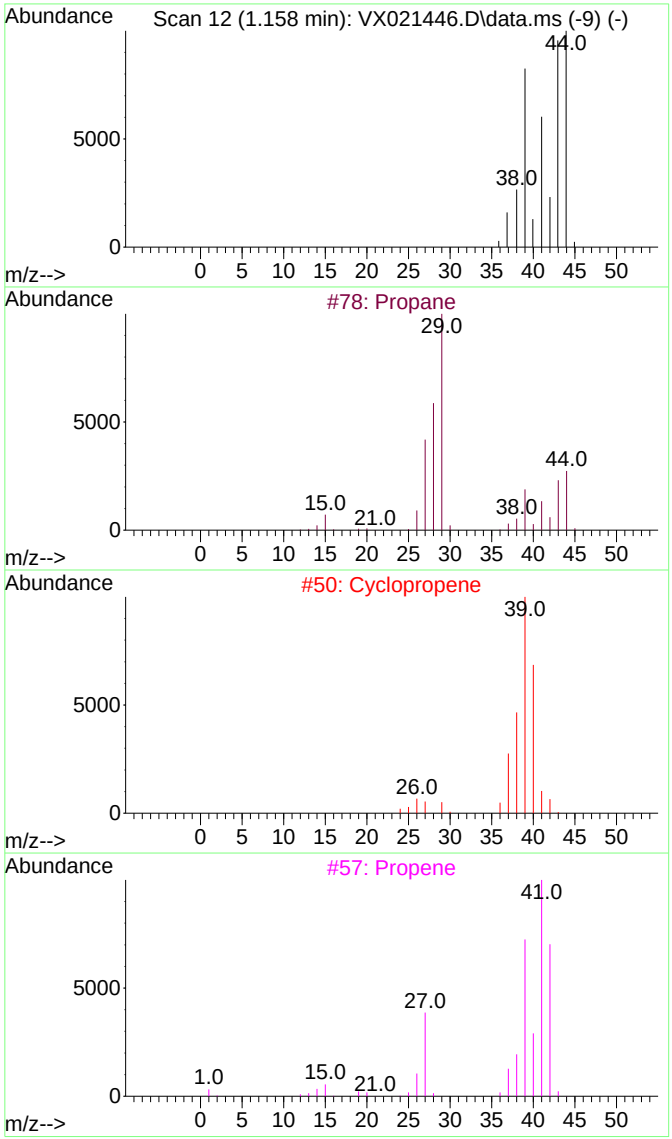
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

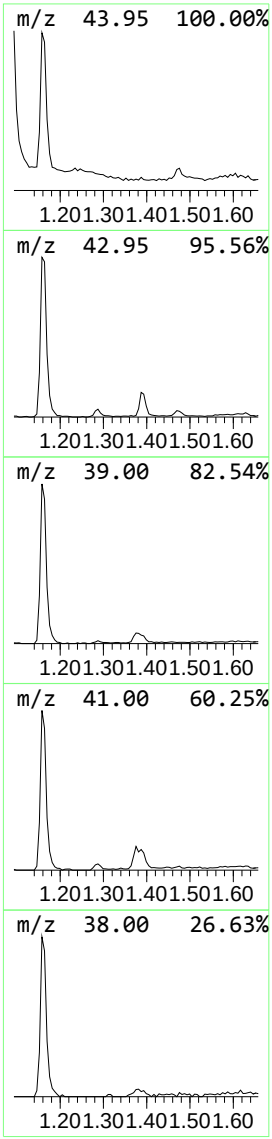
****

Peak Number 1 Propane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.158	17.57 ug/l	73783	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Cyclopropene	40	C3H4	002781-85-3	39
3	Propene	42	C3H6	000115-07-1	9
4	Acetaldehyde	44	C2H4O	000075-07-0	4
5	Ethanamine, 2-propoxy-	103	C5H13NO	042185-03-5	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

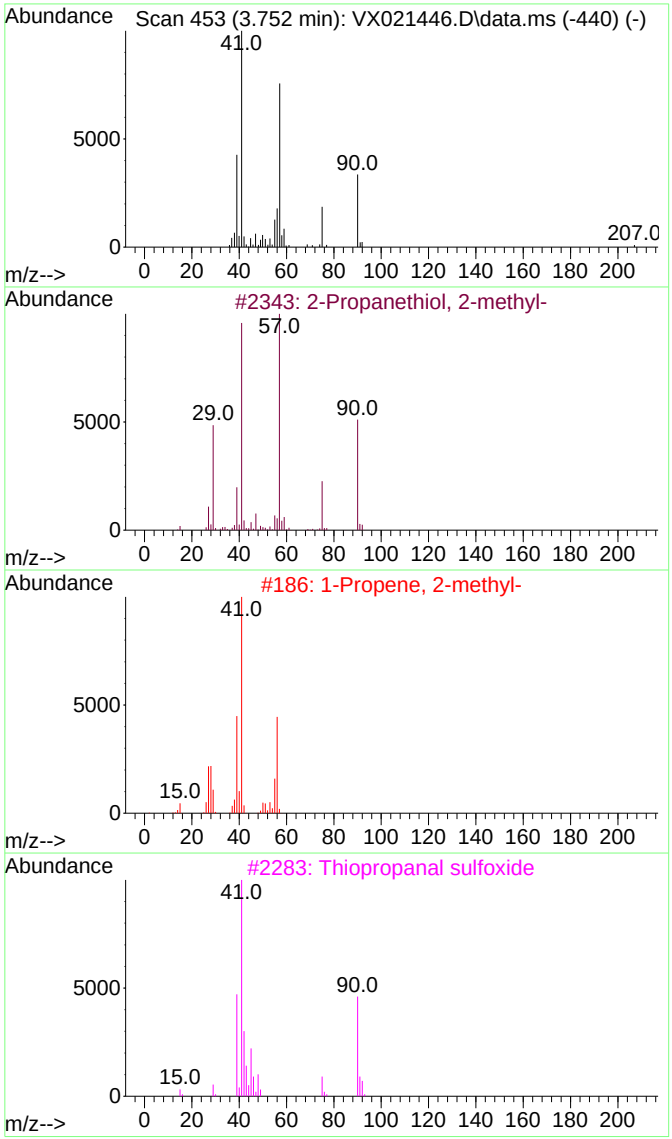
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

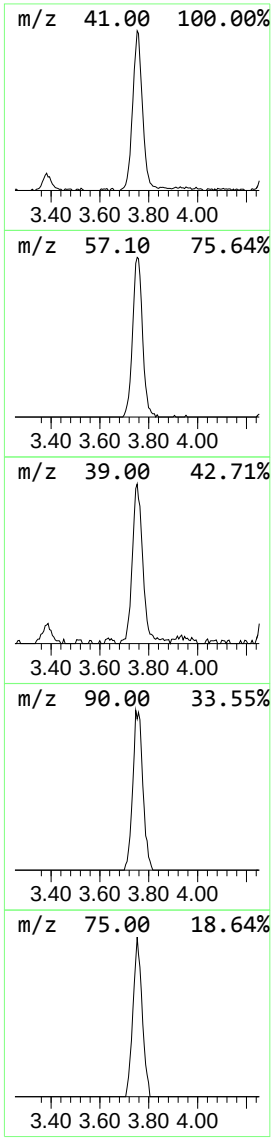
****

Peak Number 2 unknown3.752 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.752	18.57 ug/l	77987	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	46
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	30
3	Thiopropanal sulfoxide	90	C3H6OS	1000322-28-4	28
4	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	14
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

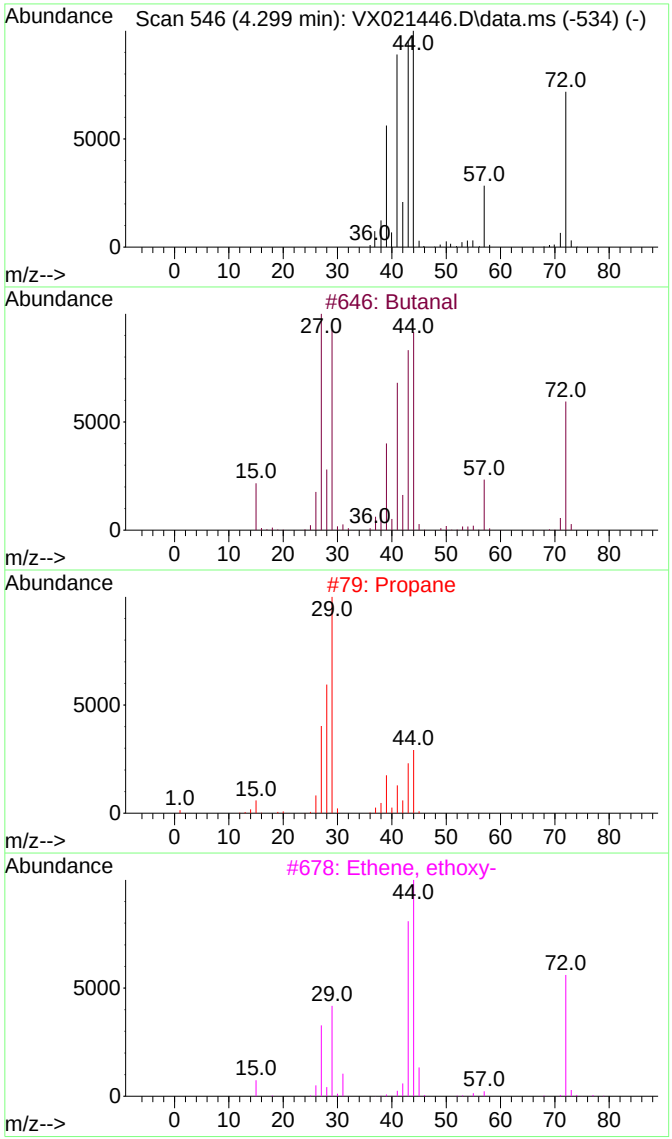
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

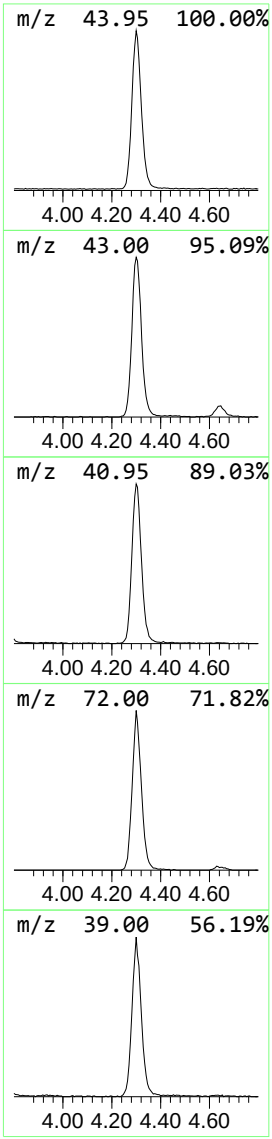
****

Peak Number 3 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	79.57 ug/l	334196	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	47
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Methacrolein	70	C4H6O	000078-85-3	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

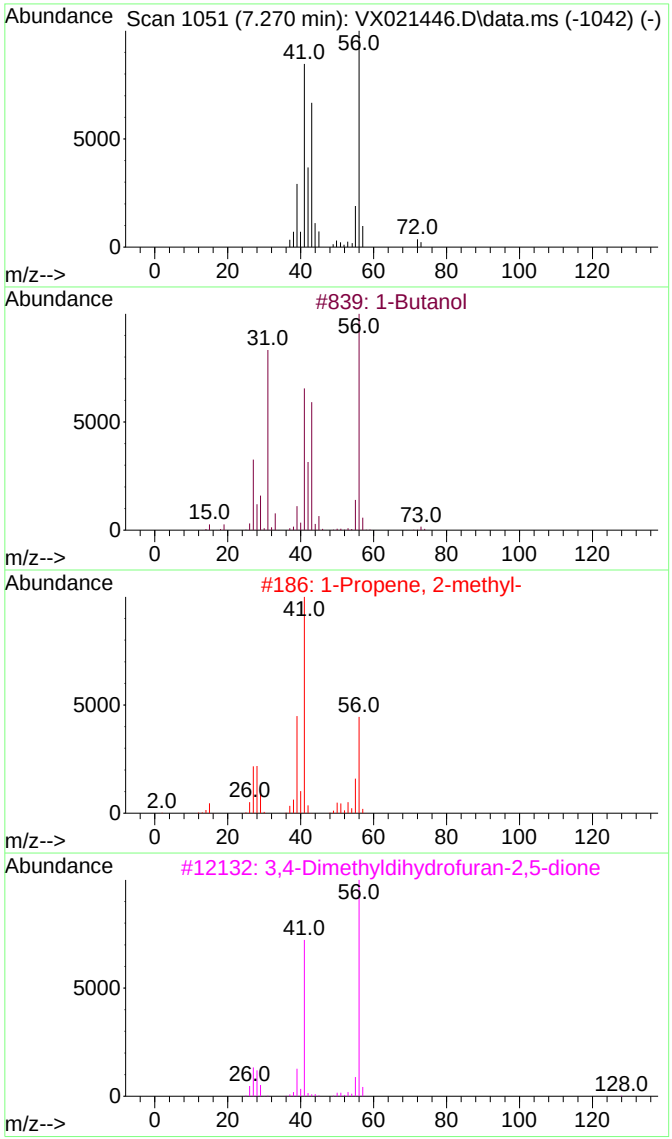
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

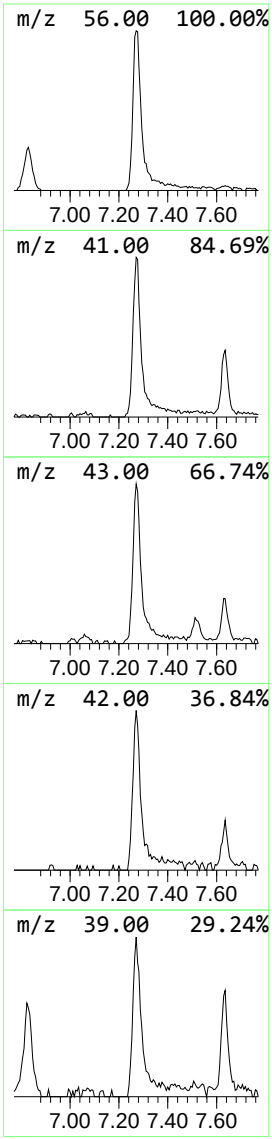
****

Peak Number 4 1-Butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.270	8.63 ug/l	51639	1,4-Difluorobenzene	6.829

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	72
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	42
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
4	2-Butene, (Z)-	56	C4H8	000590-18-1	17
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

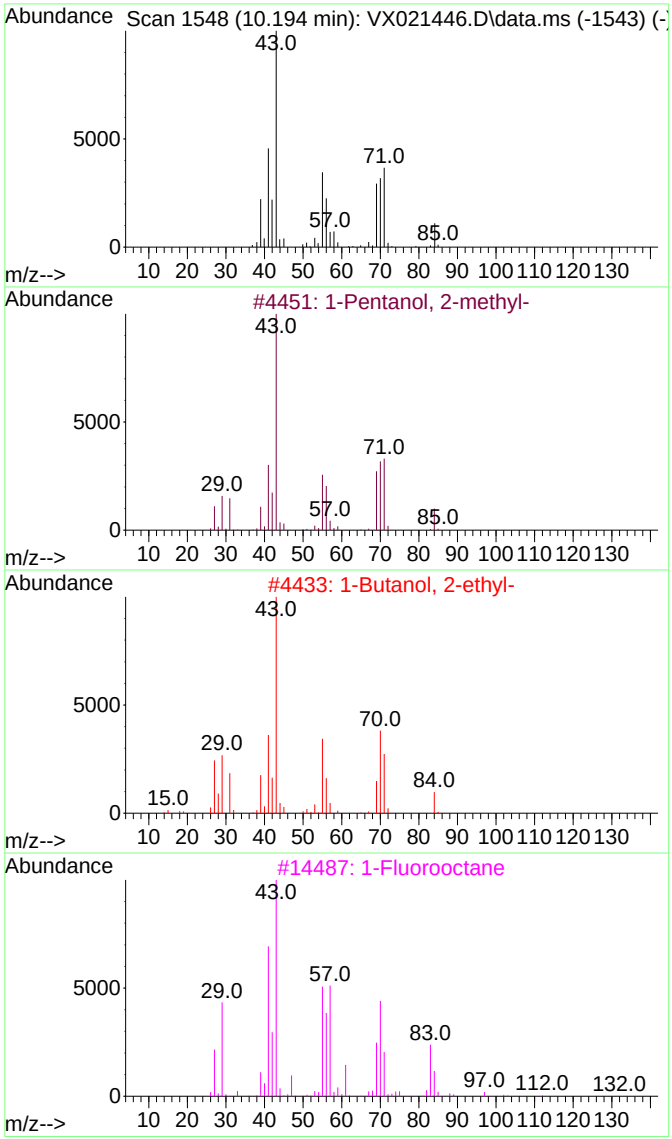
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

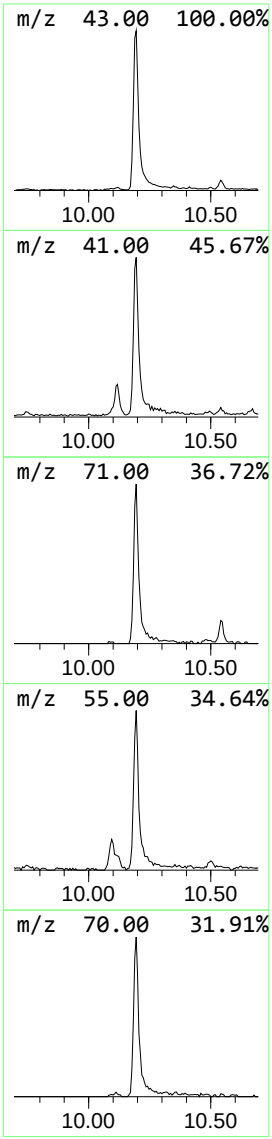
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Pentanol, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.194	13.99 ug/l	115654	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	64
3	1-Fluorooctane	132	C8H17F	000463-11-6	45
4	Pyrrolidine	71	C4H9N	000123-75-1	42
5	Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30807

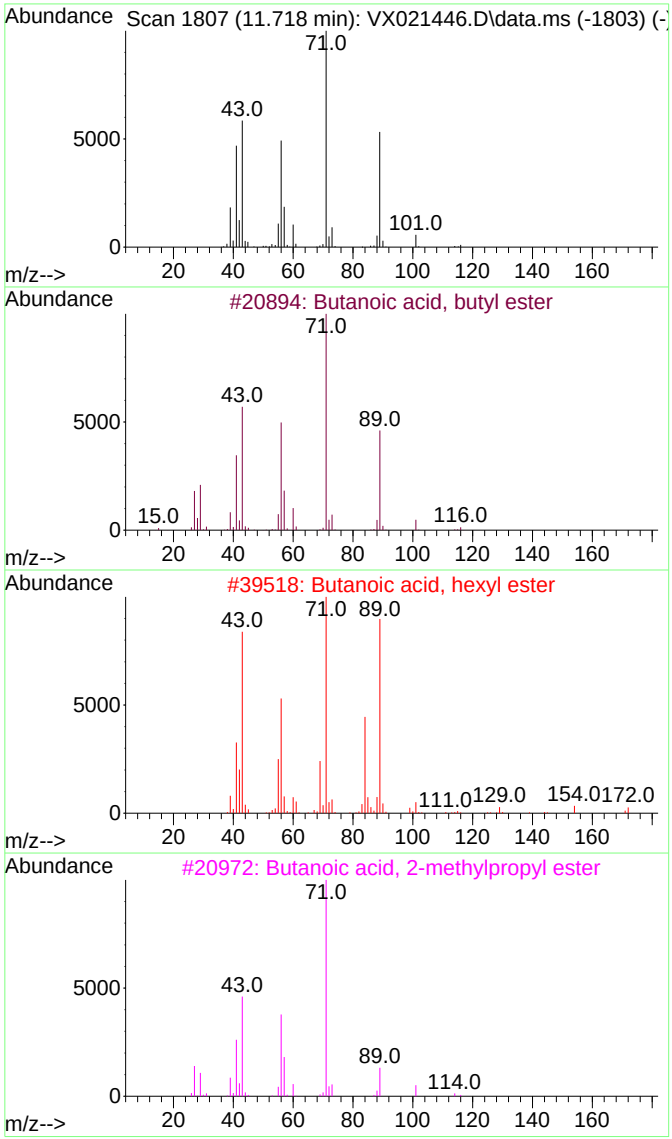
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

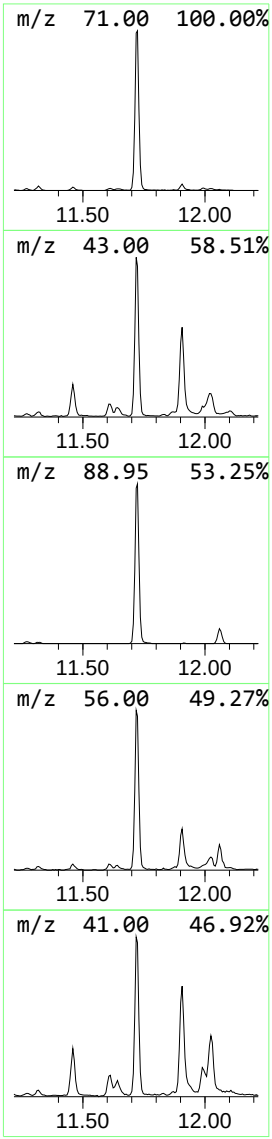
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.718	23.44 ug/l	182028	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

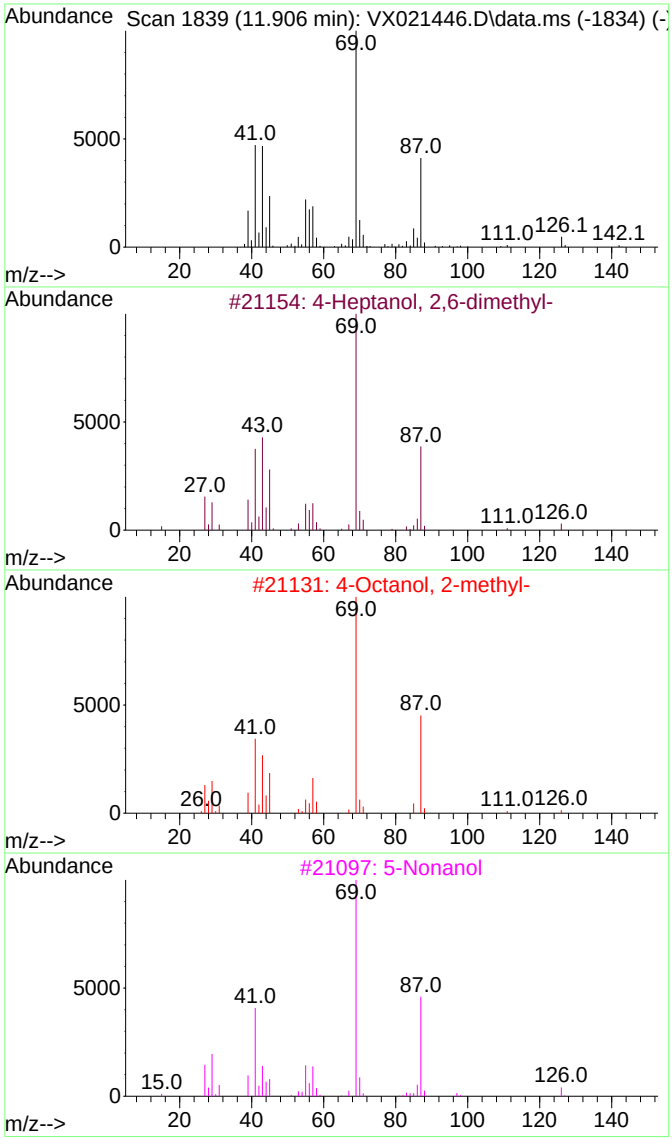
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

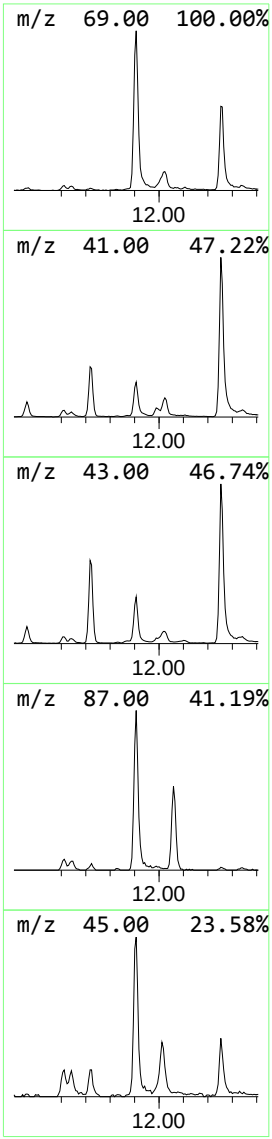
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Heptanol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.906	17.81 ug/l	138308	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	78
3	5-Nonanol	144	C9H20O	000623-93-8	72
4	4,5-Octanediol, 2,7-dimethyl-	174	C10H22O2	1000153-20-8	72
5	3-Heptanol, 2-methyl-	130	C8H18O	018720-62-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

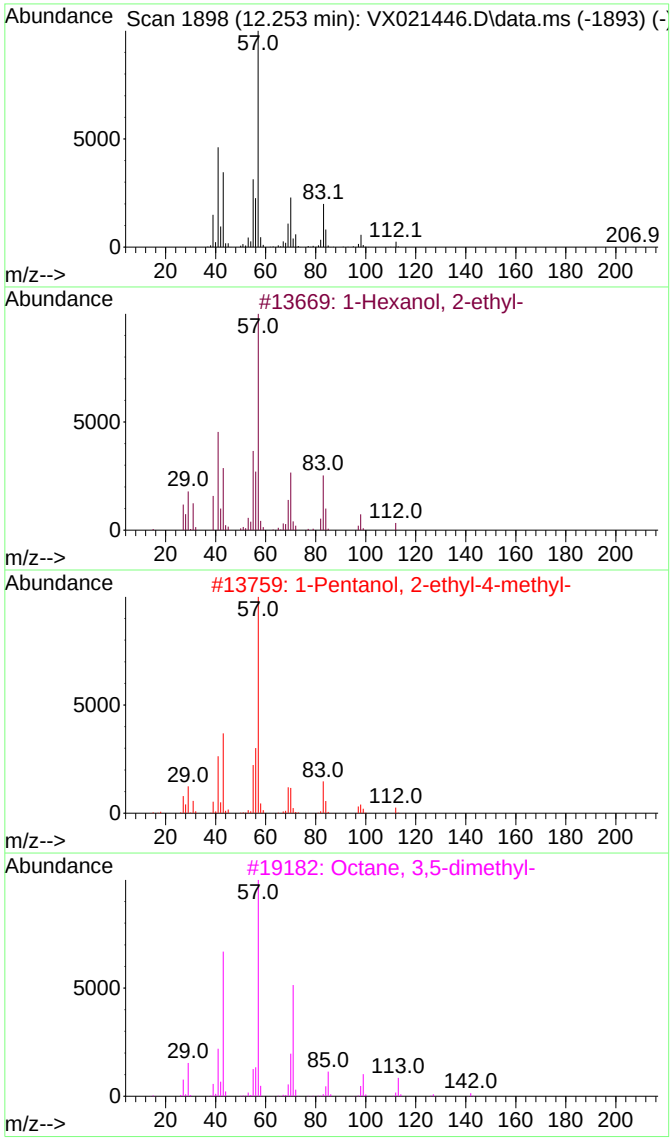
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

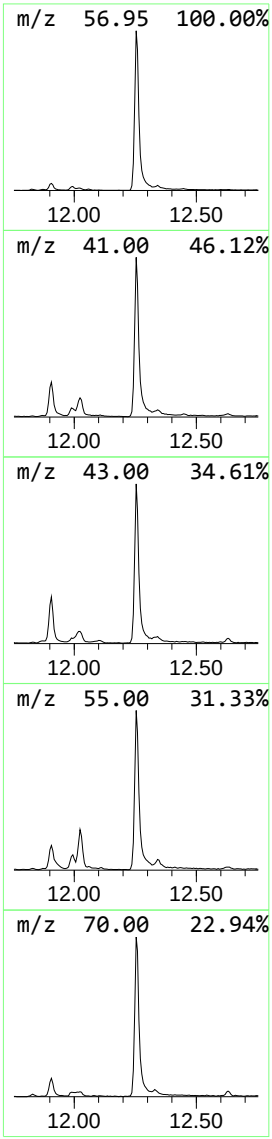
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	77.28 ug/l	600040	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

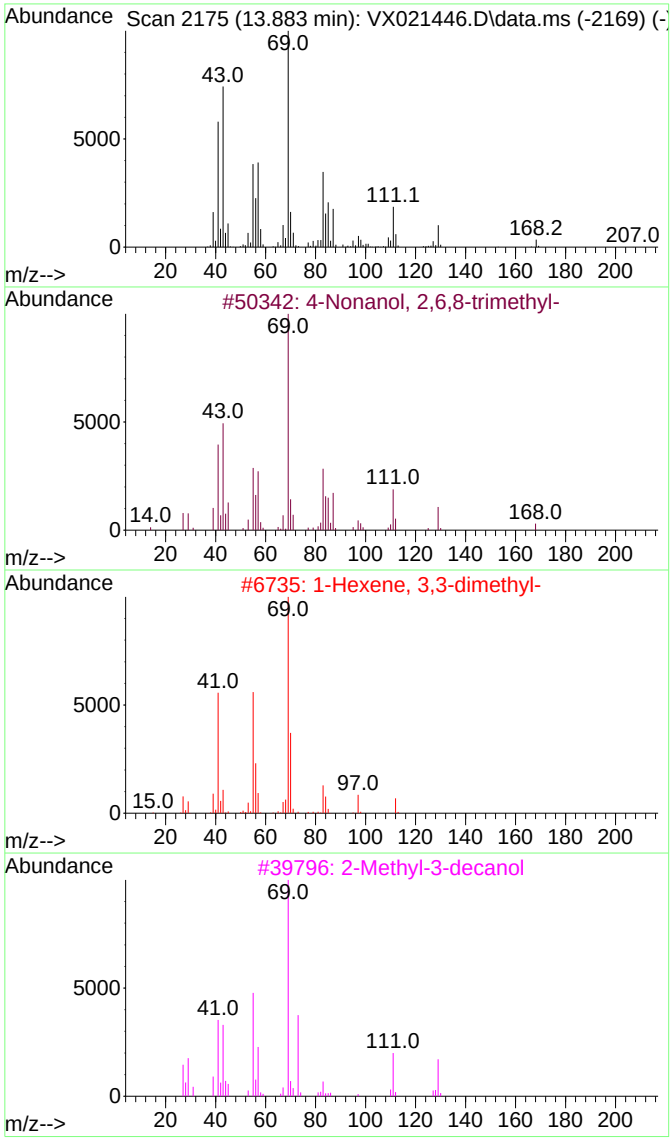
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

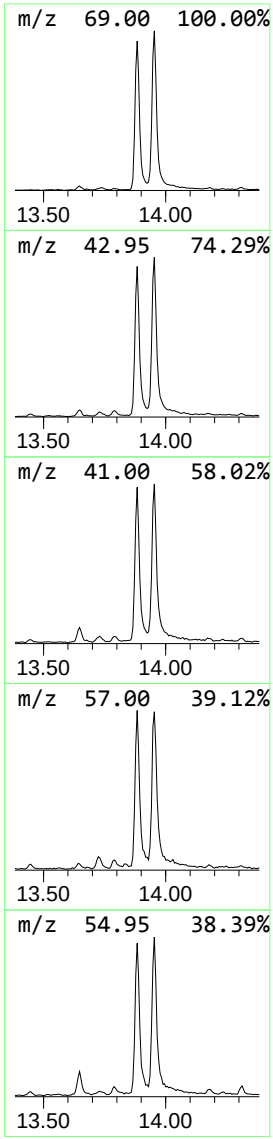
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Nonanol, 2,6,8-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.883	40.08 ug/l	311178	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonanol, 2,6,8-trimethyl-	186	C12H26O	000123-17-1	86
2	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	50
3	2-Methyl-3-decanol	172	C11H24O	083909-79-9	47
4	Cyclopropanecarboxylic acid,isob...	142	C8H14O2	064969-79-5	47
5	Cyclooctane, butyl-	168	C12H24	016538-93-5	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

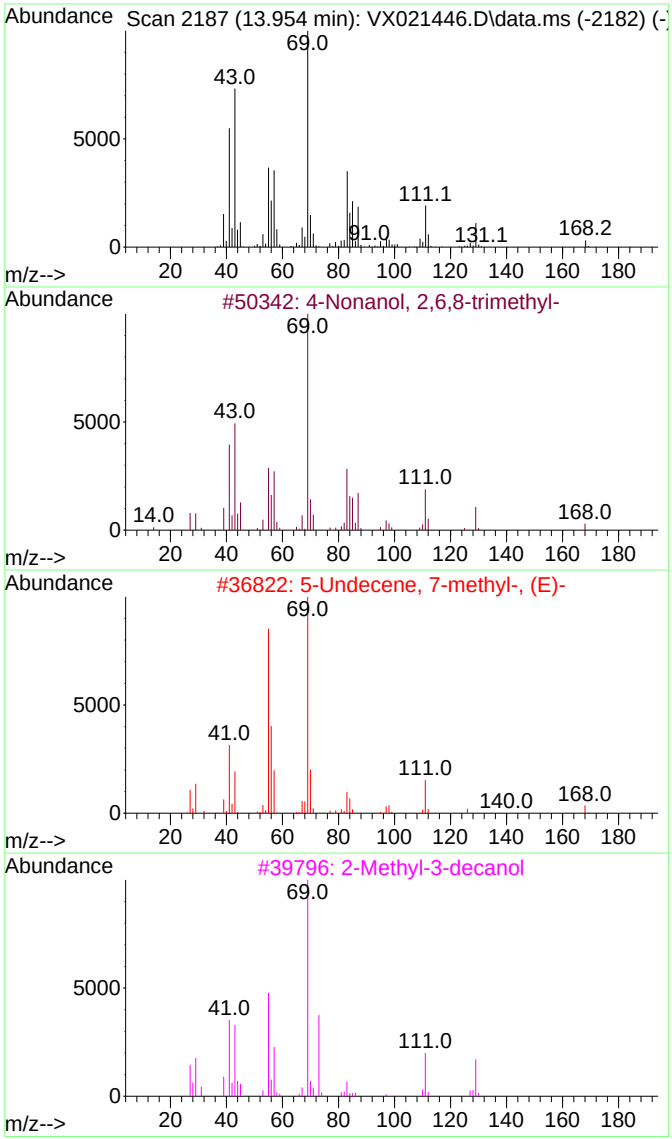
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

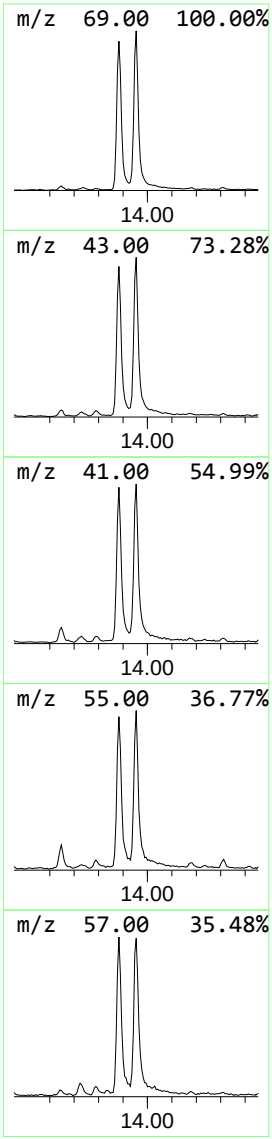
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 5-Undecene, 7-methyl-, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.954	40.87 ug/l	317293	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonanol, 2,6,8-trimethyl-	186	C12H26O	000123-17-1	87
2	5-Undecene, 7-methyl-, (E)-	168	C12H24	074630-66-3	50
3	2-Methyl-3-decanol	172	C11H24O	083909-79-9	47
4	Cyclooctane, ethyl-	140	C10H20	013152-02-8	43
5	2-Hexene, 4-methyl-, (E)-	98	C7H14	003683-22-5	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021446.D
Acq On : 24 Mar 2021 19:10
Operator : JC/MD
Sample : M1774-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30807

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.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
Propane	1.158	17.6	ug/l	73783	1	5.629	209994	50.0
unknown3.752	3.752	18.6	ug/l	77987	1	5.629	209994	50.0
Butanal	4.299	79.6	ug/l	334196	1	5.629	209994	50.0
1-Butanol	7.270	8.6	ug/l	51639	2	6.829	299105	50.0
1-Pentanol, 2-m...	10.194	14.0	ug/l	115654	3	10.094	413347	50.0
Butanoic acid, ...	11.718	23.4	ug/l	182028	4	12.059	388206	50.0
4-Heptanol, 2,6...	11.906	17.8	ug/l	138308	4	12.059	388206	50.0
1-Hexanol, 2-et...	12.253	77.3	ug/l	600040	4	12.059	388206	50.0
4-Nonanol, 2,6,...	13.883	40.1	ug/l	311178	4	12.059	388206	50.0
5-Undecene, 7-m...	13.954	40.9	ug/l	317293	4	12.059	388206	50.0