LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

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\82X042523W.M
Title : SW846 8260

Signal : TIC: VX035595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	86	rBV	10087030	14526669	100.00%	30.142%
2	2.203	158	183	184	rBV	1649388	7202793	49.58%	14.945%
3	2.392	208	214	230	rVB	1064241	2269825	15.63%	4.710%
4	2.617	237	251	277	rVB2	156079	1051859	7.24%	2.183%
5	4.227	504	515	527	rBV	75399	209102	1.44%	0.434%
6	4.562	560	570	590	rVB	156735	476578	3.28%	0.989%
7	5.007	631	643	655	rBV	414946	1408366	9.70%	2.922%
8	5.385	693	705	721	rBV2	181200	530909	3.65%	1.102%
9	5.550	721	732	749	rVB	318107	916417	6.31%	1.902%
10	5.952	788	798	810	rBV	178553	474599	3.27%	0.985%
11	6.617	893	907	921	rBV4	43435	163064	1.12%	0.338%
12	6.757	921	930	943	rVV	484837	1168457	8.04%	2.424%
13	7.257	1001	1012	1030	rBV2	101912	422476	2.91%	0.877%
14	8.647	1234	1240	1247	rBV	1036811	1607586	11.07%	3.336%
15	10.055	1465	1471	1479	rVB	1006904	1413090	9.73%	2.932%
16	10.299	1507	1511	1518	rVB	186944	248861	1.71%	0.516%
17	10.506	1539	1545	1550	rBV	228091	294162	2.02%	0.610%
18	10.640	1563	1567	1570	rVV	116301	158616	1.09%	0.329%
19	10.768	1582	1588	1594	rVV	212765	265526	1.83%	0.551%
20	11.012	1622	1628	1635	rBV2	176033	431307	2.97%	0.895%
21	11.079	1635	1639	1650	rVB	948769	1202103	8.28%	2.494%
22	11.378	1683	1688	1693	rBV	113352	179056	1.23%	0.372%
23	11.750	1745	1749	1756	rVB	268418	335012	2.31%	0.695%
24	12.018	1789	1793	1800	rVB	1161637	1514415	10.43%	3.142%
25	12.085	1800	1804	1812	rVB	114937	165590	1.14%	0.344%
26	12.219	1821	1826	1833	rBV	2696962	3499674	24.09%	7.262%
27	12.317	1838	1842	1847	rVB3	96720	170123	1.17%	0.353%
28	12.768	1912	1916	1919	rBV	143320	174486	1.20%	0.362%
29	12.817	1919	1924	1928	rVV2	114090	145982	1.00%	0.303%
30	12.969	1944	1949	1955	rBV2	147707	219311	1.51%	0.455%
31	13.067	1955	1965	1967	rBV3	123436	182127	1.25%	0.378%
32	13.097	1967	1970	1974	rVV	276443	358374	2.47%	0.744%
33	13.158	1974	1980	1987	rVB	970445	1439309	9.91%	2.986%
34	13.292	1998	2002	2006	rVB2	200147	269580	1.86%	0.559%
35	13.426	2019	2024	2033	rBV2	274274	454169	3.13%	0.942%
36	13.731	2069	2074	2078	rBV2	187157	314260	2.16%	0.652%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

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\82X042523W.M
Title : SW846 8260

37	13.774	2078	2081	2088	rVB	232850	317504	2.19%	0.659%
38	13.859	2089	2095	2098	rBV2	112439	204400	1.41%	0.424%
39	14.231	2147	2156	2164	rVB4	178463	376140	2.59%	0.780%
40	14.481	2193	2197	2202	rVB2	121672	161754	1.11%	0.336%
41	14.633	2215	2222	2226	rBV2	189025	309512	2.13%	0.642%
42	14.780	2241	2246	2250	rBV	117311	153905	1.06%	0.319%
43	15.182	2303	2312	2320	rBV2	73247	176002	1.21%	0.365%
44	15.542	2365	2371	2378	rBV	218808	321744	2.21%	0.668%
45	16.468	2517	2523	2537	rVB	165012	309090	2.13%	0.641%

Sum of corrected areas: 48193884

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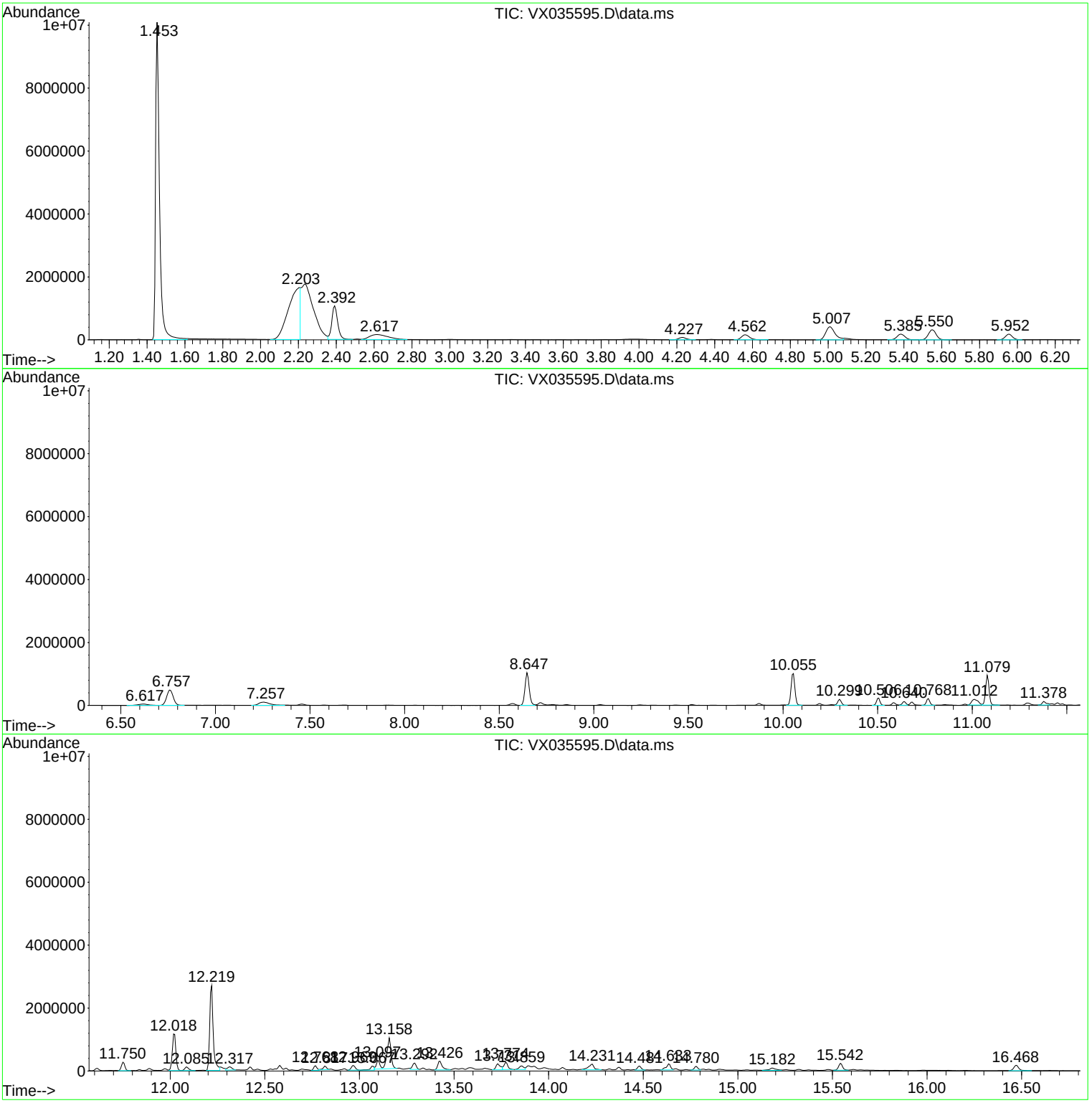
MSVOA_X
ClientSampleId :
PL-OILYWATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

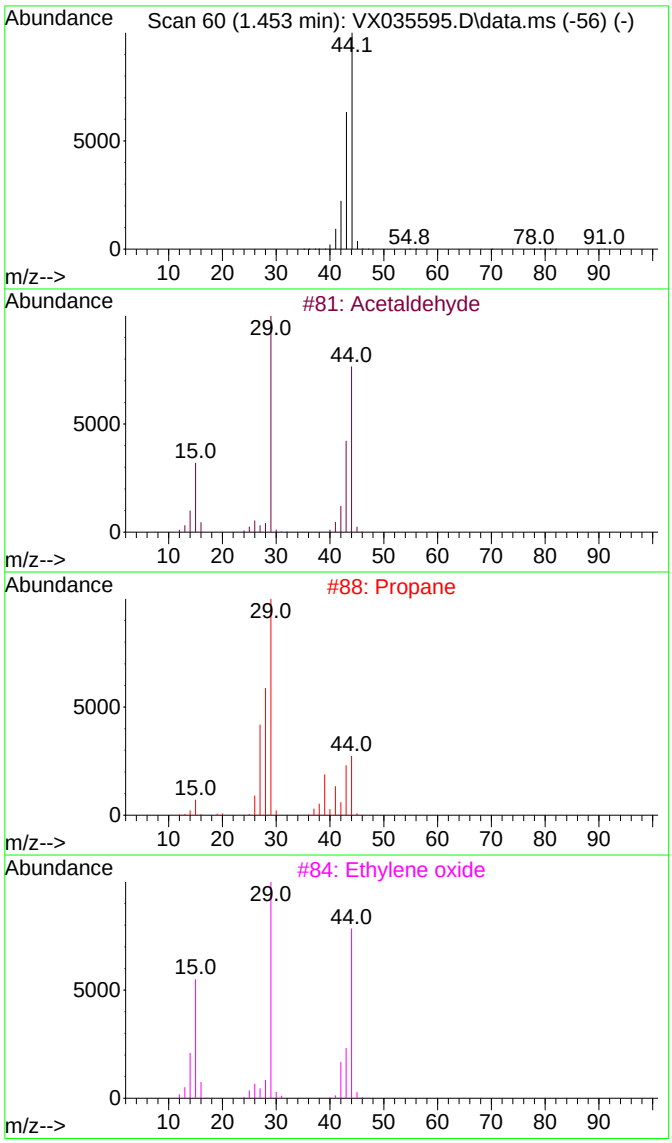
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

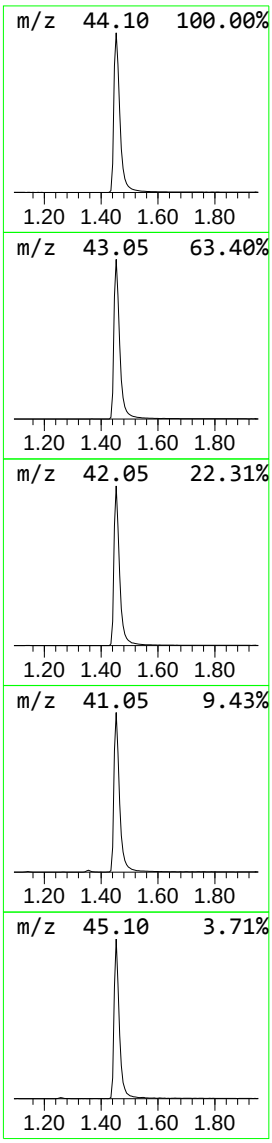
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	792.58 ug/l	14526700	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

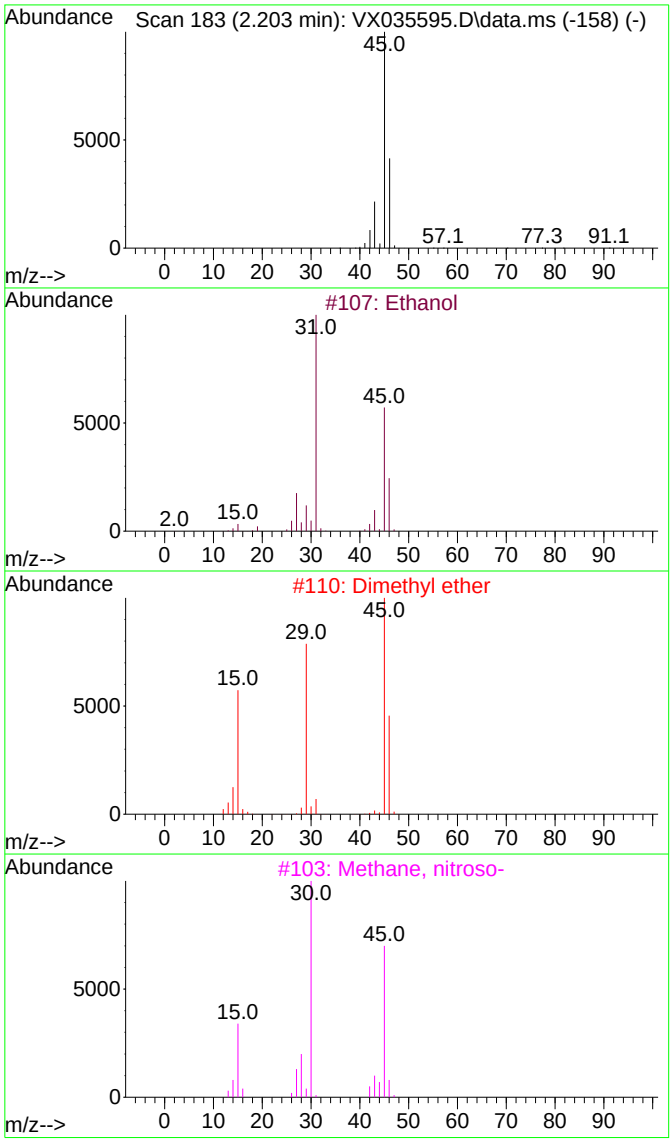
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

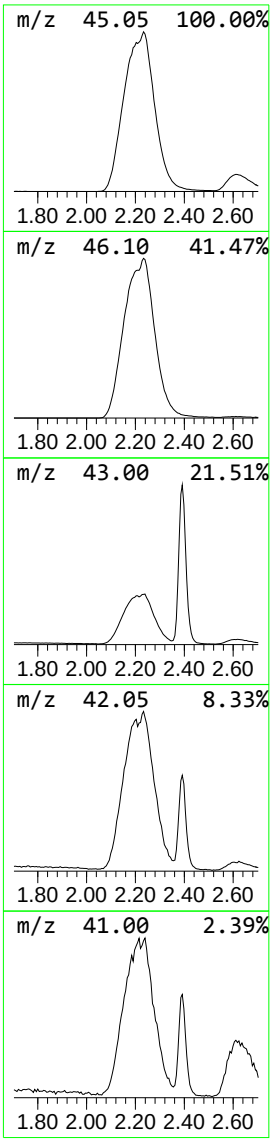
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.203	392.99 ug/l	7202790	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

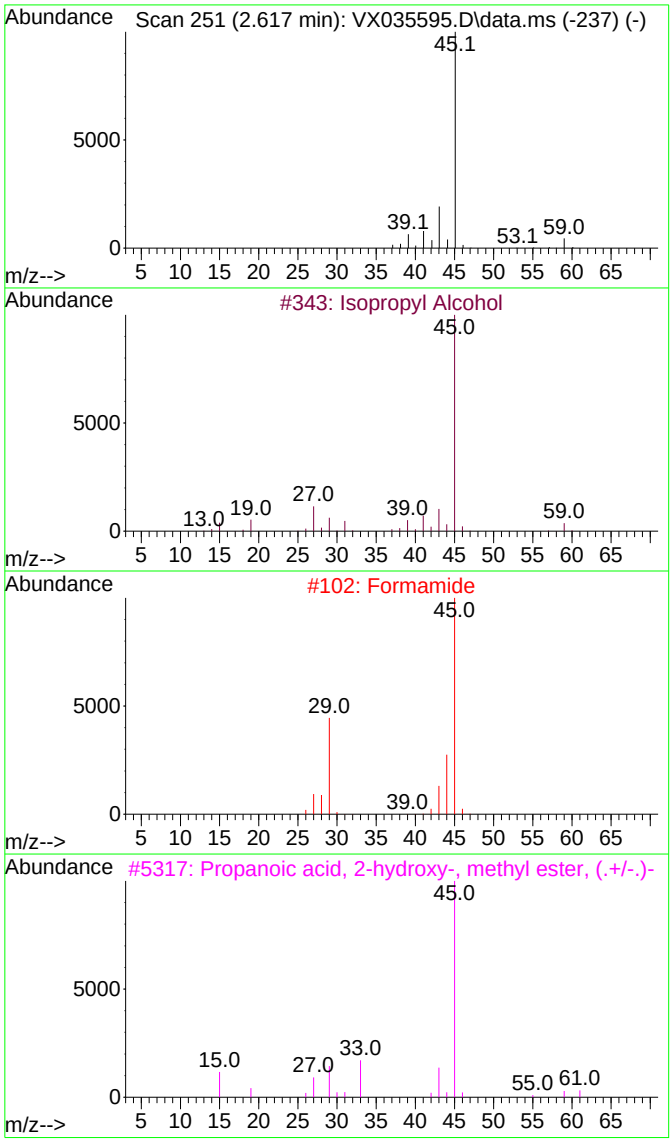
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

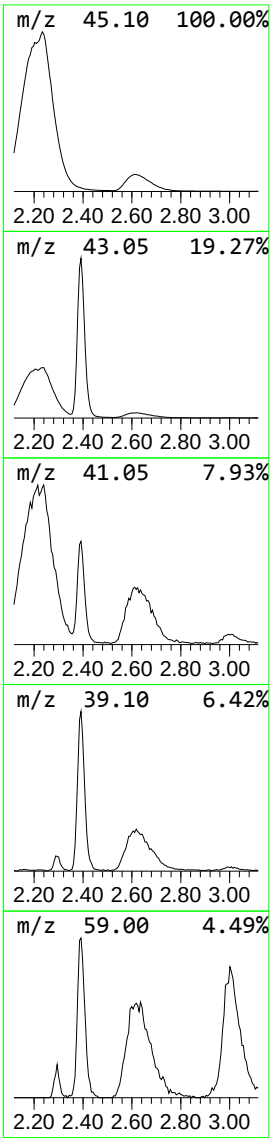
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.617	57.39 ug/l	1051860	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Formamide	45	CH3NO	000075-12-7	4
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4
4	Methane, nitroso-	45	CH3NO	000865-40-7	3
5	2,3-Butanediol	90	C4H10O2	000513-85-9	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

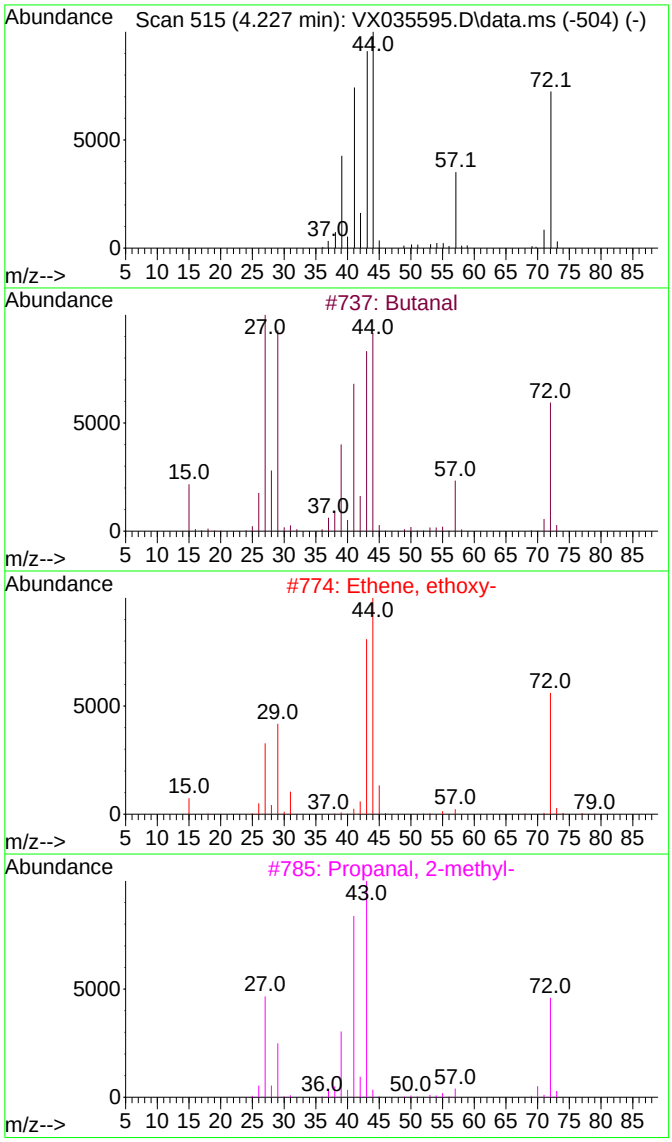
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

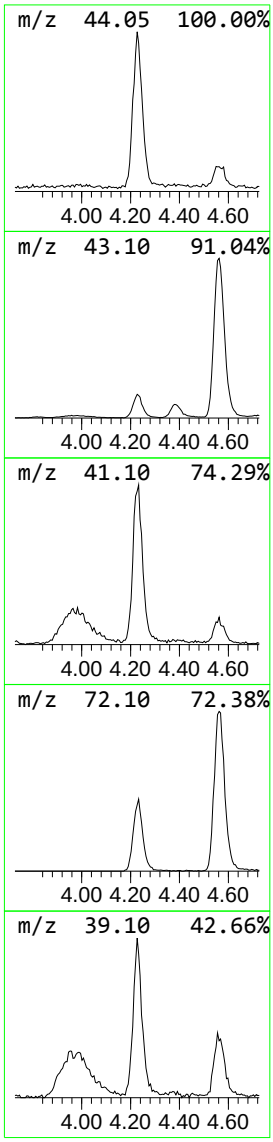
****

Peak Number 4 Butanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	11.41 ug/l	209102	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	90
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

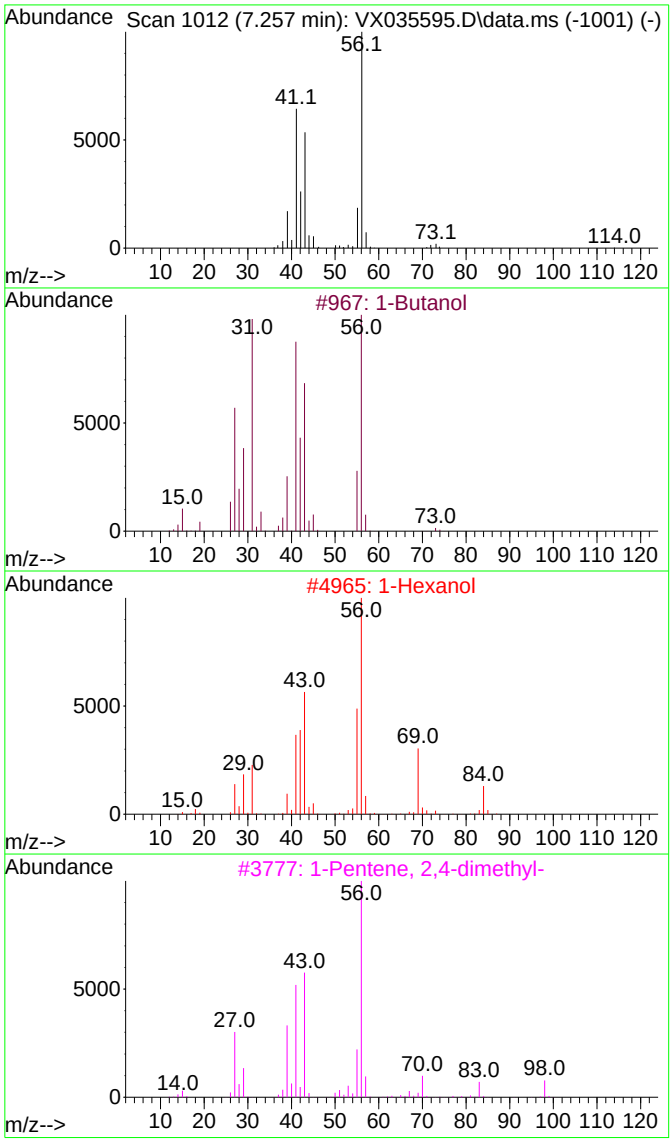
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

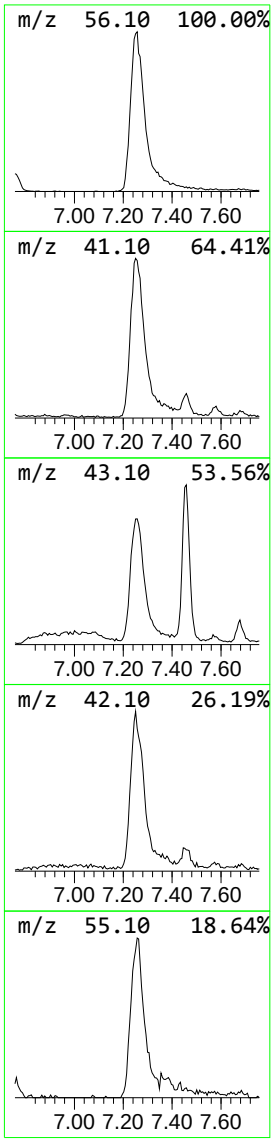
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.257	18.08 ug/l	422476	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	1-Hexanol	102	C6H14O	000111-27-3	40
3	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

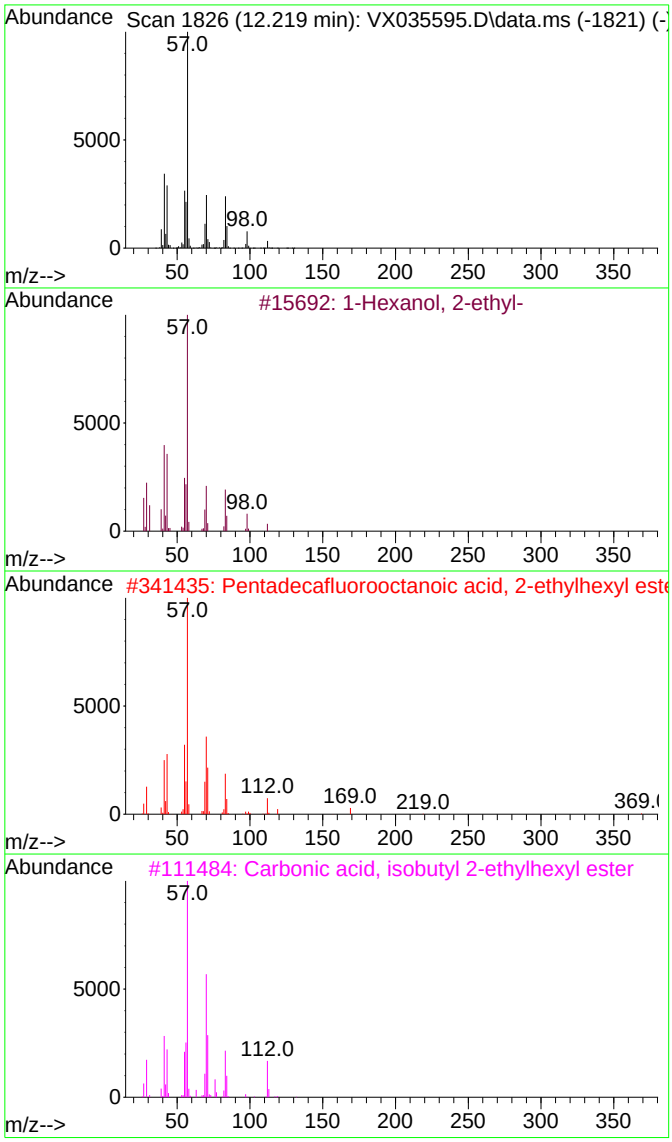
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

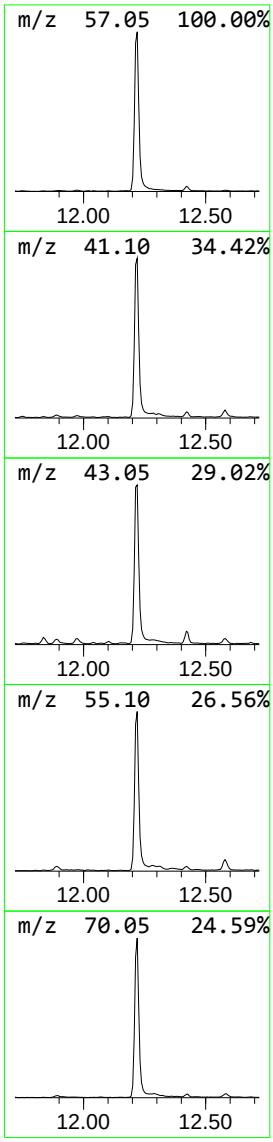
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	115.55 ug/l	3499670	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	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

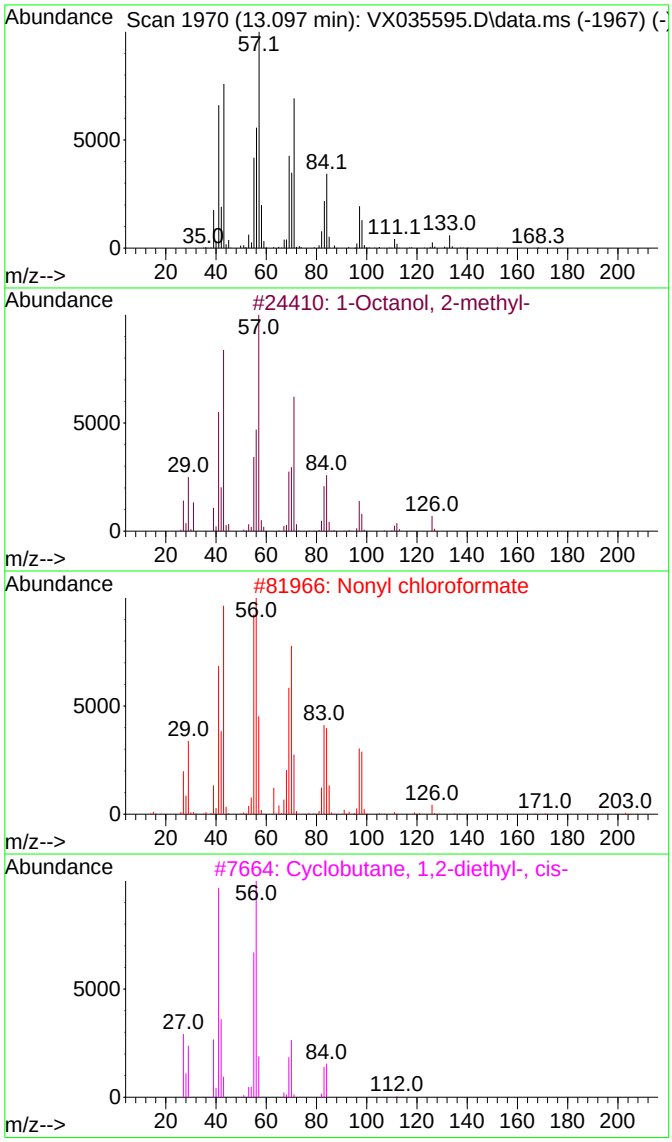
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

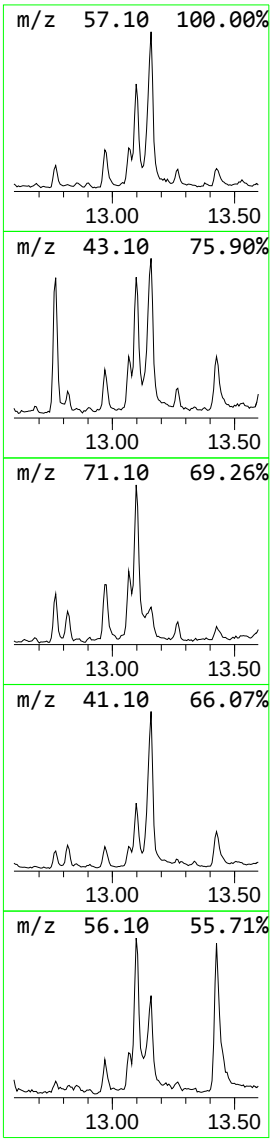
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Octanol, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.097	11.83 ug/l	358374	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	72
2	Nonyl chloroformate	206	C10H19ClO2	057045-82-6	50
3	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	43
4	Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	43
5	Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	38





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

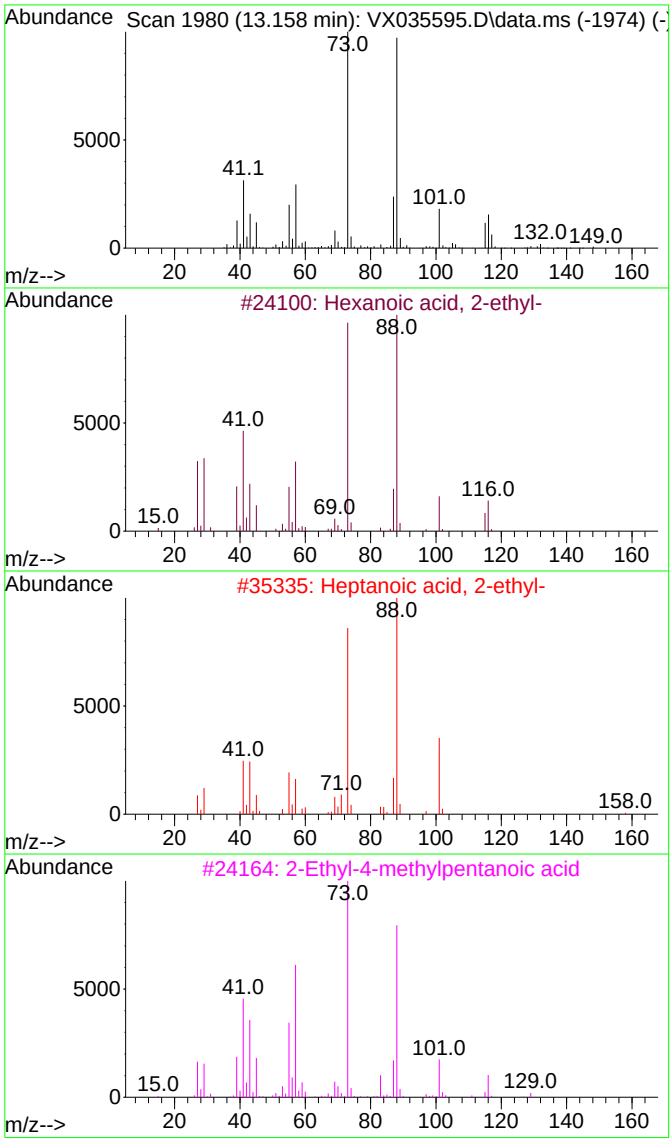
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

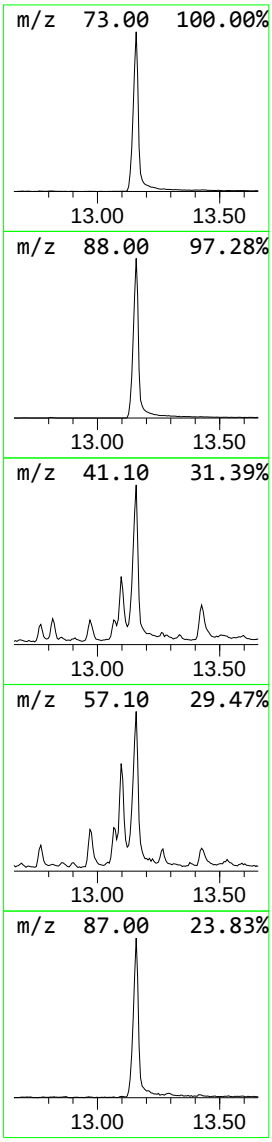
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.158	47.52 ug/l	1439310	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	47
5	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	47





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

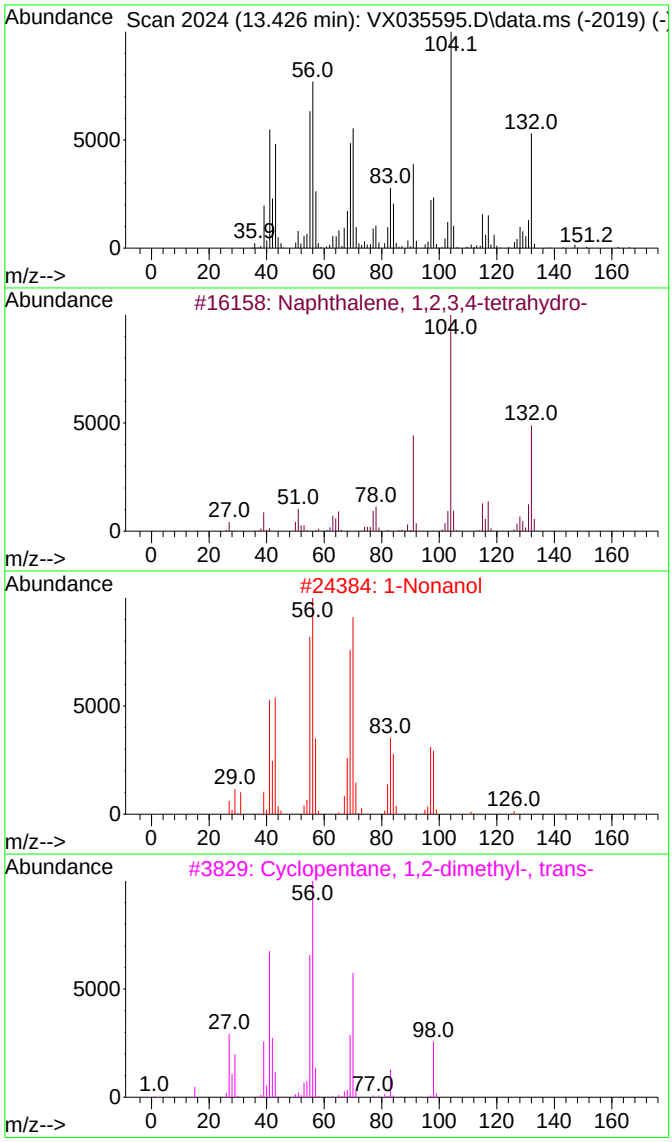
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

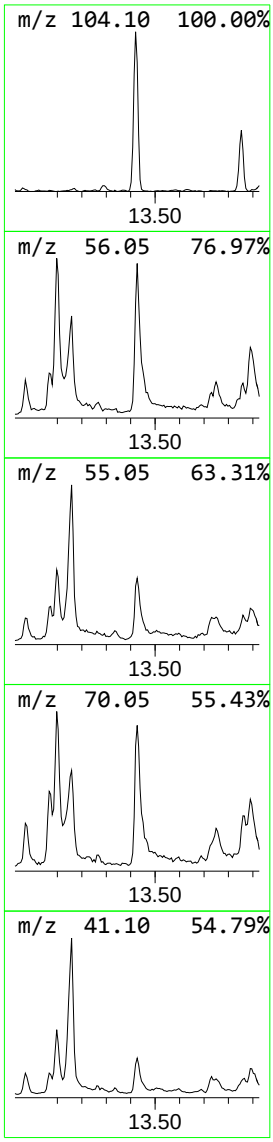
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	14.99 ug/l	454169	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	81
2	1-Nonanol	144	C9H20O	000143-08-8	49
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	42
4	Cycloheptane	98	C7H14	000291-64-5	38
5	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

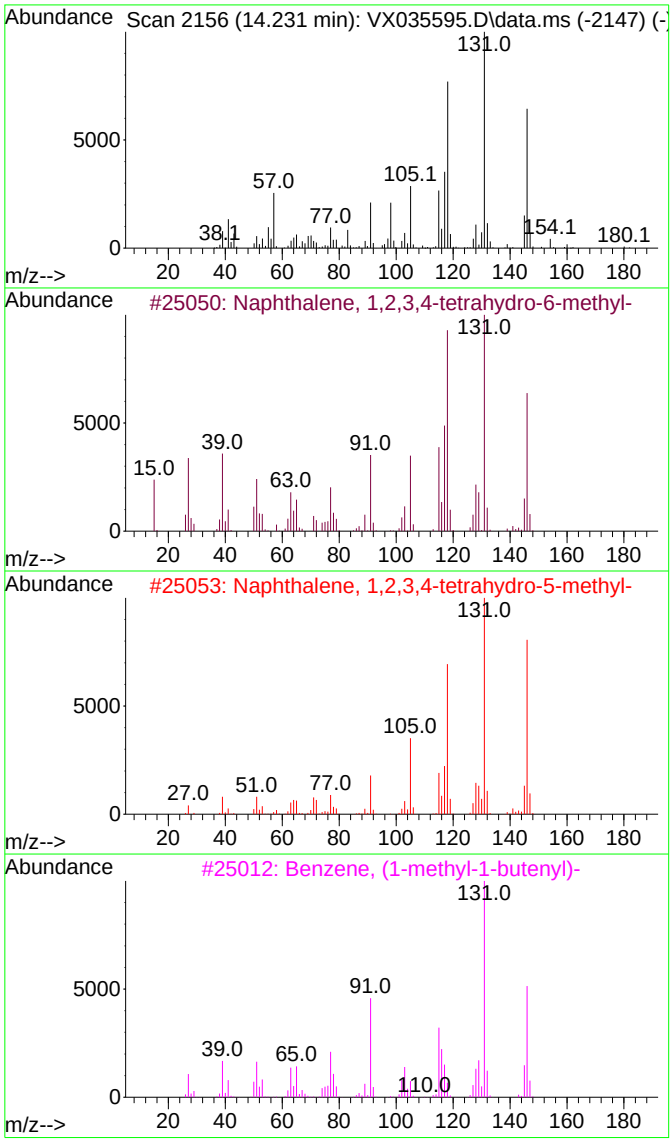
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

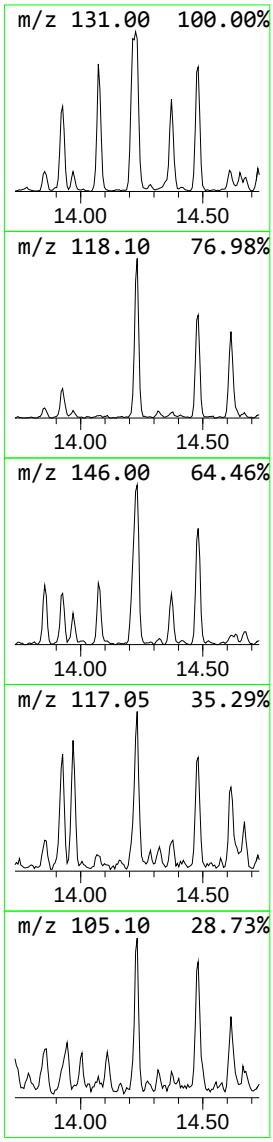
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	12.42 ug/l	376140	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	60
4	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	60
5	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
Data File : VX035595.D
Acq On : 10 May 2023 18:43
Operator : JC/MD
Sample : 02744-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PL-OILYWATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.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
Acetaldehyde	1.453	792.6	ug/l	14526700	1	5.550	916417	50.0
Ethanol	2.203	393.0	ug/l	7202790	1	5.550	916417	50.0
Isopropyl Alcohol	2.617	57.4	ug/l	1051860	1	5.550	916417	50.0
Butanal	4.227	11.4	ug/l	209102	1	5.550	916417	50.0
1-Butanol	7.257	18.1	ug/l	422476	2	6.763	1168460	50.0
1-Hexanol, 2-et...	12.219	115.6	ug/l	3499670	4	12.024	1514420	50.0
1-Octanol, 2-me...	13.097	11.8	ug/l	358374	4	12.024	1514420	50.0
Hexanoic acid, ...	13.158	47.5	ug/l	1439310	4	12.024	1514420	50.0
Naphthalene, 1,...	13.426	15.0	ug/l	454169	4	12.024	1514420	50.0
Naphthalene, 1,...	14.231	12.4	ug/l	376140	4	12.024	1514420	50.0