LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090923\
Data File : VX037633.D
Acq On : 09 Sep 2023 17:26
Operator : JC/MD
Sample : 04297-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

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\82X090823W.M
Title : SW846 8260

Signal : TIC: VX037633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	206	212	224	rBV	58246	95558	12.30%	1.348%
2	2.544	228	239	248	rBV	11368	21926	2.82%	0.309%
3	2.965	298	308	317	rBV2	4648	11538	1.49%	0.163%
4	4.233	509	516	533	rBV2	6966	20920	2.69%	0.295%
5	4.556	555	569	588	rBV	279698	776716	100.00%	10.955%
6	5.007	633	643	661	rBV2	45547	158225	20.37%	2.232%
7	5.385	695	705	720	rVB	79296	233195	30.02%	3.289%
8	5.550	720	732	749	rVB	151009	427134	54.99%	6.025%
9	5.958	789	799	812	rBV	84395	224579	28.91%	3.168%
10	6.763	922	931	948	rBV	217271	528053	67.99%	7.448%
11	7.464	1040	1046	1058	rBV2	4948	11918	1.53%	0.168%
12	7.653	1071	1077	1089	rVB3	3380	8727	1.12%	0.123%
13	8.647	1234	1240	1248	rVV	451087	712181	91.69%	10.045%
14	8.720	1248	1252	1260	rVB3	5597	10136	1.30%	0.143%
15	10.055	1460	1471	1489	rBV	442970	606655	78.11%	8.557%
16	10.195	1489	1494	1501	rVB	8198	11133	1.43%	0.157%
17	10.299	1501	1511	1521	rBV	64941	92076	11.85%	1.299%
18	10.506	1541	1545	1556	rVB	73473	94735	12.20%	1.336%
19	10.640	1563	1567	1571	rBV	20908	27605	3.55%	0.389%
20	10.683	1571	1574	1580	rVB	17994	23019	2.96%	0.325%
21	10.756	1580	1586	1594	rBV	281786	404950	52.14%	5.712%
22	11.079	1634	1639	1644	rBV	364485	461698	59.44%	6.512%
23	11.134	1644	1648	1655	rVB	115968	146900	18.91%	2.072%
24	11.305	1673	1676	1682	rVB2	8387	11299	1.45%	0.159%
25	11.378	1682	1688	1696	rBV	42393	78329	10.08%	1.105%
26	11.451	1696	1700	1707	rVB	26571	32624	4.20%	0.460%
27	11.573	1715	1720	1723	rBV	144649	194770	25.08%	2.747%
28	11.604	1723	1725	1744	rVV3	127302	207896	26.77%	2.932%
29	11.750	1745	1749	1756	rVV	103417	129338	16.65%	1.824%
30	11.829	1756	1762	1765	rVV	35959	53459	6.88%	0.754%
31	11.866	1765	1768	1782	rVV	104241	178127	22.93%	2.512%
32	11.975	1782	1786	1789	rVV2	16905	26400	3.40%	0.372%
33	12.018	1789	1793	1800	rVV	433370	571853	73.62%	8.066%
34	12.085	1800	1804	1809	rVB	22605	28479	3.67%	0.402%
35	12.244	1821	1830	1838	rBV4	26562	54594	7.03%	0.770%
36	12.317	1838	1842	1850	rVB3	14816	26639	3.43%	0.376%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
713-G-DIP

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\82X090823W.M
Title : SW846 8260

37	12.536	1873	1878	1879	rVV	10634	15287	1.97%	0.216%
38	12.567	1879	1883	1887	rVV4	28856	52225	6.72%	0.737%
39	12.609	1887	1890	1895	rVV	18814	28063	3.61%	0.396%
40	12.695	1899	1904	1913	rVB3	8400	15707	2.02%	0.222%
41	12.920	1937	1941	1945	rBV	16744	22085	2.84%	0.311%
42	12.963	1945	1948	1952	rVB	15561	17649	2.27%	0.249%
43	13.170	1977	1982	1986	rBV	10101	12560	1.62%	0.177%
44	13.256	1990	1996	1998	rVV6	5537	11633	1.50%	0.164%
45	13.292	1998	2002	2008	rVB2	17753	24838	3.20%	0.350%
46	13.689	2057	2067	2075	rVB5	5419	12184	1.57%	0.172%
47	13.774	2077	2081	2088	rVB	18645	24711	3.18%	0.349%
48	13.847	2088	2093	2100	rBV	27660	46943	6.04%	0.662%
49	13.914	2100	2104	2111	rBV	34409	51167	6.59%	0.722%
50	14.640	2217	2223	2233	rVB	23510	32753	4.22%	0.462%
51	14.780	2241	2246	2253	rVB	14117	18736	2.41%	0.264%

Sum of corrected areas: 7089925

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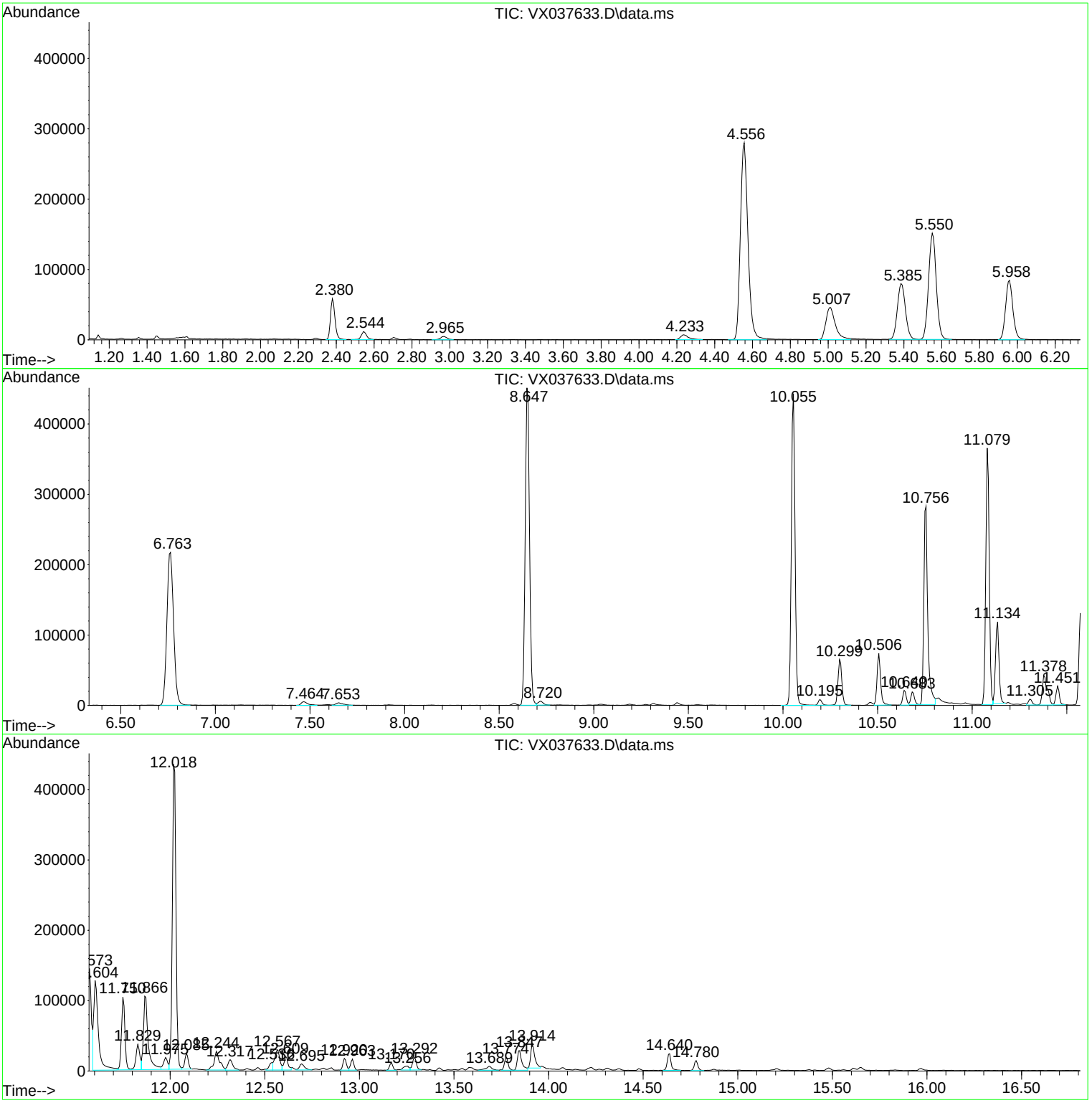
Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090923\
Data File : VX037633.D
Acq On : 09 Sep 2023 17:26
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

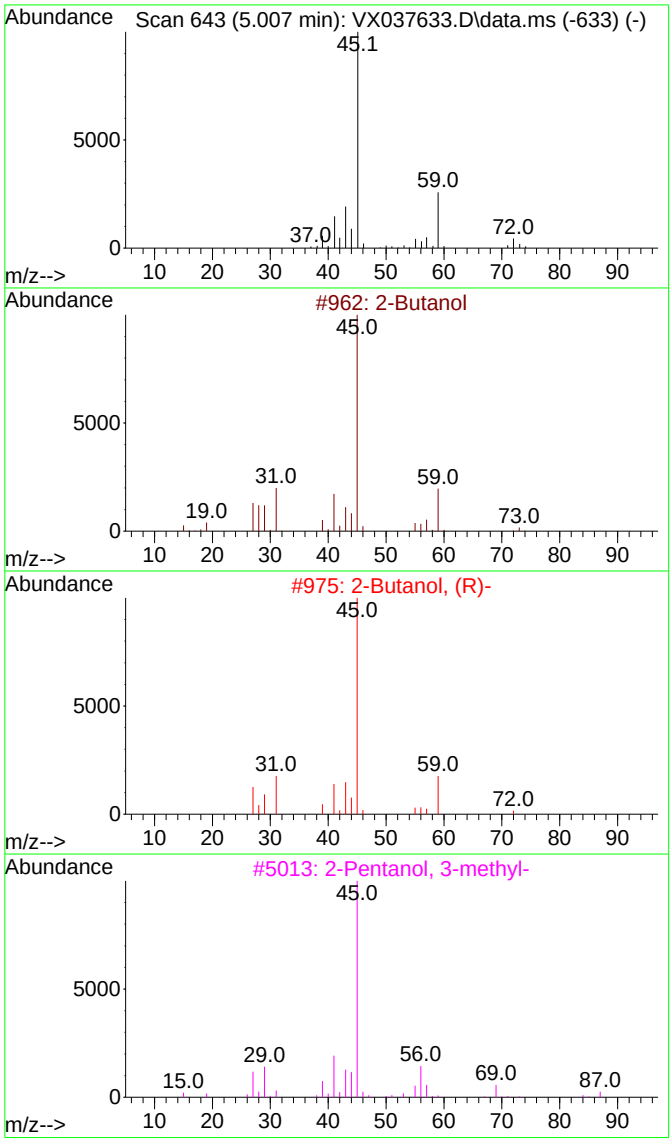
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

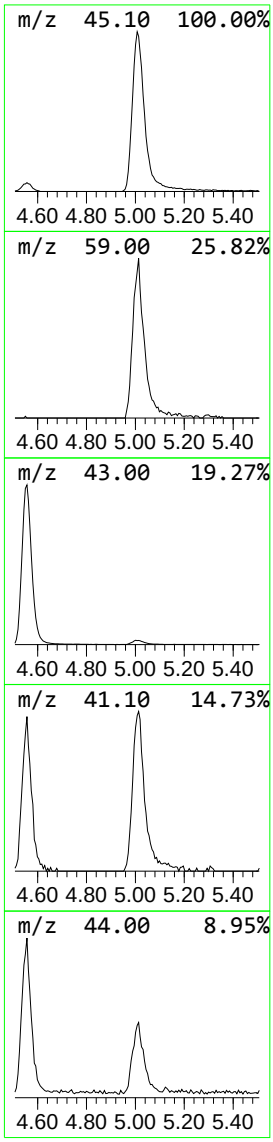
****

Peak Number 1 2-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.007	18.52 ug/l	158225	Pentafluorobenzene	5.550

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	78
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	53
5	2-Hexanol, (R)-	102	C6H14O	026549-24-6	38





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Data File : VX037633.D
Acq On : 09 Sep 2023 17:26
Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

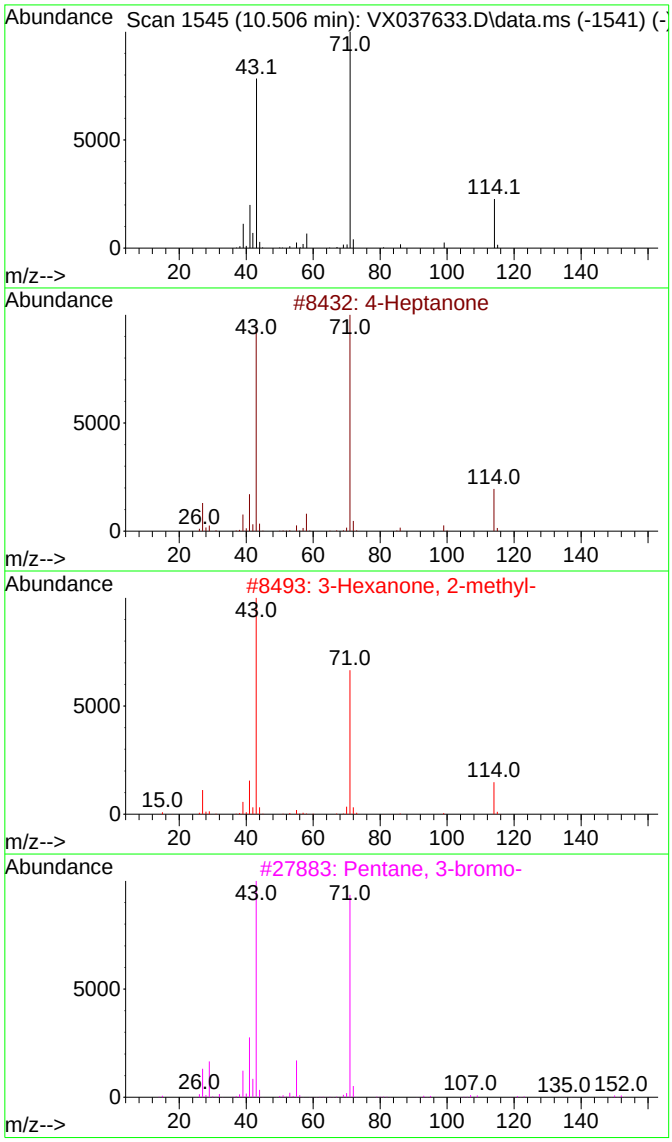
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

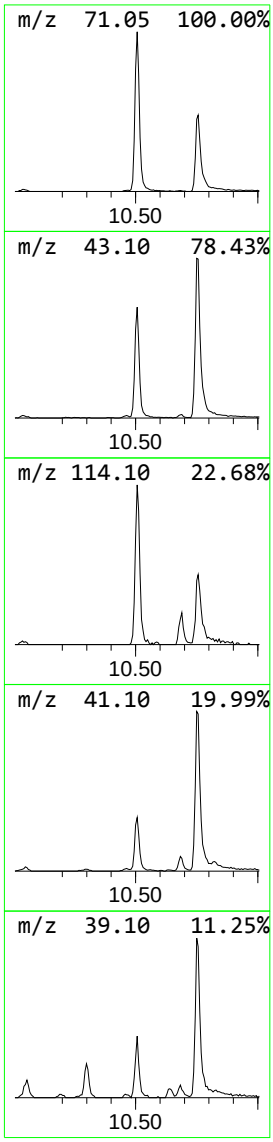
****

Peak Number 2 4-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.506	7.81 ug/l	94735	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone	114	C7H14O	000123-19-3	91
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
3	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	59
4	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	50
5	1-Ethoxy-3-methyl-2-butene	114	C7H14O	1000432-34-5	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090923\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

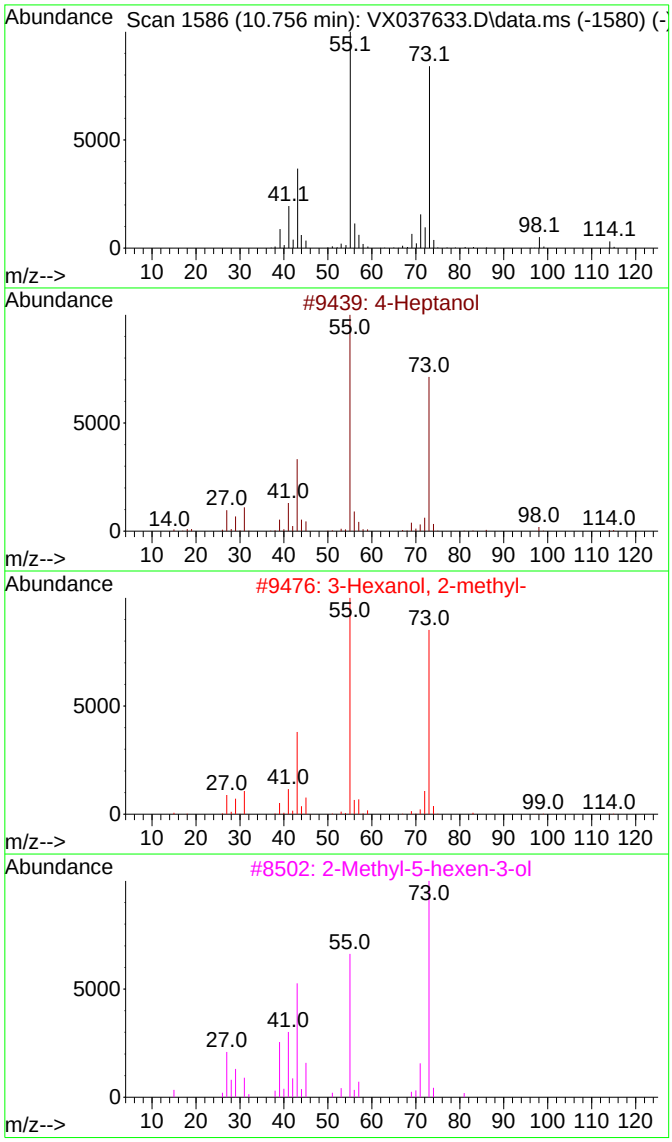
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

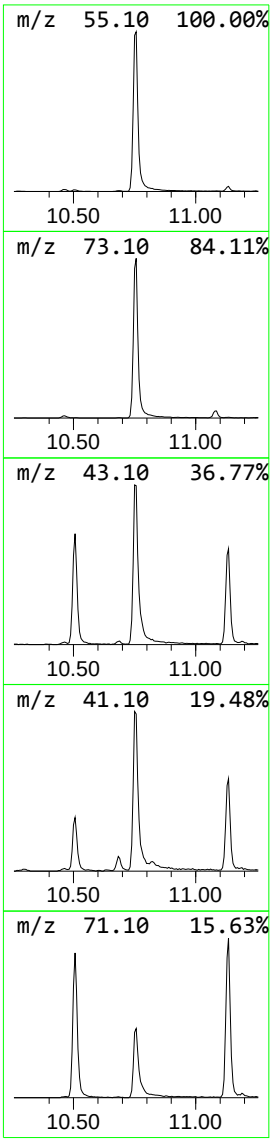
****

Peak Number 3 4-Heptanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	33.38 ug/l	404950	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	78
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	50
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4	Isobutylamine	73	C4H11N	000078-81-9	32
5	Oxalic acid, cyclobutyl hexyl ester	228	C12H20O4	1000309-69-7	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090923\
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Sample : 04297-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

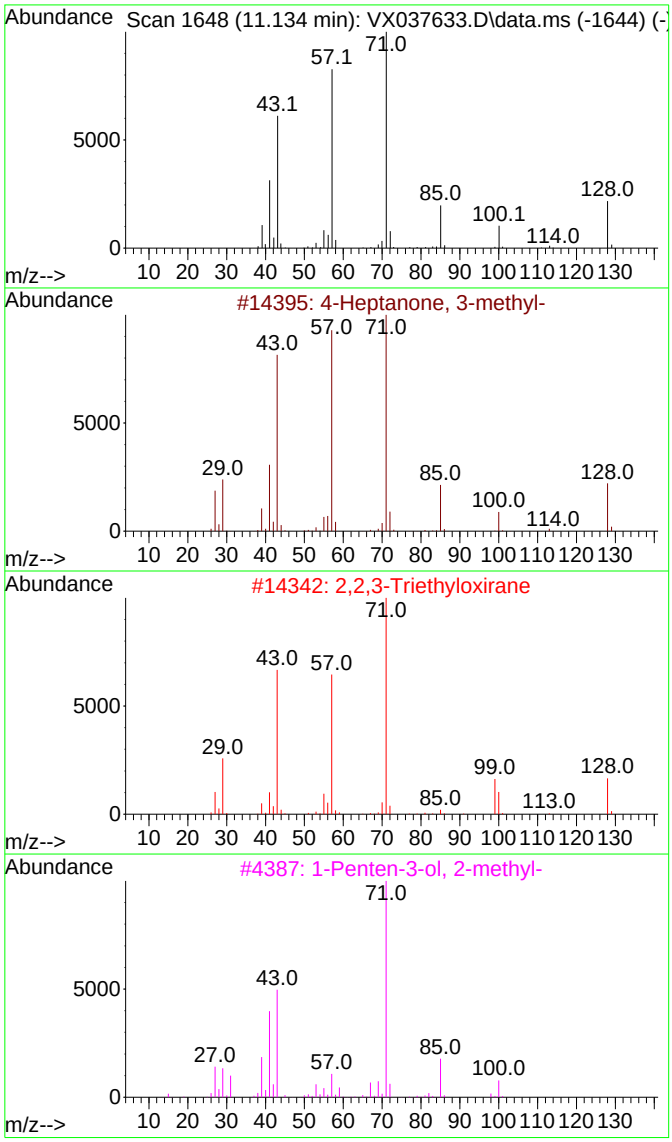
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

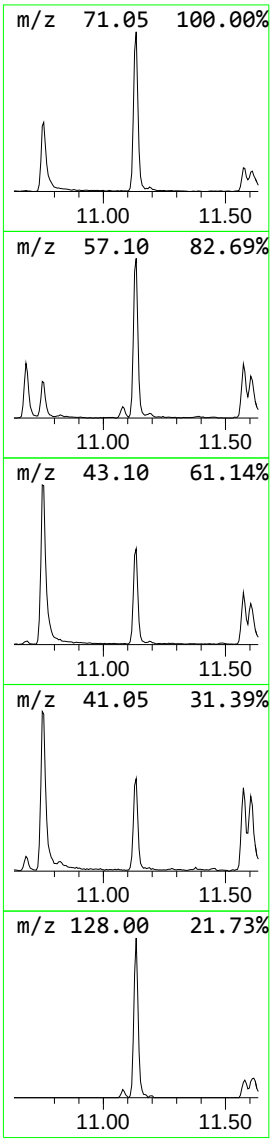
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4-Heptanone, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.134	12.84 ug/l	146900	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	95
2	2,2,3-Triethyloxirane	128	C8H16O	053229-40-6	80
3	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	59
4	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	50
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	50





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Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

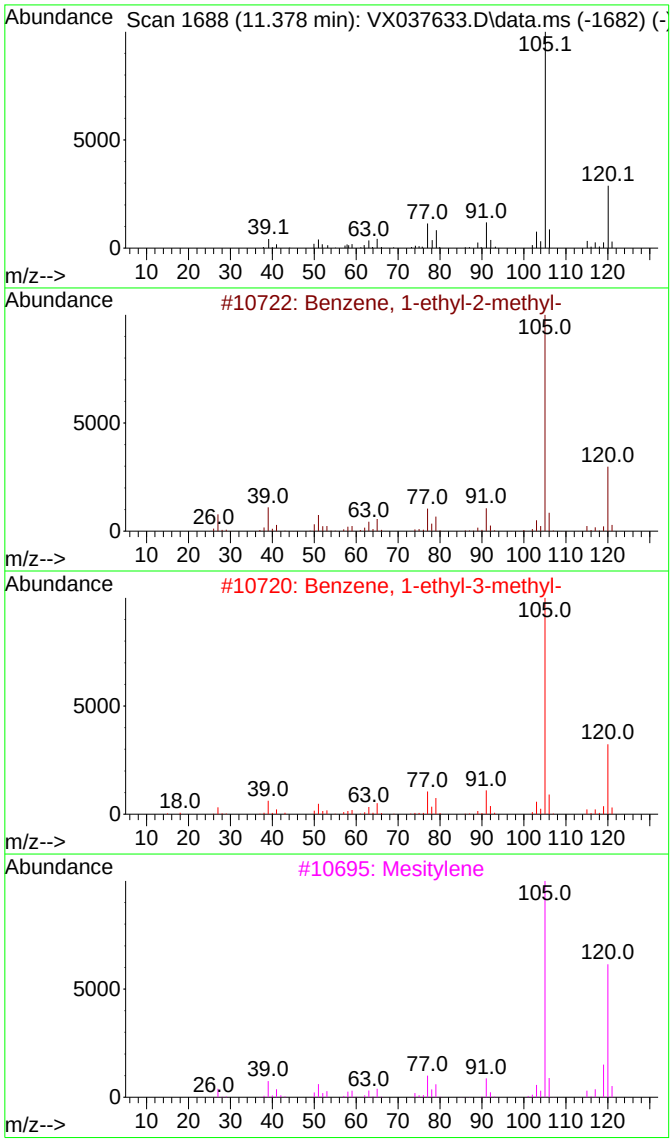
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

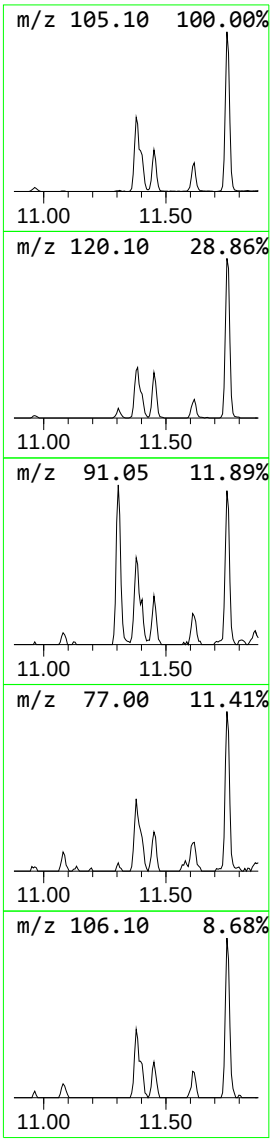
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	6.85 ug/l	78329	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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Data File : VX037633.D
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Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

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

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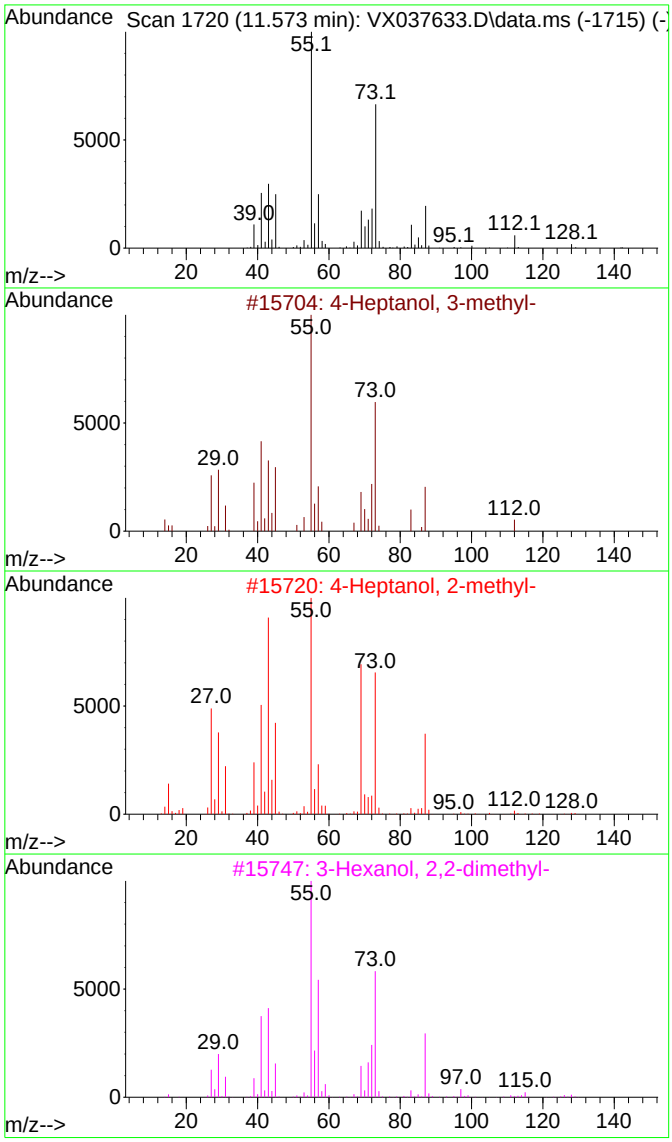
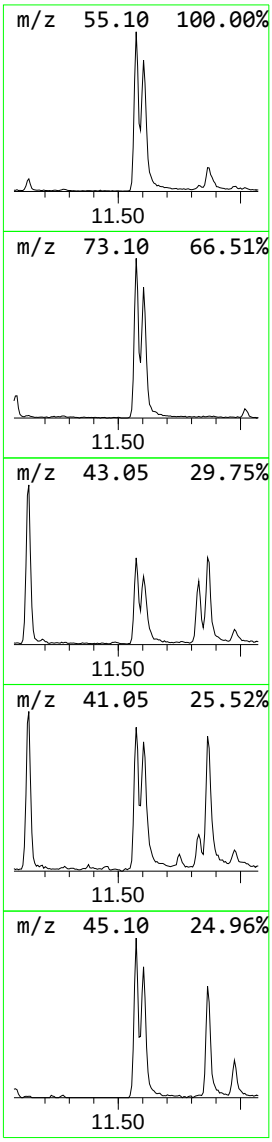
Peak Number 6 4-Heptanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	17.03 ug/l	194770	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	78
2	4-Heptanol, 2-methyl-	130	C8H18O	021570-35-4	42
3	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	38
4	4-Heptanol, 3-ethyl-	144	C9H20O	019780-42-8	37
5	5-Ethyl-4-nonanol	172	C11H24O	019780-73-5	32





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

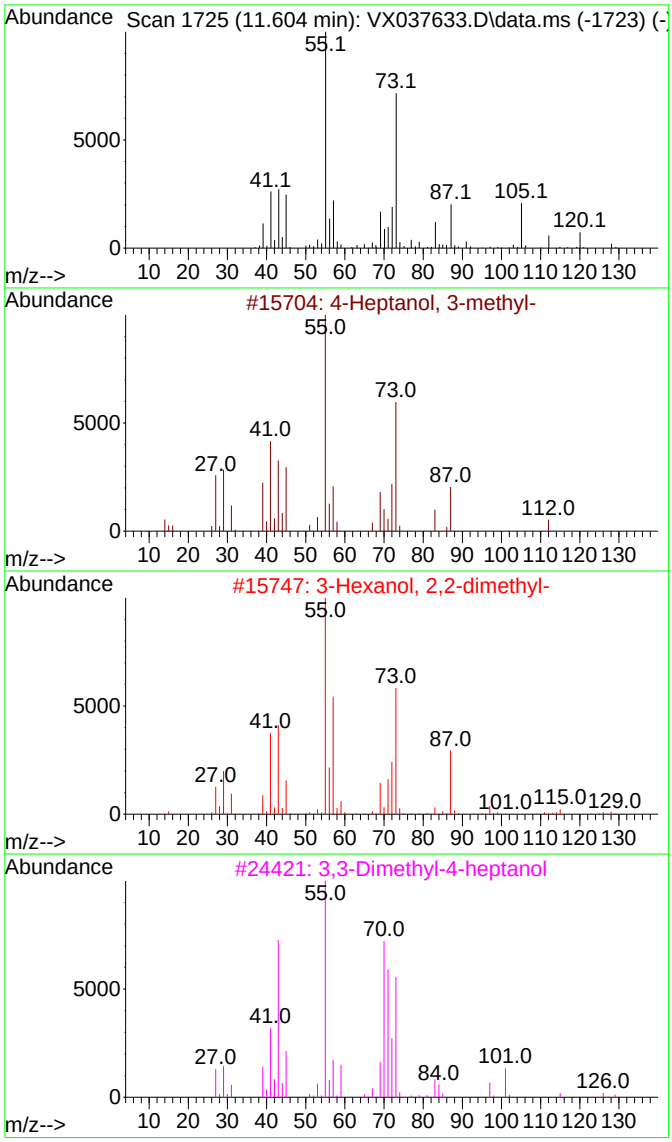
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

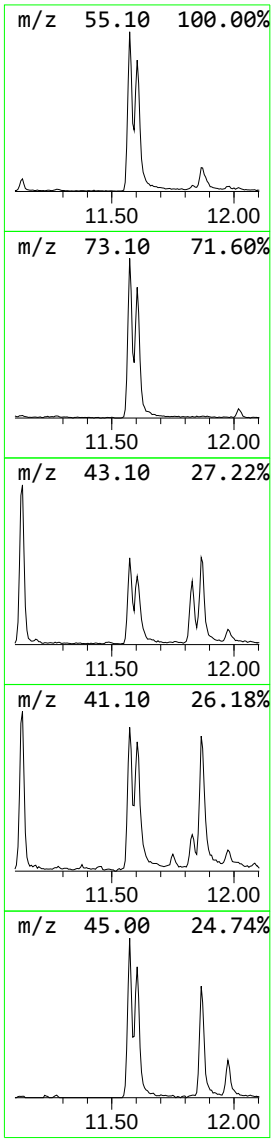
****

Peak Number 7 unknown11.604 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	18.18 ug/l	207896	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	59
2	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	33
3	3,3-Dimethyl-4-heptanol	144	C9H20O	019549-78-1	25
4	1-Butene, 3-propoxy-	114	C7H14O	037027-59-1	17
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090923\
Data File : VX037633.D
Acq On : 09 Sep 2023 17:26
Operator : JC/MD
Sample : 04297-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

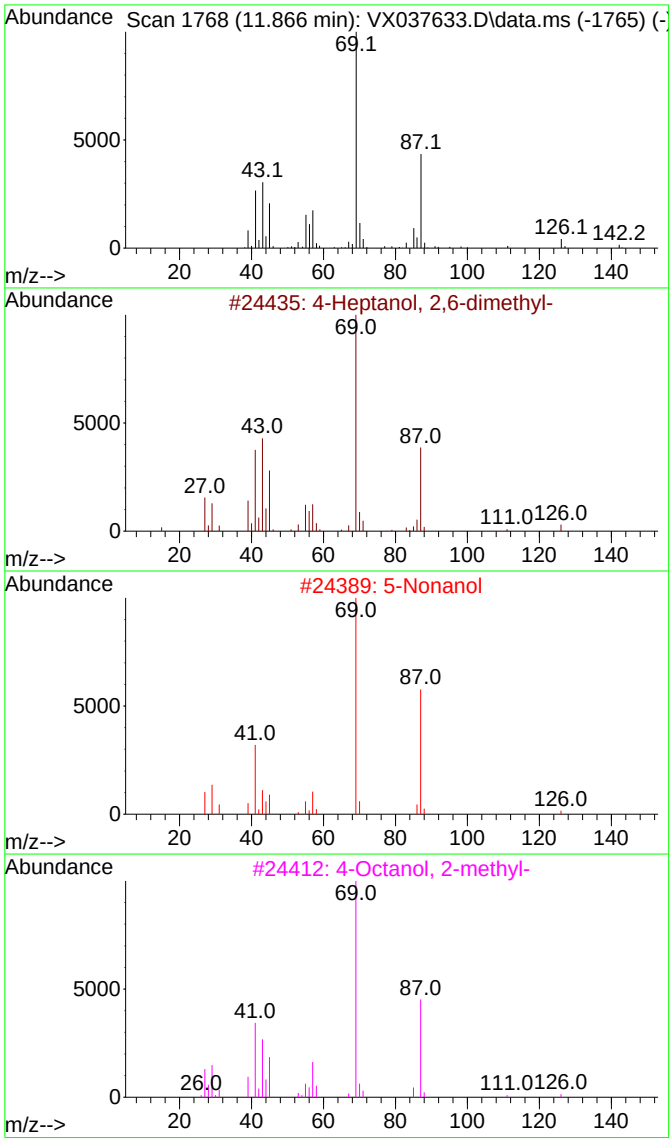
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
Quant Title : SW846 8260

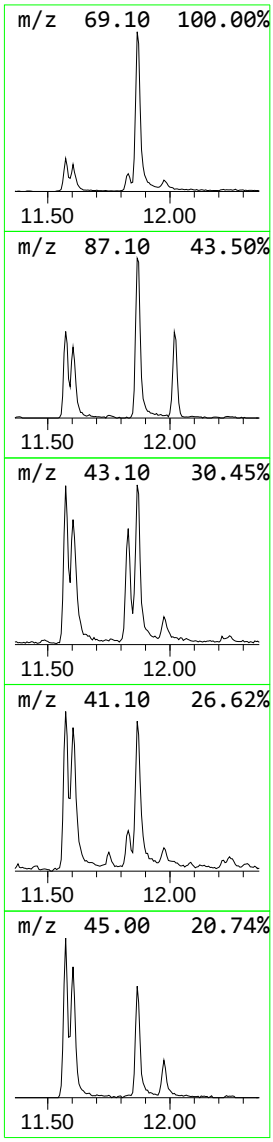
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.866	15.57 ug/l	178127	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	78
2	5-Nonanol	144	C9H20O	000623-93-8	64
3	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64
4	Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	59
5	5-Dodecanol	186	C12H26O	010203-33-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090923\
Data File : VX037633.D
Acq On : 09 Sep 2023 17:26
Operator : JC/MD
Sample : 04297-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-G-DIP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090823W.M
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
2-Butanol	5.007	18.5	ug/l	158225	1	5.550	427134	50.0
4-Heptanone	10.506	7.8	ug/l	94735	3	10.055	606655	50.0
4-Heptanol	10.756	33.4	ug/l	404950	3	10.055	606655	50.0
4-Heptanone, 3-...	11.134	12.8	ug/l	146900	4	12.024	571853	50.0
Benzene, 1-ethy...	11.378	6.8	ug/l	78329	4	12.024	571853	50.0
4-Heptanol, 2-m...	11.573	17.0	ug/l	194770	4	12.024	571853	50.0
unknown11.604	11.604	18.2	ug/l	207896	4	12.024	571853	50.0
4-Heptanol, 2,6...	11.866	15.6	ug/l	178127	4	12.024	571853	50.0