LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091923\
Data File : VX037807.D
Acq On : 19 Sep 2023 15:40
Operator : JC/MD
Sample : 04479-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

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\82X091523W.M
Title : SW846 8260

Signal : TIC: VX037807.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	20	rBV	68578	72970	2.45%	0.536%
2	1.453	56	60	65	rBV	42198	45783	1.54%	0.336%
3	2.380	206	212	220	rBV	52418	85889	2.88%	0.631%
4	3.331	359	368	378	rBV	18377	43147	1.45%	0.317%
5	4.233	504	516	536	rBV	1135718	2977779	100.00%	21.886%
6	4.556	559	569	586	rBV	314992	886135	29.76%	6.513%
7	5.001	631	642	662	rBV	33280	113772	3.82%	0.836%
8	5.385	695	705	722	rBV	130928	388728	13.05%	2.857%
9	5.556	722	733	749	rVB	225788	644436	21.64%	4.736%
10	5.958	788	799	809	rBV	143960	388295	13.04%	2.854%
11	6.111	819	824	838	rVB3	13415	36036	1.21%	0.265%
12	6.763	921	931	944	rBV	353791	844451	28.36%	6.206%
13	7.208	996	1004	1024	rBV	110817	257051	8.63%	1.889%
14	7.580	1058	1065	1075	rBV	59602	115176	3.87%	0.846%
15	8.653	1234	1241	1248	rBV	730675	1176603	39.51%	8.648%
16	10.055	1465	1471	1483	rBV	804661	1076554	36.15%	7.912%
17	10.299	1504	1511	1522	rVB	20286	32682	1.10%	0.240%
18	10.750	1580	1585	1595	rBV	137272	195730	6.57%	1.439%
19	11.079	1634	1639	1645	rBV	672901	856368	28.76%	6.294%
20	11.134	1645	1648	1653	rVB	25343	33854	1.14%	0.249%
21	11.573	1715	1720	1722	rBV	65079	78426	2.63%	0.576%
22	11.604	1722	1725	1735	rVB2	61801	85924	2.89%	0.632%
23	11.866	1765	1768	1776	rVB2	40428	66603	2.24%	0.490%
24	12.024	1789	1794	1801	rVB	902502	1157562	38.87%	8.508%
25	12.219	1820	1826	1837	rBV	1347766	1751529	58.82%	12.873%
26	12.305	1838	1840	1852	rVB4	22497	47915	1.61%	0.352%
27	13.750	2072	2077	2085	rBV2	69039	115474	3.88%	0.849%
28	13.847	2090	2093	2100	rVV2	19474	31283	1.05%	0.230%

Sum of corrected areas: 13606155

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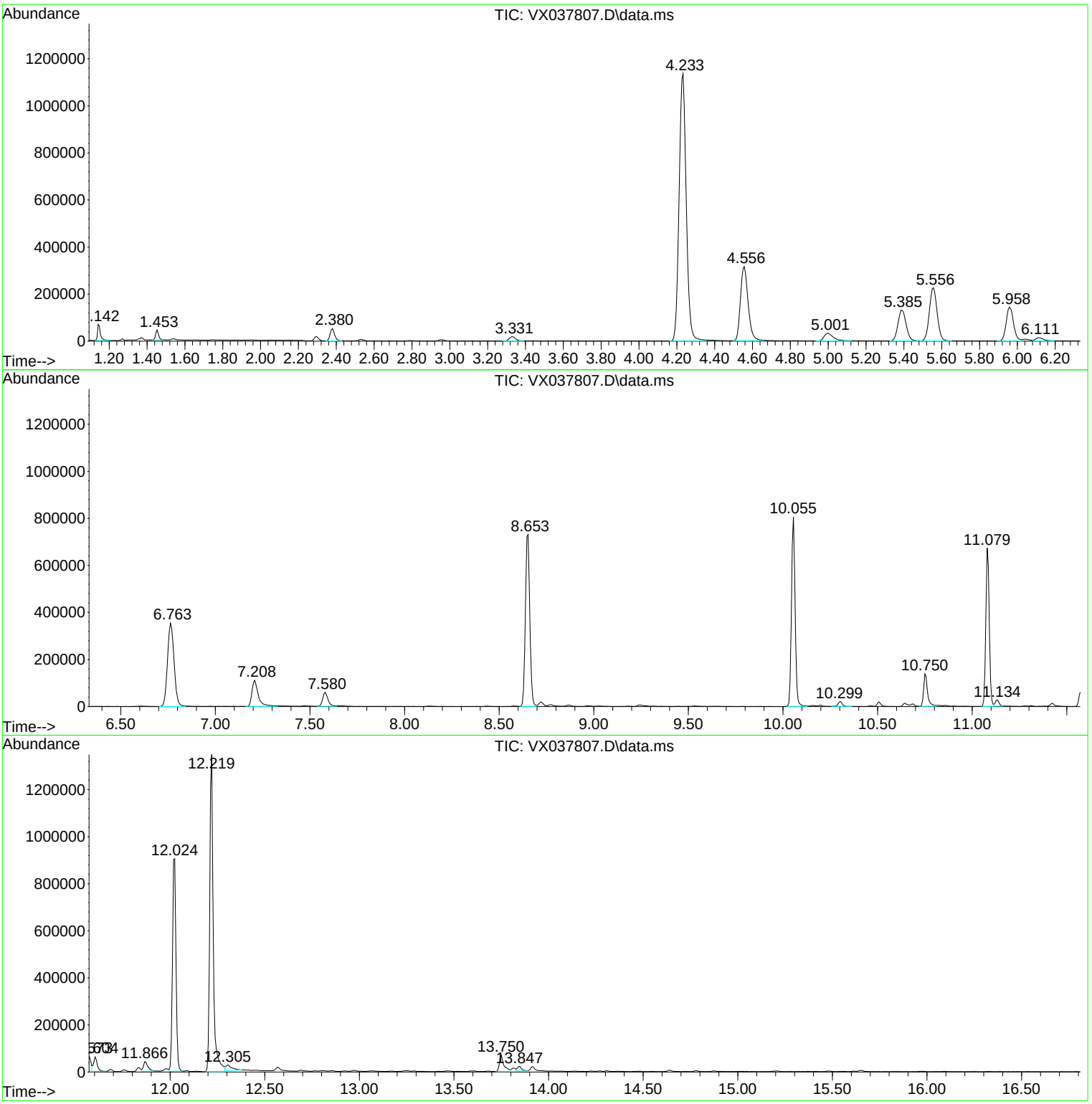
ClientSampleId :
1027

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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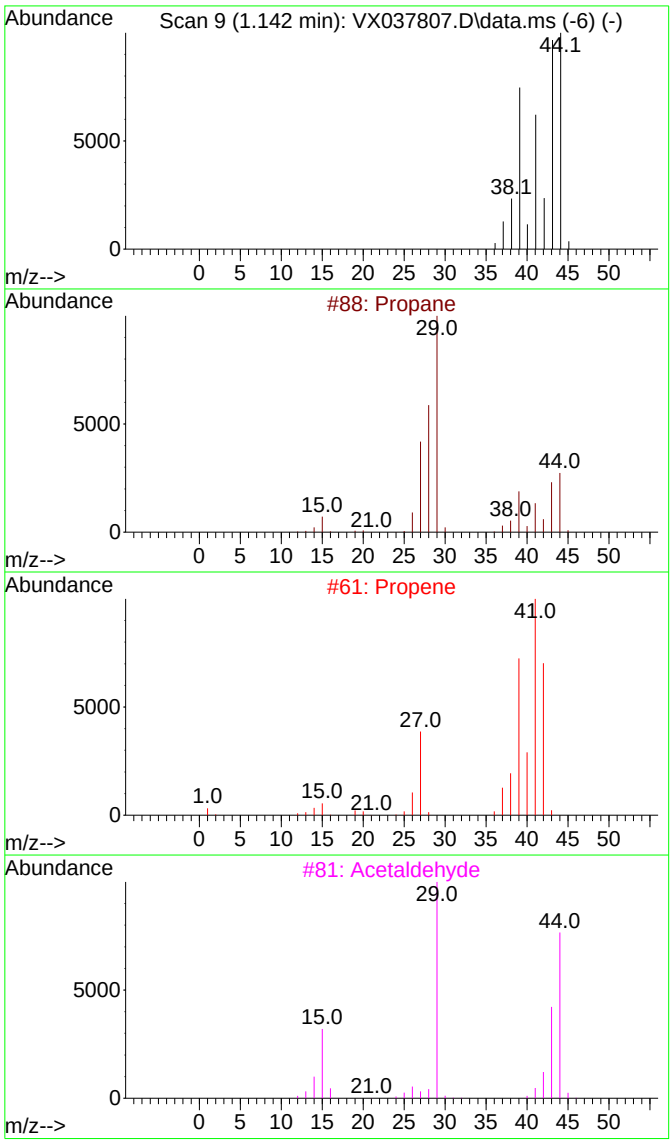
Quant Title : SW846 8260

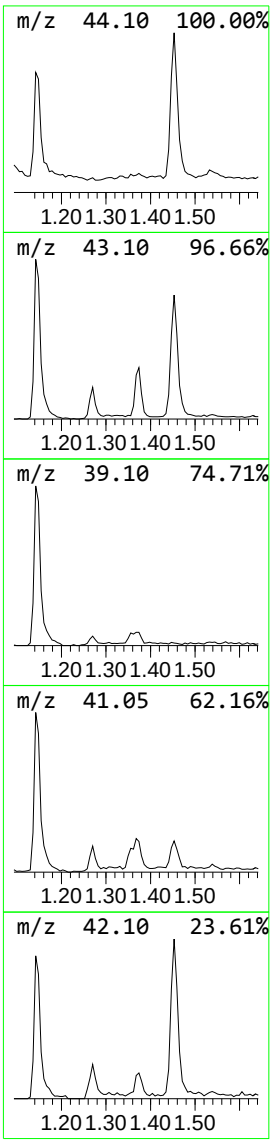
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	5.66 ug/l	72970	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Acetaldehyde	44	C2H4O	000075-07-0	5
4	Cyclopropene	40	C3H4	002781-85-3	2
5	Alanine	89	C3H7NO2	000056-41-7	2





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Data File : VX037807.D
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Operator : JC/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

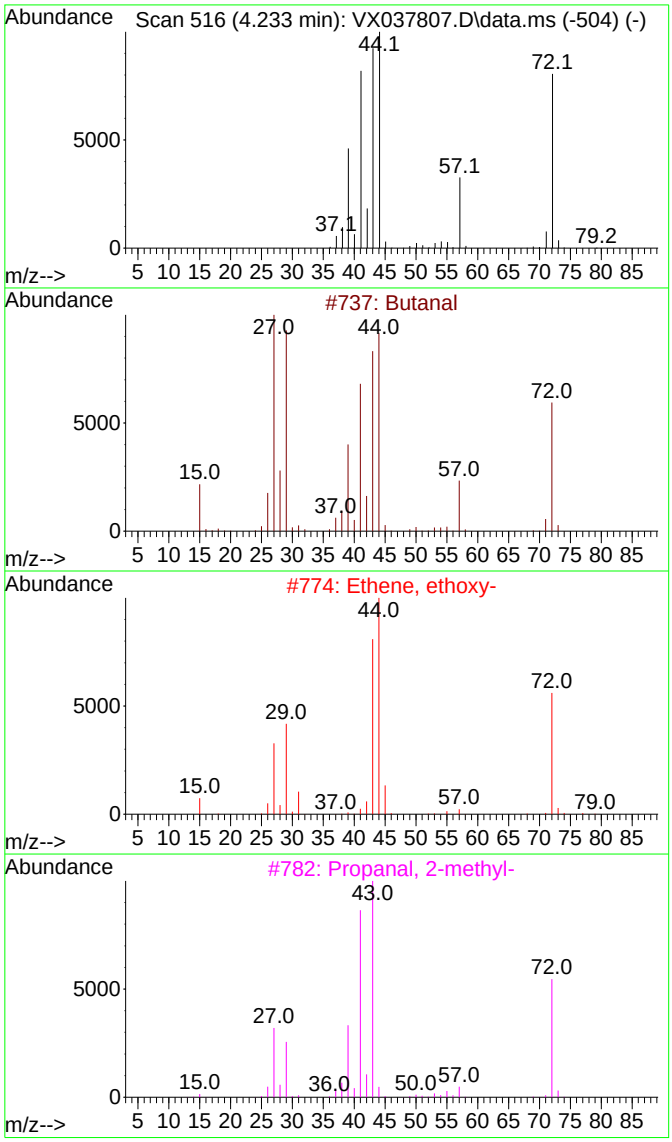
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

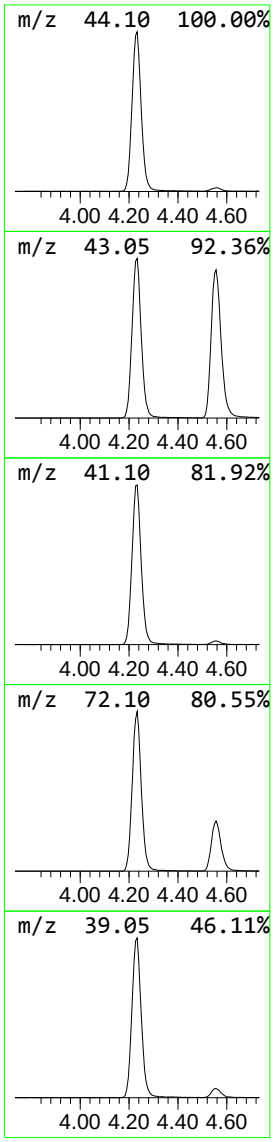
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	231.04 ug/l	2977780	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

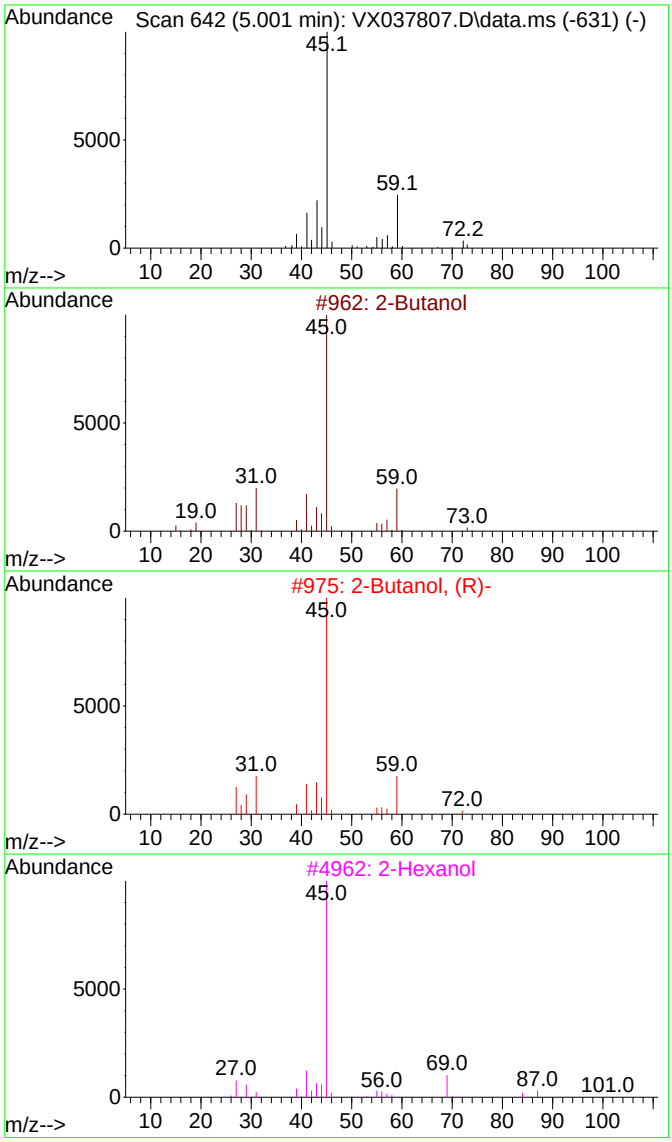
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

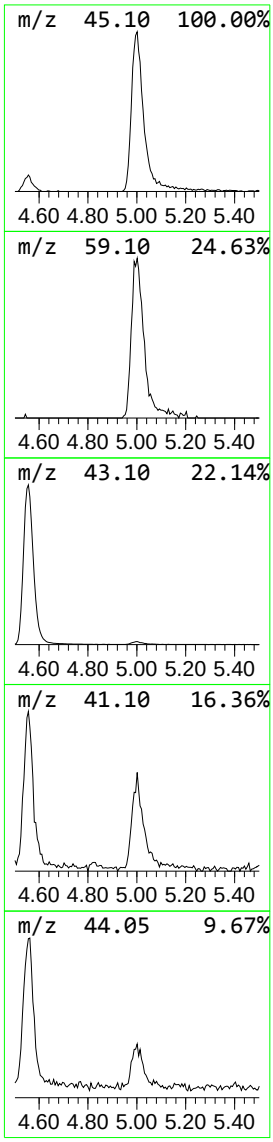
****

Peak Number 3 2-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.001	8.83 ug/l	113772	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
3	2-Hexanol	102	C6H14O	000626-93-7	38
4	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	38
5	1-Pentanol, 5-methoxy-	118	C6H14O2	004799-62-6	38





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

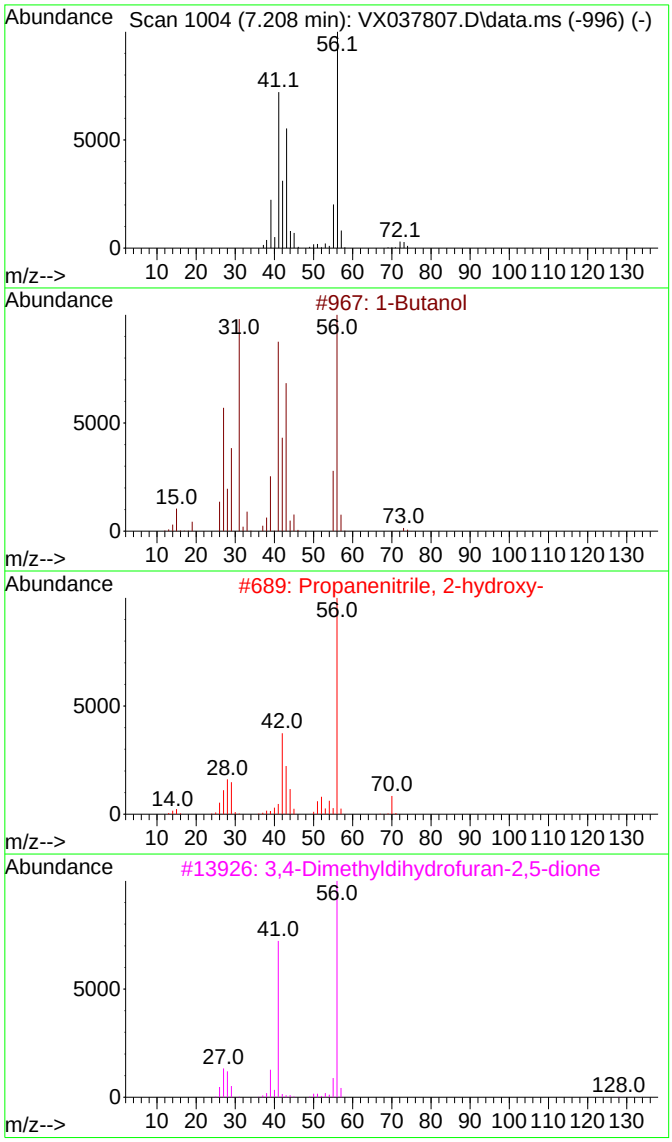
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

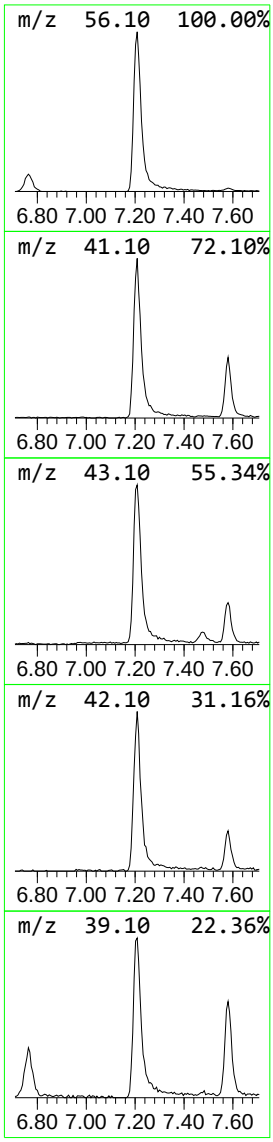
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	15.22 ug/l	257051	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	56
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9





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Acq On : 19 Sep 2023 15:40
Operator : JC/MD
Sample : 04479-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

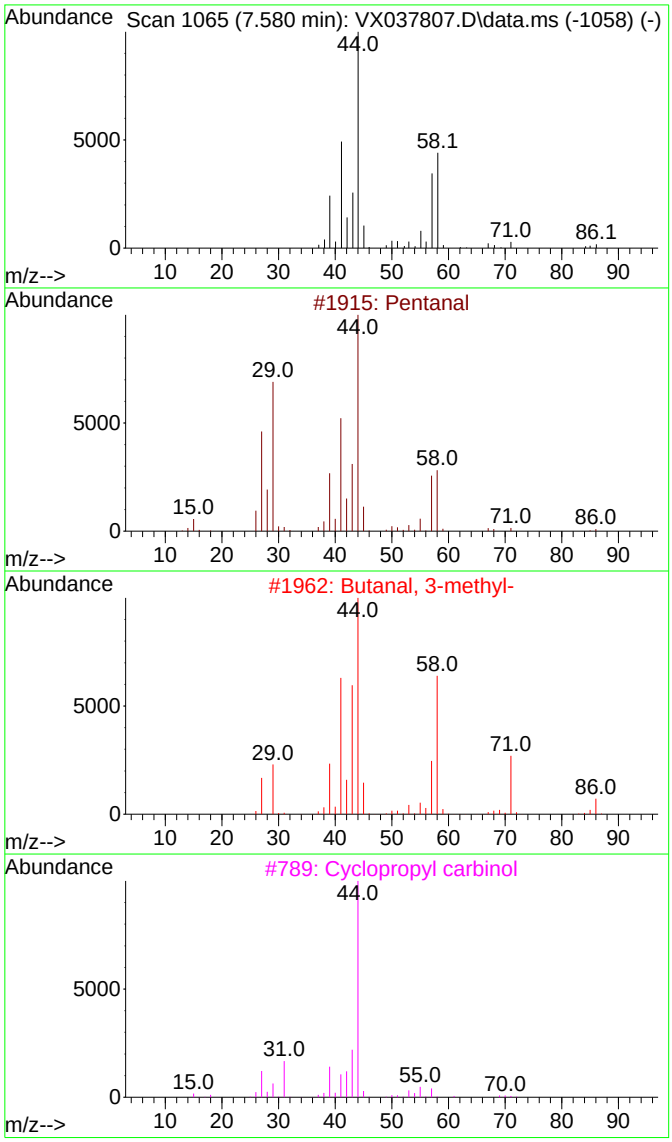
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

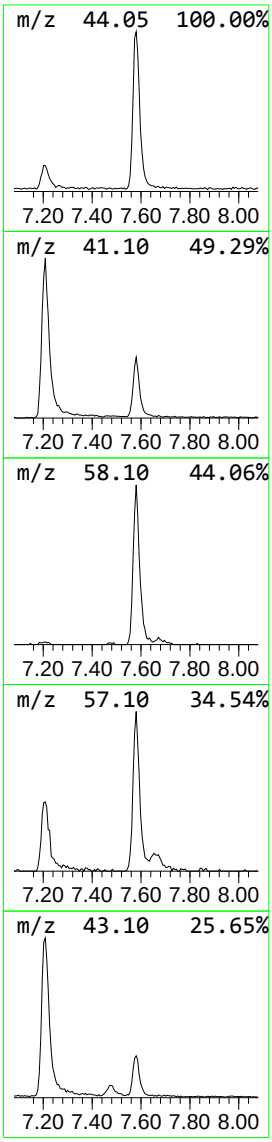
****

Peak Number 5 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.580	6.82 ug/l	115176	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	90
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
4	2-Formylhistamine	139	C6H9N3O	1000132-95-8	28
5	Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	10





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

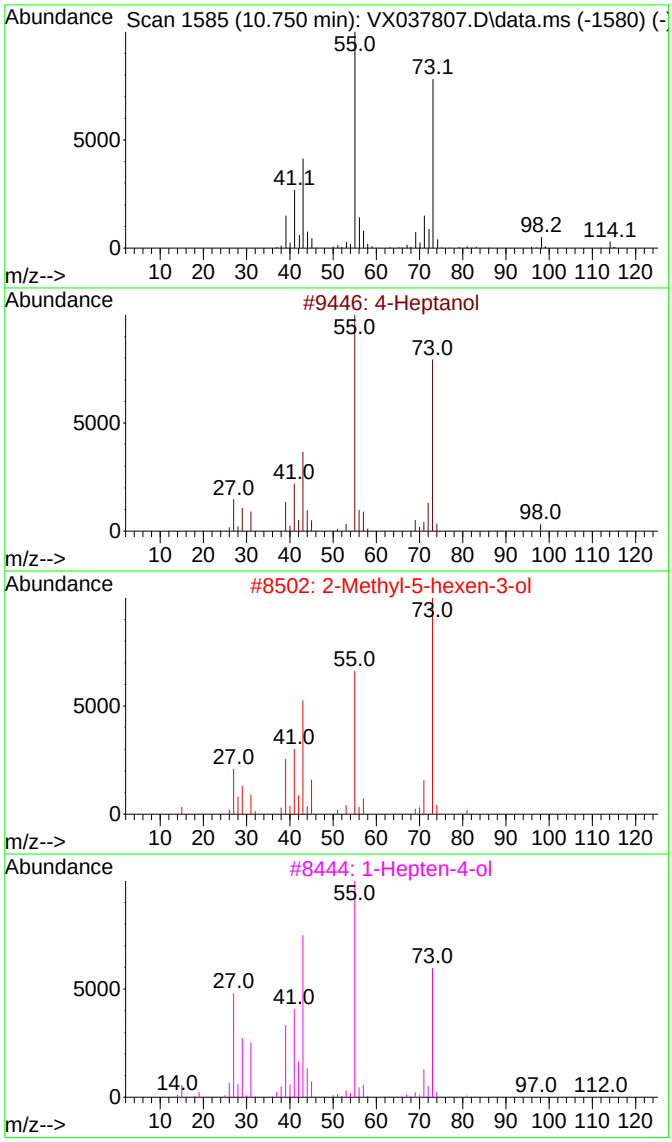
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

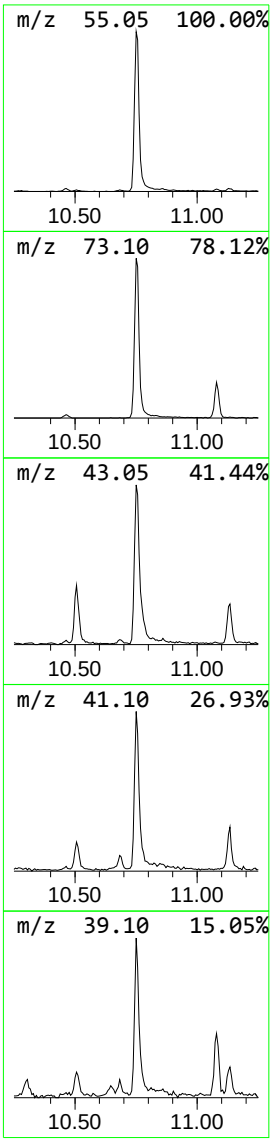
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	9.09 ug/l	195730	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3	1-Hepten-4-ol	114	C7H14O	003521-91-3	45
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	42
5	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	32





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ClientSampleId :
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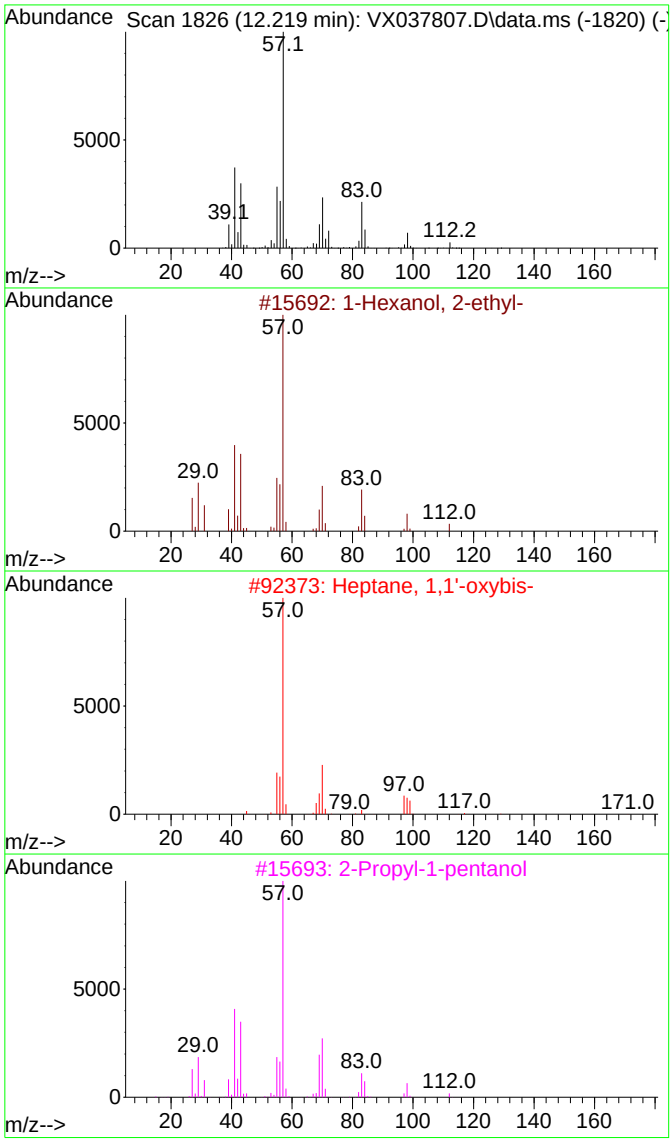
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091523W.M
Quant Title : SW846 8260

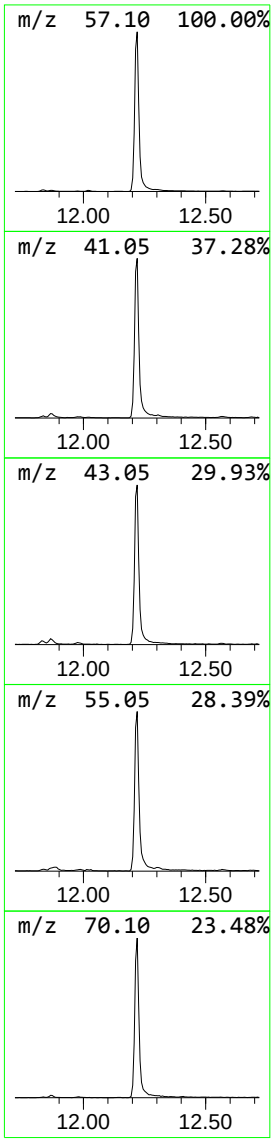
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	75.66 ug/l	1751530	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.142	5.7	ug/l	72970	1	5.556	644436	50.0
Butanal	4.233	231.0	ug/l	2977780	1	5.556	644436	50.0
2-Butanol	5.001	8.8	ug/l	113772	1	5.556	644436	50.0
1-Butanol	7.208	15.2	ug/l	257051	2	6.763	844451	50.0
Pentanal	7.580	6.8	ug/l	115176	2	6.763	844451	50.0
4-Heptanol	10.750	9.1	ug/l	195730	3	10.055	1076550	50.0
1-Hexanol, 2-et...	12.219	75.7	ug/l	1751530	4	12.024	1157560	50.0