LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021224.D
Acq On : 16 Mar 2021 01:31
Operator : JC/MD
Sample : M1647-22
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP3-30788:89

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\82X031521W.M
Title : SW846 8260

Signal : TIC: VX021224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.164	10	13	20	rVB2	15564	15153	3.25%	0.323%
2	1.281	29	33	36	rBV2	4594	5099	1.09%	0.109%
3	1.376	46	49	55	rVB2	6663	7955	1.71%	0.170%
4	1.476	62	66	76	rVV	51590	57391	12.32%	1.225%
5	1.599	79	87	91	rVB5	4911	11940	2.56%	0.255%
6	2.093	166	171	179	rBV	12929	20221	4.34%	0.432%
7	2.334	206	212	220	rVB	4567	7184	1.54%	0.153%
8	2.423	220	227	232	rBV	40603	68016	14.60%	1.452%
9	2.582	245	254	260	rBV2	6286	14020	3.01%	0.299%
10	2.752	276	283	293	rVB	20070	35525	7.62%	0.758%
11	3.011	316	327	338	rBV	17205	39291	8.43%	0.839%
12	3.388	384	391	401	rVB2	2693	6375	1.37%	0.136%
13	3.758	444	454	464	rBV2	7427	20764	4.46%	0.443%
14	4.076	497	508	515	rVB6	2884	7924	1.70%	0.169%
15	4.299	534	546	561	rBV	66365	185263	39.76%	3.955%
16	4.441	561	570	584	rVB3	5651	21229	4.56%	0.453%
17	4.641	593	604	612	rBV2	4486	13683	2.94%	0.292%
18	5.464	733	744	757	rBV	55636	158078	33.93%	3.375%
19	5.629	761	772	788	rVB	84526	235104	50.46%	5.019%
20	6.029	828	840	847	rBV	63395	166191	35.67%	3.548%
21	6.111	847	854	864	rVV2	55168	148342	31.84%	3.167%
22	6.182	864	866	877	rVB4	3171	6565	1.41%	0.140%
23	6.829	967	976	987	rBV	144061	338449	72.64%	7.225%
24	7.265	1038	1050	1060	rBV	20109	49530	10.63%	1.057%
25	7.512	1086	1092	1100	rVB	2797	5587	1.20%	0.119%
26	7.629	1107	1112	1119	rVB2	6087	11612	2.49%	0.248%
27	8.618	1274	1280	1286	rBV2	3461	5595	1.20%	0.119%
28	8.694	1286	1293	1300	rBV	298727	465934	100.00%	9.946%
29	8.765	1300	1305	1311	rVB	61260	95385	20.47%	2.036%
30	9.277	1386	1392	1401	rBV	9943	18155	3.90%	0.388%
31	9.488	1421	1428	1431	rBV3	7028	12900	2.77%	0.275%
32	9.530	1431	1435	1446	rVB	38527	60865	13.06%	1.299%
33	10.094	1520	1531	1536	rBV	318837	435022	93.37%	9.287%
34	10.194	1543	1548	1552	rBV	21528	32123	6.89%	0.686%
35	10.235	1552	1555	1560	rVB	9575	12557	2.70%	0.268%
36	10.341	1568	1573	1579	rVB	39860	55226	11.85%	1.179%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021224.D
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Operator : JC/MD
Sample : M1647-22
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP3-30788:89

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\82X031521W.M
Title : SW846 8260

37	10.441	1585	1590	1594	rBV3	7904	11512	2.47%	0.246%
38	10.612	1613	1619	1624	rBV5	3280	6008	1.29%	0.128%
39	10.683	1624	1631	1641	rVB3	21906	37484	8.04%	0.800%
40	10.789	1645	1649	1654	rBV	13020	19636	4.21%	0.419%
41	10.894	1662	1667	1672	rBV6	6204	10496	2.25%	0.224%
42	11.118	1698	1705	1711	rBV	266530	338655	72.68%	7.229%
43	11.171	1711	1714	1718	rVV	10976	14656	3.15%	0.313%
44	11.212	1718	1721	1725	rVB2	4351	5635	1.21%	0.120%
45	11.318	1736	1739	1742	rBV3	4787	7221	1.55%	0.154%
46	11.606	1784	1788	1791	rBV	10046	13718	2.94%	0.293%
47	11.642	1791	1794	1803	rVV4	8320	16681	3.58%	0.356%
48	11.724	1803	1808	1815	rVB	78032	103047	22.12%	2.200%
49	11.789	1815	1819	1824	rBV	10305	13037	2.80%	0.278%
50	11.906	1831	1839	1848	rBV	29612	48631	10.44%	1.038%
51	11.995	1850	1854	1855	rVV	7951	9940	2.13%	0.212%
52	12.024	1855	1859	1861	rVV	43115	55028	11.81%	1.175%
53	12.059	1861	1865	1873	rVV	318468	407190	87.39%	8.692%
54	12.124	1873	1876	1881	rVB	4072	4878	1.05%	0.104%
55	12.253	1893	1898	1909	rBV	282131	403325	86.56%	8.610%
56	12.342	1909	1913	1920	rVB6	13437	24176	5.19%	0.516%
57	12.453	1927	1932	1936	rVB2	11529	14836	3.18%	0.317%
58	12.630	1955	1962	1969	rVB8	4589	10999	2.36%	0.235%
59	12.836	1987	1997	2003	rBV3	9216	19469	4.18%	0.416%
60	12.942	2011	2015	2020	rBV5	2803	5603	1.20%	0.120%
61	12.995	2020	2024	2028	rVV4	5175	8246	1.77%	0.176%
62	13.330	2077	2081	2086	rVB3	3720	5415	1.16%	0.116%
63	13.454	2097	2102	2109	rVB5	3203	6377	1.37%	0.136%
64	13.648	2126	2135	2143	rBV5	12780	28431	6.10%	0.607%
65	13.818	2156	2164	2170	rBV2	45276	67476	14.48%	1.440%
66	13.883	2170	2175	2182	rVV3	23703	36912	7.92%	0.788%
67	13.954	2182	2187	2201	rVB	21833	36788	7.90%	0.785%
68	14.518	2278	2283	2294	rVB5	5576	9545	2.05%	0.204%
69	14.677	2306	2310	2316	rVB	11143	14617	3.14%	0.312%
70	14.818	2330	2334	2341	rBV2	7490	10100	2.17%	0.216%
71	16.024	2533	2539	2548	rVB6	4505	8414	1.81%	0.180%

Sum of corrected areas: 4684435

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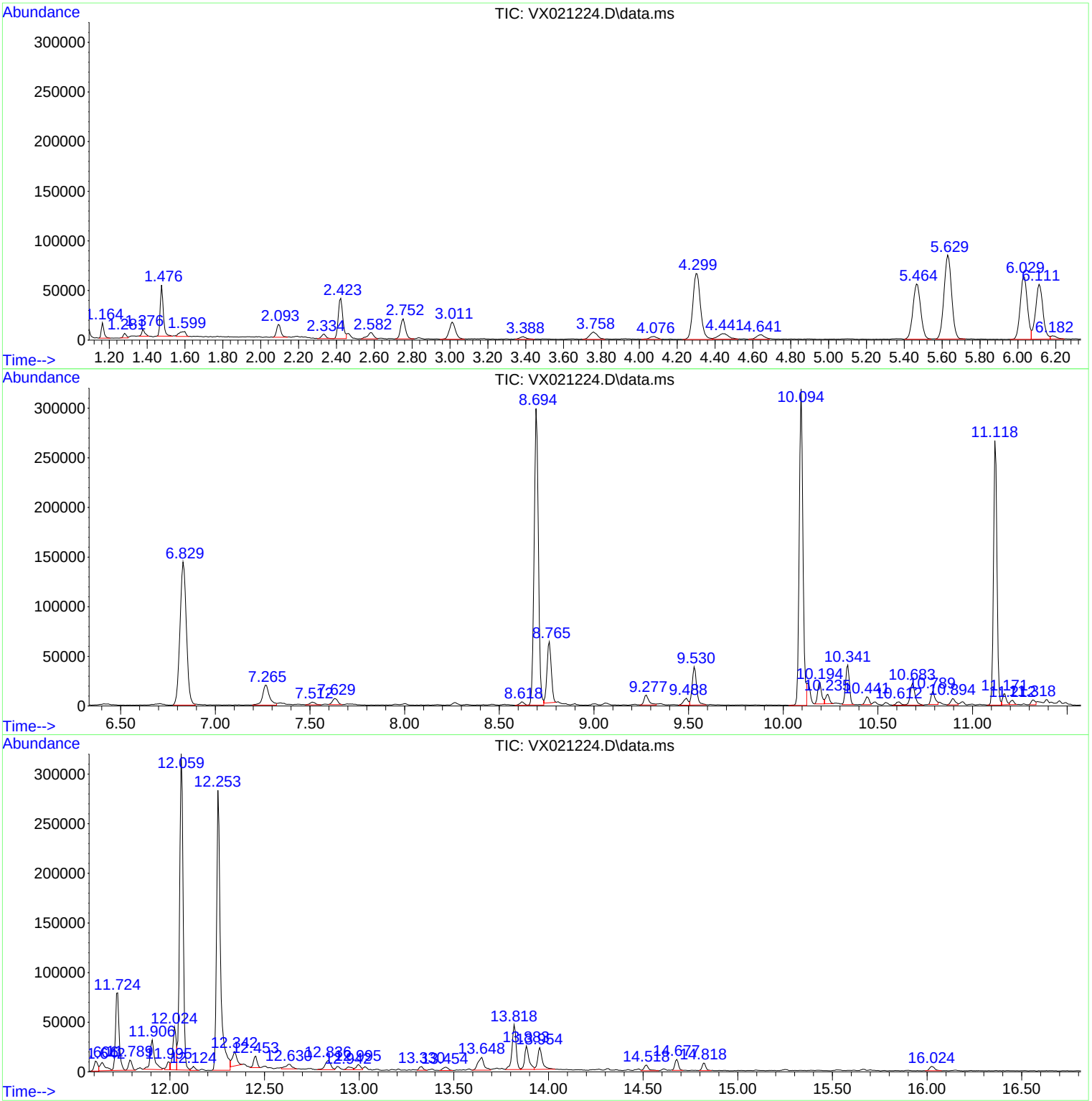
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP3-30788:89

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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



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Data File : VX021224.D
Acq On : 16 Mar 2021 01:31
Operator : JC/MD
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

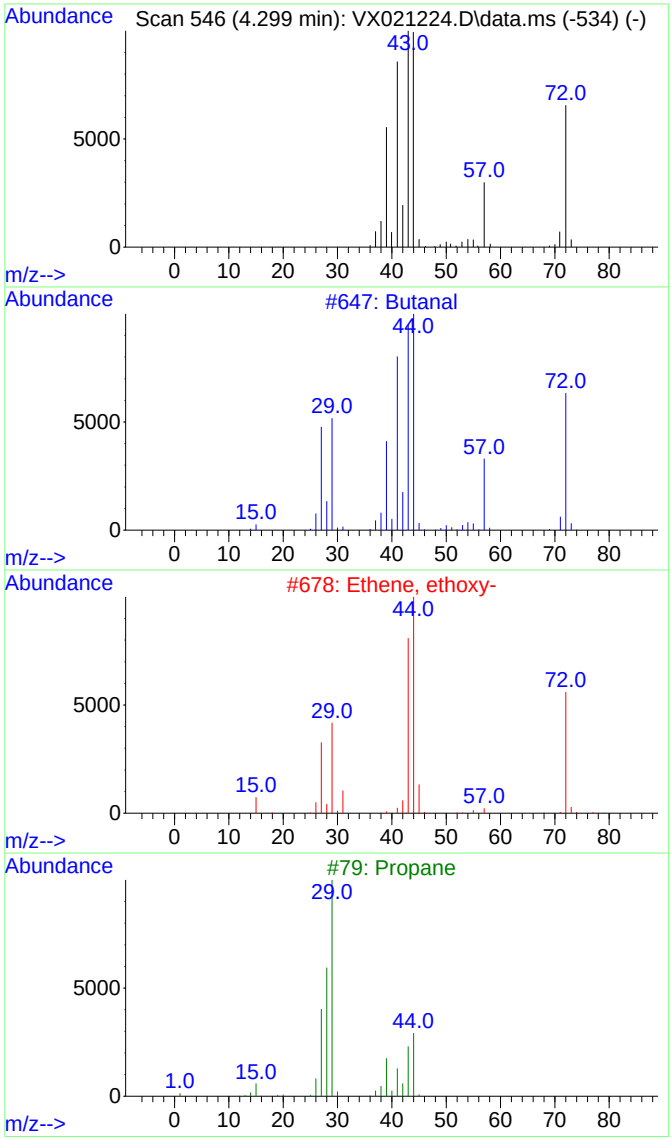
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

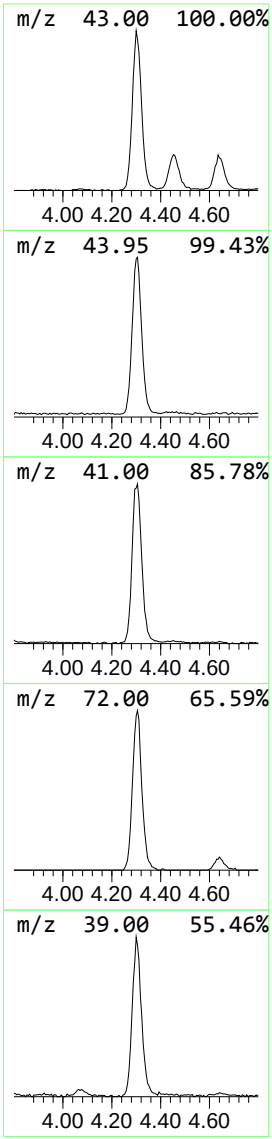
****

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	39.40 ug/l	185263	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	Propane	44	C3H8	000074-98-6	43
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\VX031521\
Data File : VX021224.D
Acq On : 16 Mar 2021 01:31
Operator : JC/MD
Sample : M1647-22
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP3-30788:89

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

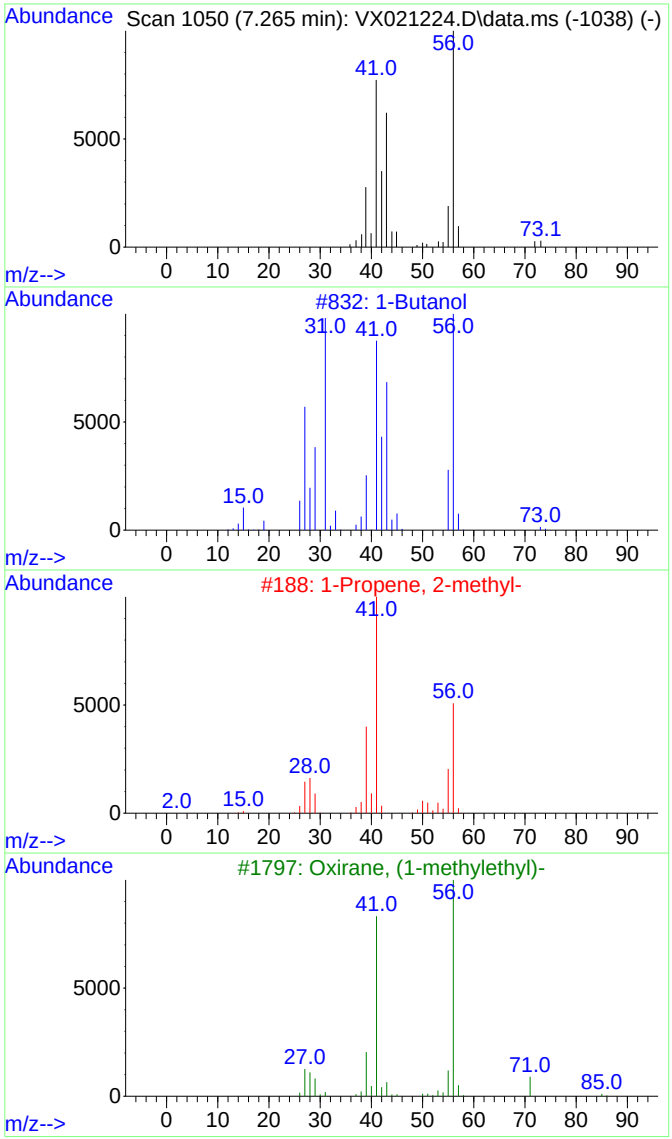
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

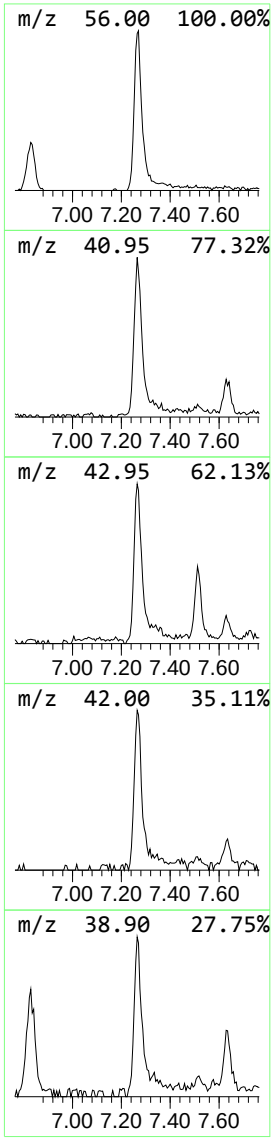
****

Peak Number 3 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.265	7.32 ug/l	49530	1,4-Difluorobenzene	6.829

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	50
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
4	2-Butene	56	C4H8	000107-01-7	40
5	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9





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Instrument :
MSVOA_X
ClientSampleId :
COMP3-30788:89

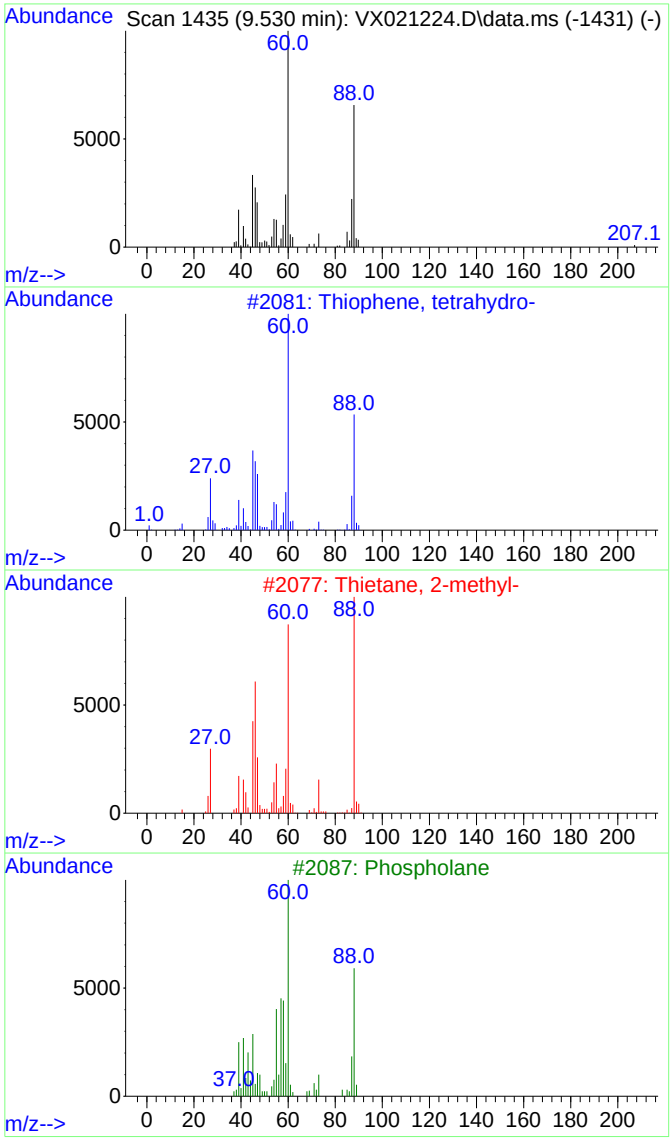
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

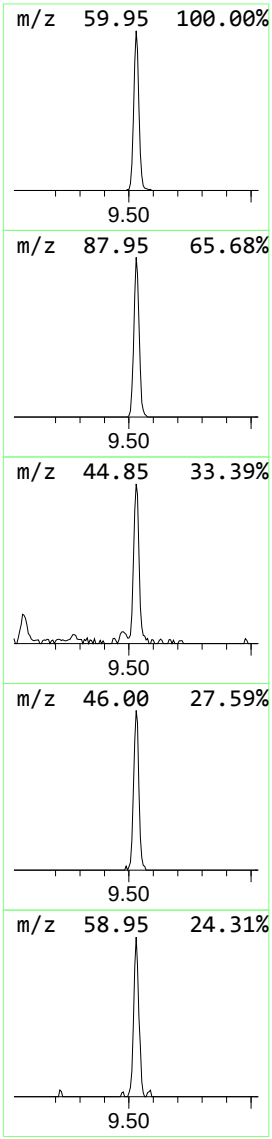
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Thiophene, tetrahydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.530	7.00 ug/l	60865	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3	Phospholane	88	C4H9P	003466-00-0	50
4	Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
5	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
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Acq On : 16 Mar 2021 01:31
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP3-30788:89

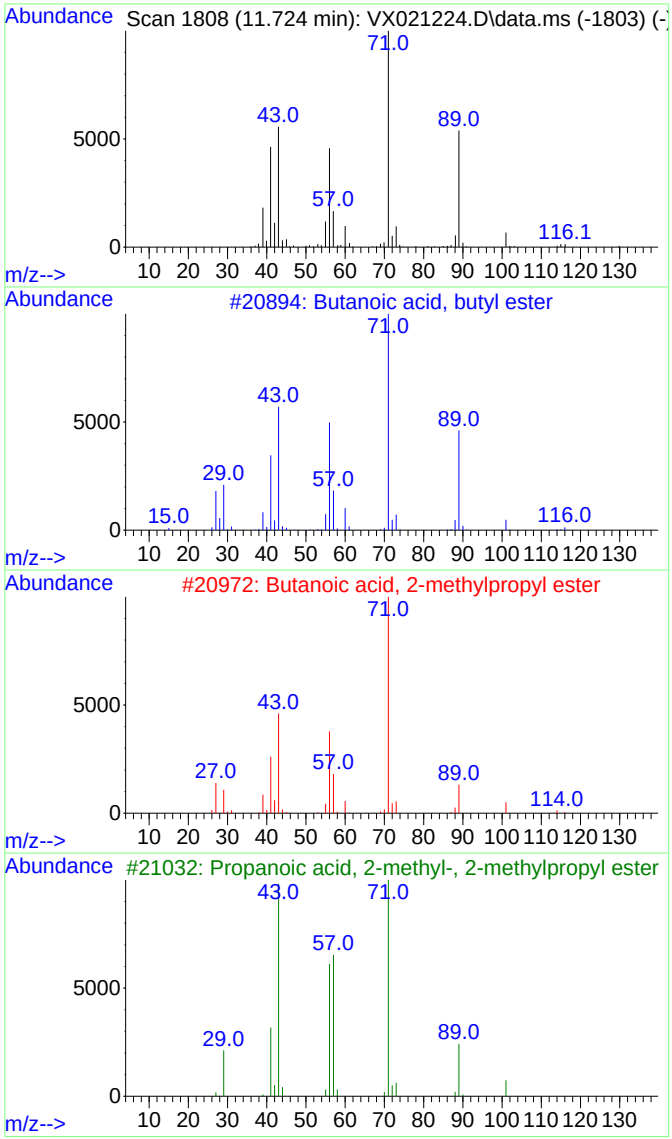
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

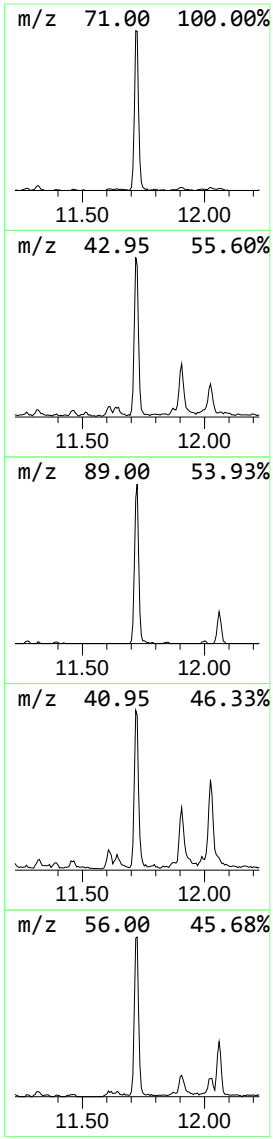
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.724	12.65 ug/l	103047	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64





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Instrument :
MSVOA_X
ClientSampleId :
COMP3-30788:89

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

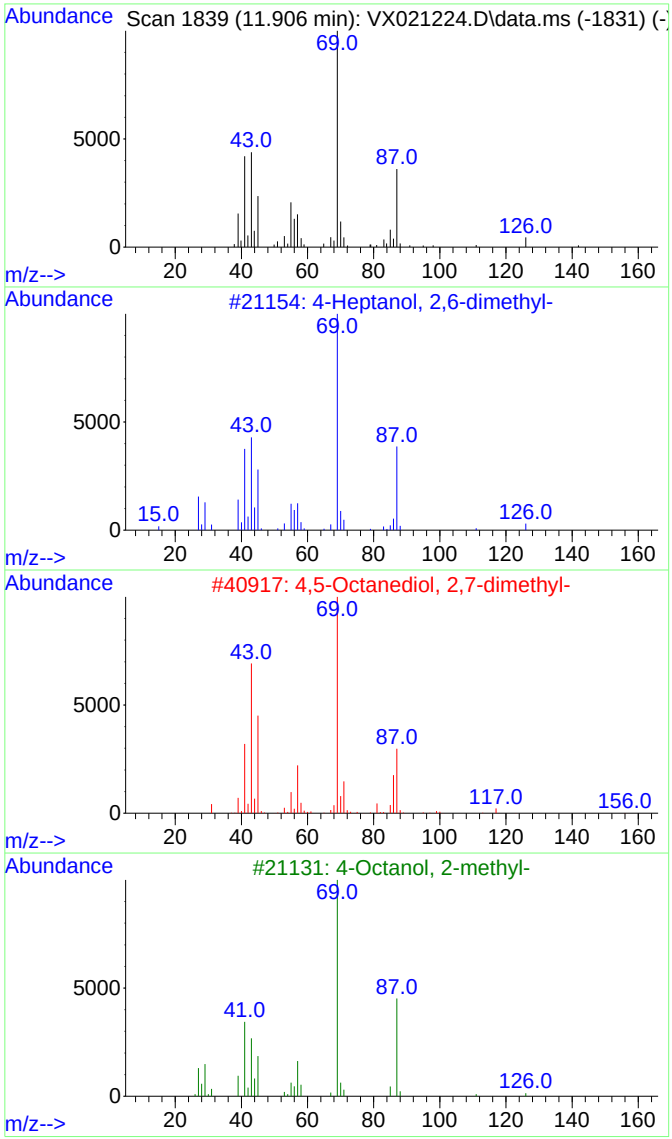
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

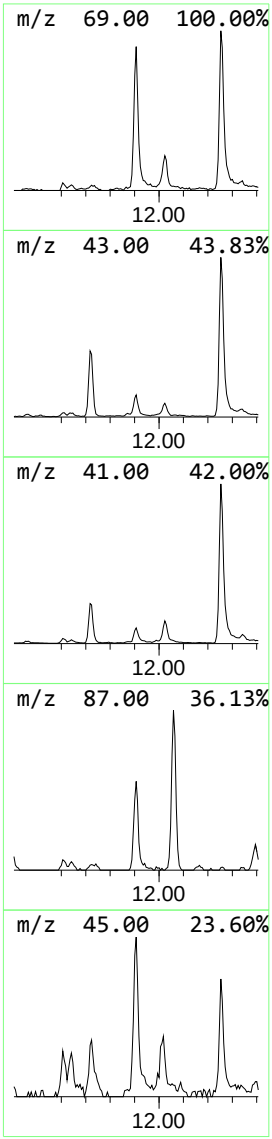
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.906	5.97 ug/l	48631	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	90
2	4,5-Octanediol, 2,7-dimethyl-	174	C10H22O2	1000153-20-8	72
3	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64
4	5-Nonanol	144	C9H20O	000623-93-8	64
5	5-Dodecanol	186	C12H26O	010203-33-5	64





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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP3-30788:89

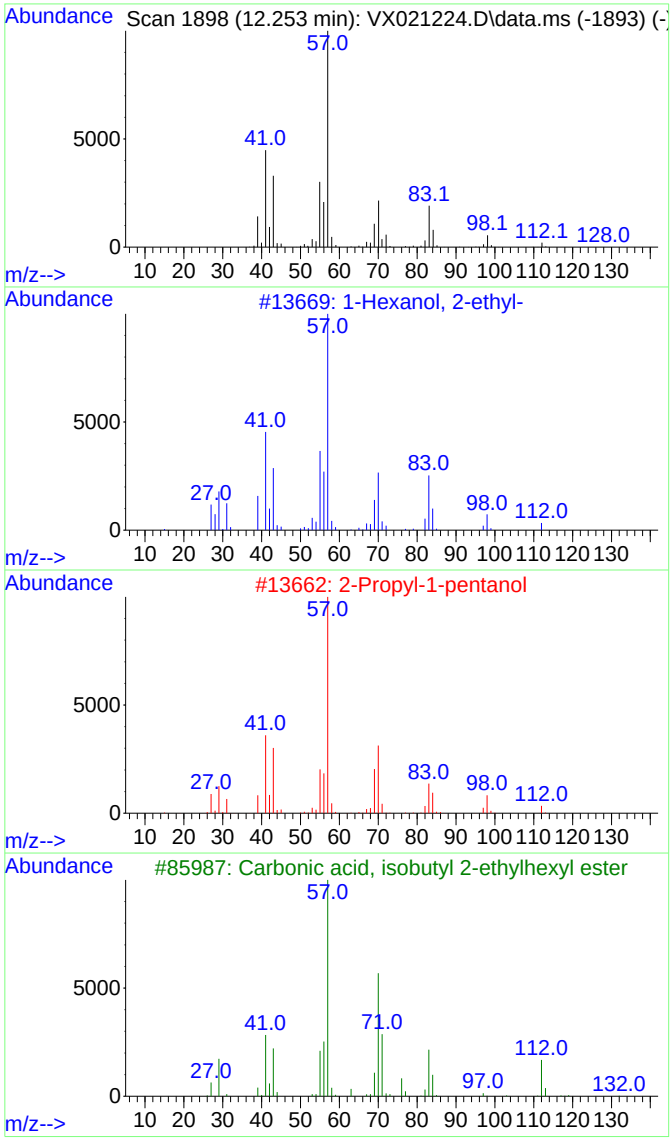
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

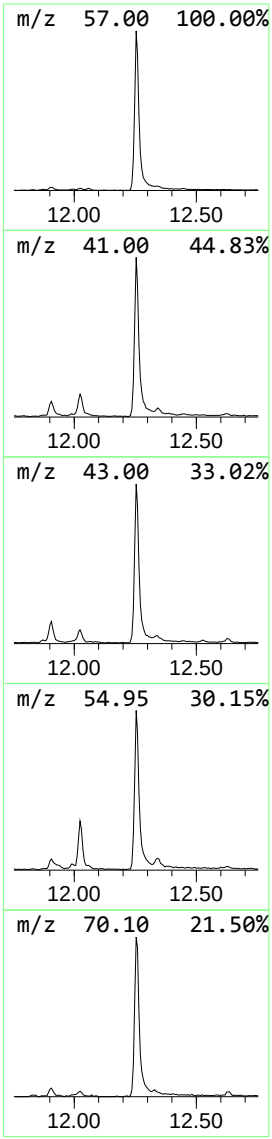
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	49.53 ug/l	403325	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	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45
4	1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	45
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	42





Tentatively Identified Compound (LSC) summary

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Data File : VX021224.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP3-30788:89

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.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
Butanal	4.299	39.4	ug/l	185263	1	5.629	235104	50.0
1-Butanol	7.265	7.3	ug/l	49530	2	6.829	338449	50.0
Thiophene, tetr...	9.530	7.0	ug/l	60865	3	10.094	435022	50.0
Butanoic acid, ...	11.724	12.7	ug/l	103047	4	12.059	407190	50.0
4-Heptanol, 2,6...	11.906	6.0	ug/l	48631	4	12.059	407190	50.0
1-Hexanol, 2-et...	12.253	49.5	ug/l	403325	4	12.059	407190	50.0