LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

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\82X090122W.M
Title : SW846 8260

Signal : TIC: VX031130.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.441	55	58	109	rBV	15429538	19723285	100.00%	42.765%
2	2.118	152	169	192	rBV	2315262	7135798	36.18%	15.472%
3	2.294	192	198	206	rVV	652744	1041313	5.28%	2.258%
4	2.386	206	213	229	rVB	1877699	3138683	15.91%	6.806%
5	2.971	300	309	321	rBV2	92021	235849	1.20%	0.511%
6	3.879	442	458	472	rBV2	232033	810992	4.11%	1.758%
7	4.233	505	516	528	rBV2	148064	403980	2.05%	0.876%
8	4.562	559	570	582	rBV	515715	1435729	7.28%	3.113%
9	4.715	583	595	609	rVB4	76606	287440	1.46%	0.623%
10	5.391	694	706	718	rBV	144370	418109	2.12%	0.907%
11	5.556	721	733	746	rBV2	221669	631042	3.20%	1.368%
12	5.836	766	779	790	rBV	137166	375653	1.90%	0.815%
13	5.958	790	799	811	rVB3	135638	359007	1.82%	0.778%
14	6.763	922	931	941	rBV2	312097	782851	3.97%	1.697%
15	6.879	941	950	964	rVB	319588	747997	3.79%	1.622%
16	7.208	996	1004	1012	rBV3	215762	488776	2.48%	1.060%
17	7.458	1038	1045	1054	rVB	403742	697973	3.54%	1.513%
18	8.653	1234	1241	1248	rBV	709647	1130100	5.73%	2.450%
19	8.805	1256	1266	1284	rVB5	61135	285112	1.45%	0.618%
20	9.433	1364	1369	1376	rBV	222370	305896	1.55%	0.663%
21	10.055	1461	1471	1484	rBV	627557	896779	4.55%	1.944%
22	10.317	1509	1514	1520	rVB	334650	467114	2.37%	1.013%
23	10.683	1570	1574	1582	rVB	193669	234703	1.19%	0.509%
24	10.768	1582	1588	1593	rBV	334759	412689	2.09%	0.895%
25	11.085	1634	1640	1645	rVB	636574	830700	4.21%	1.801%
26	11.476	1700	1704	1715	rVB	335274	428214	2.17%	0.928%
27	12.024	1790	1794	1801	rVB	752721	863969	4.38%	1.873%
28	12.219	1819	1826	1834	rBV	699982	1086120	5.51%	2.355%
29	12.762	1911	1915	1919	rBV2	219406	251860	1.28%	0.546%
30	12.884	1930	1935	1940	rBV	175049	212004	1.07%	0.460%

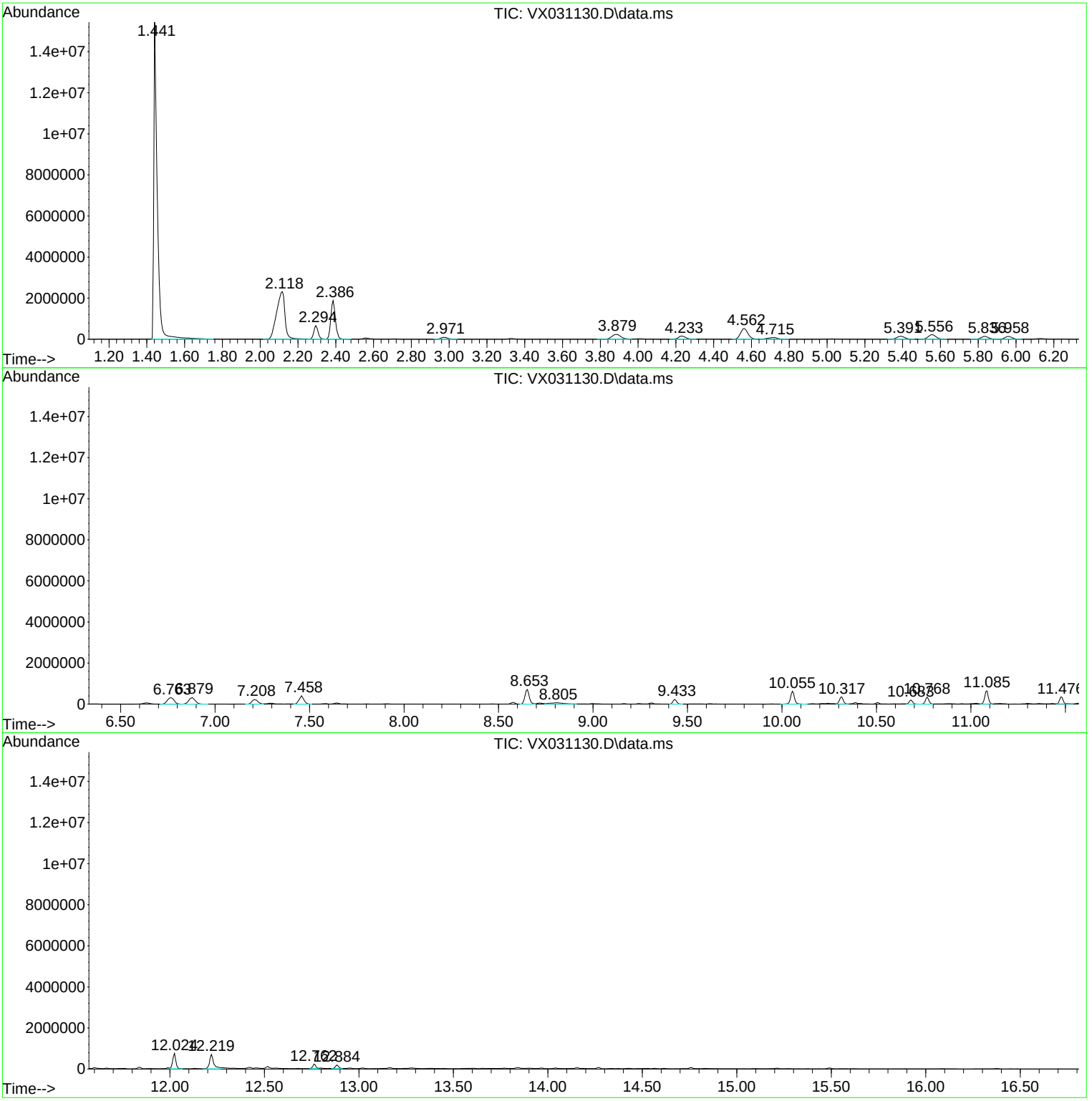
Sum of corrected areas: 46119737

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

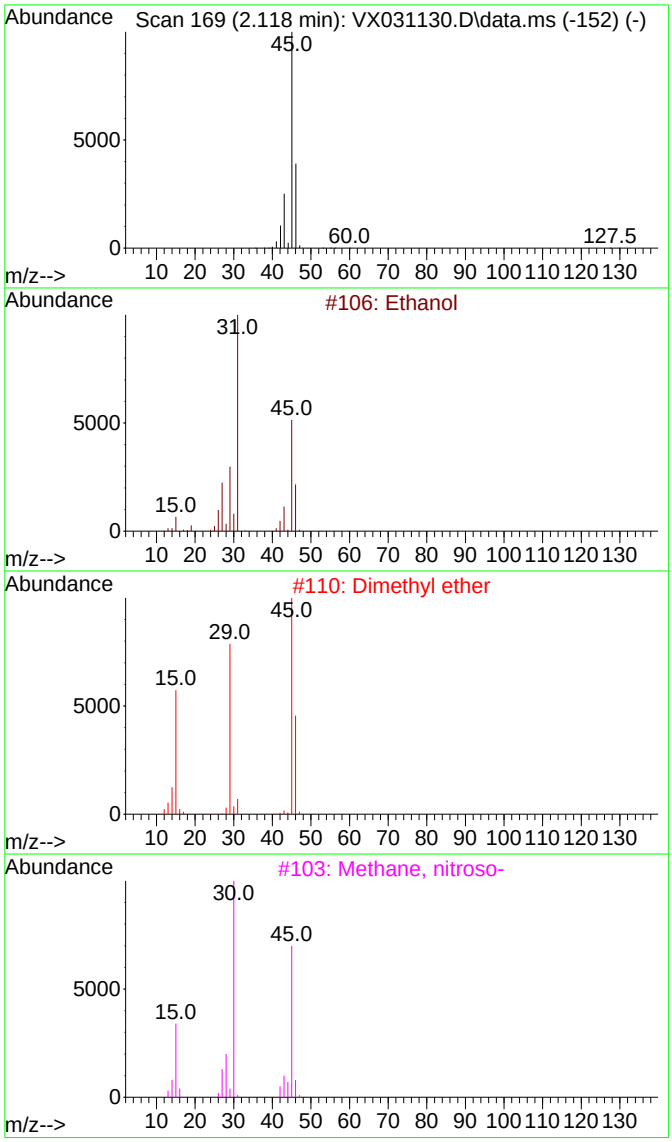
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

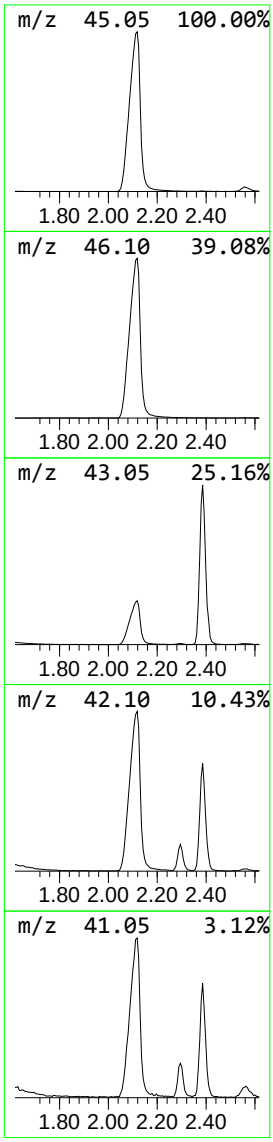
****

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.118	565.40 ug/l	7135800	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
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\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

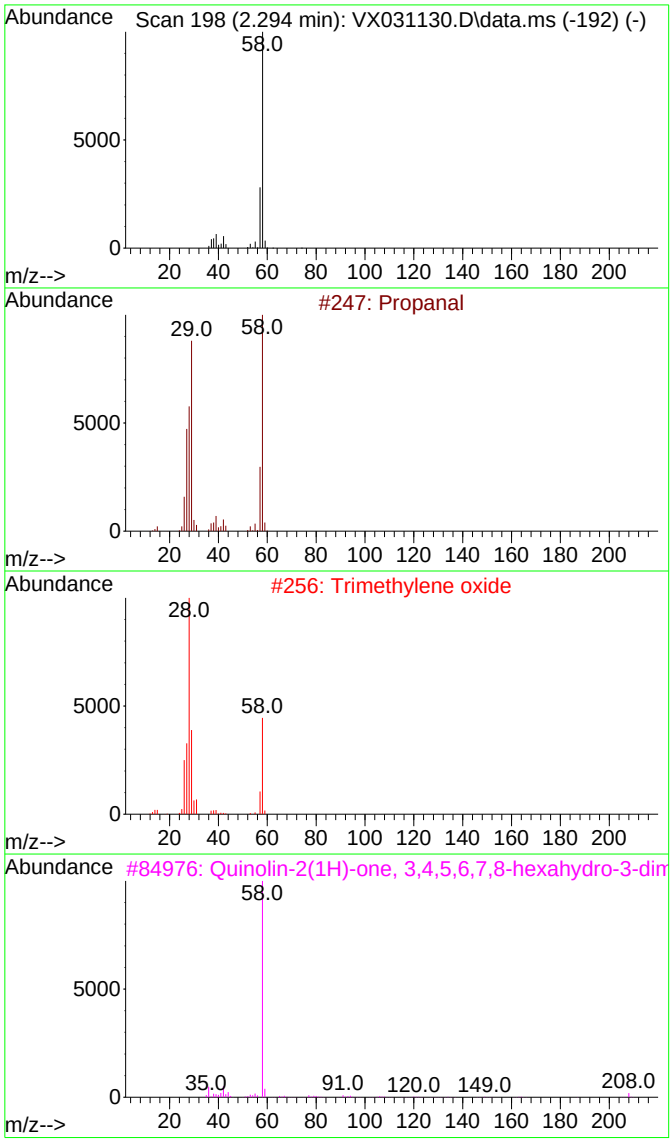
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

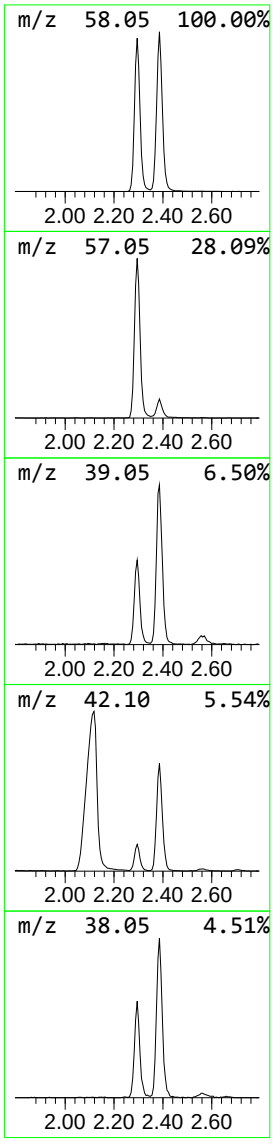
****

Peak Number 3 Propanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	82.51 ug/l	1041310	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5	Propylene oxide	58	C3H6O	000075-56-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

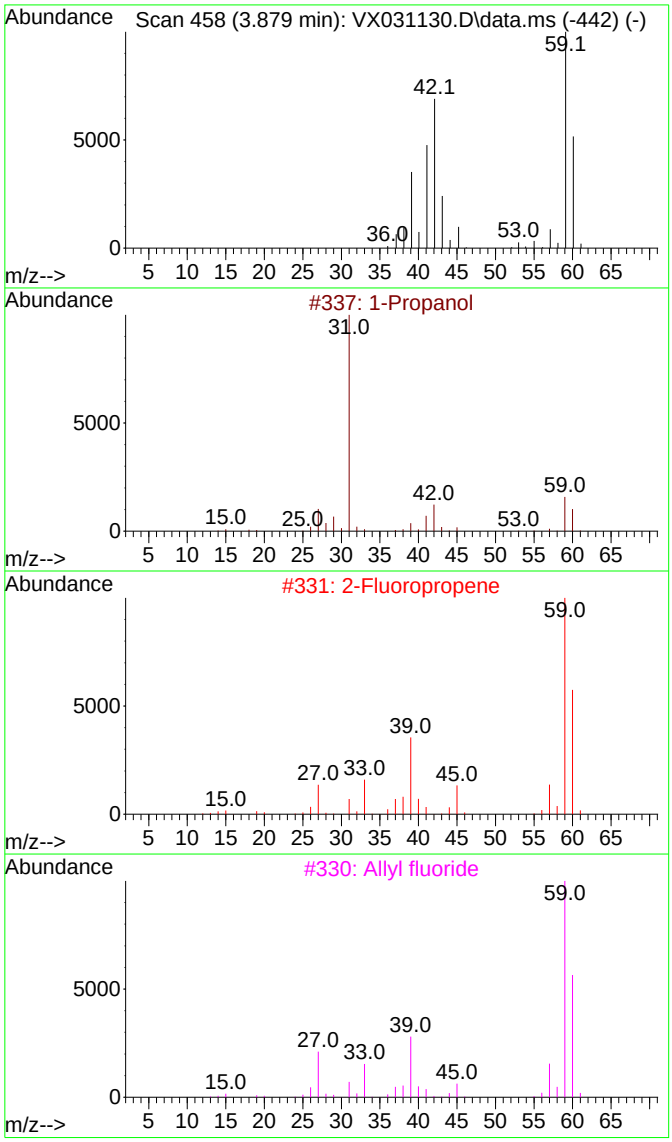
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

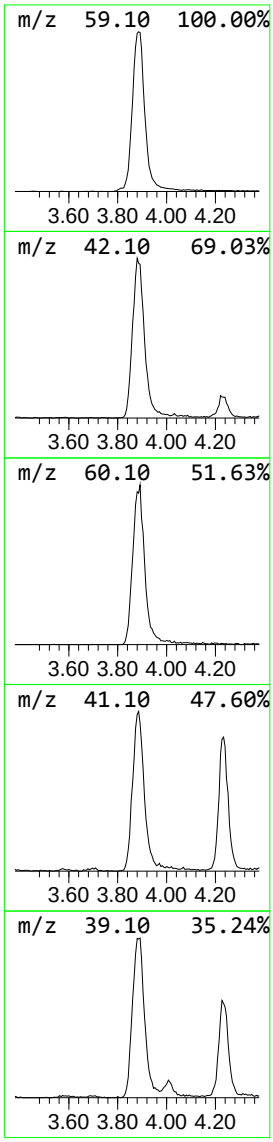
****

Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.879	64.26 ug/l	810992	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	72
2	2-Fluoropropene	60	C3H5F	001184-60-7	53
3	Allyl fluoride	60	C3H5F	000818-92-8	42
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	17
5	Cyclopropane	42	C3H6	000075-19-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

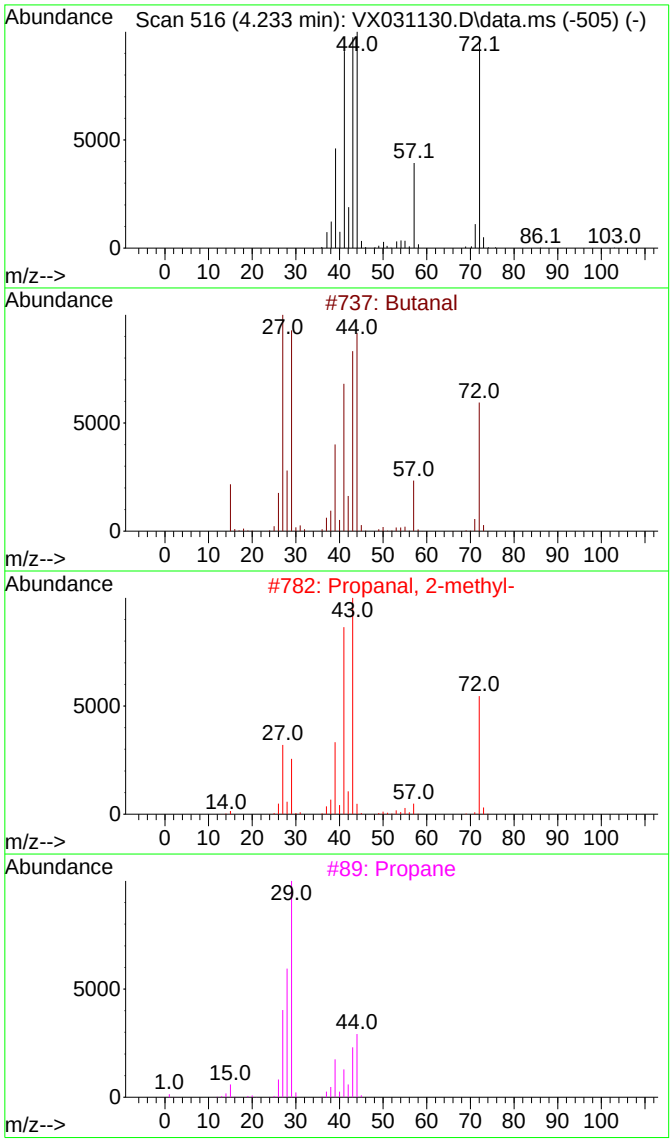
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

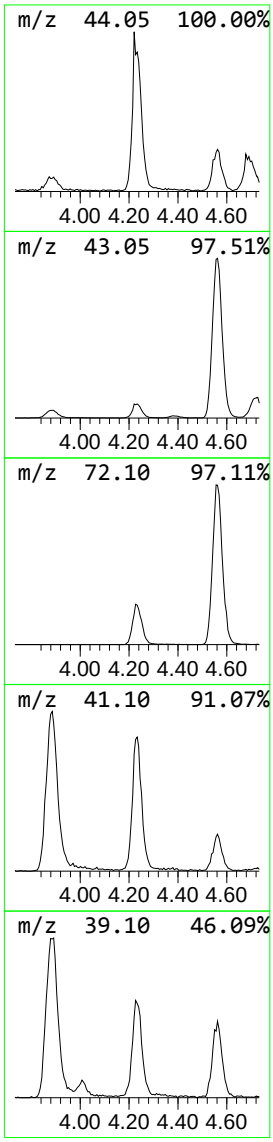
****

Peak Number 5 Butanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	32.01 ug/l	403980	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3	Propane	44	C3H8	000074-98-6	43
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	Isobutylene epoxide	72	C4H8O	000558-30-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

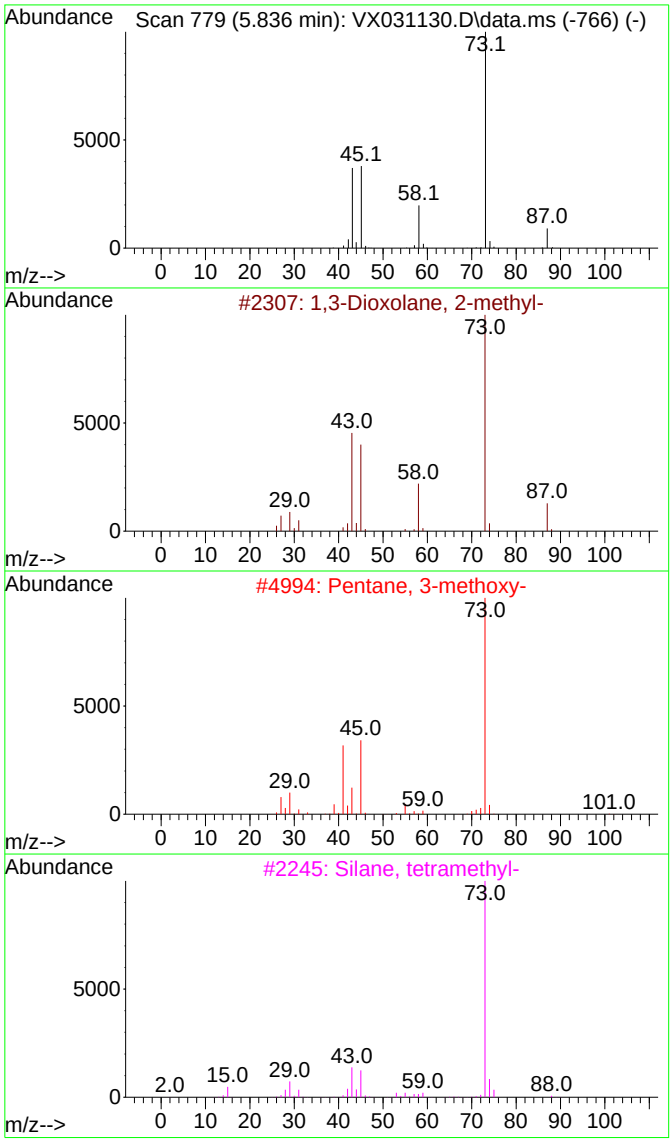
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

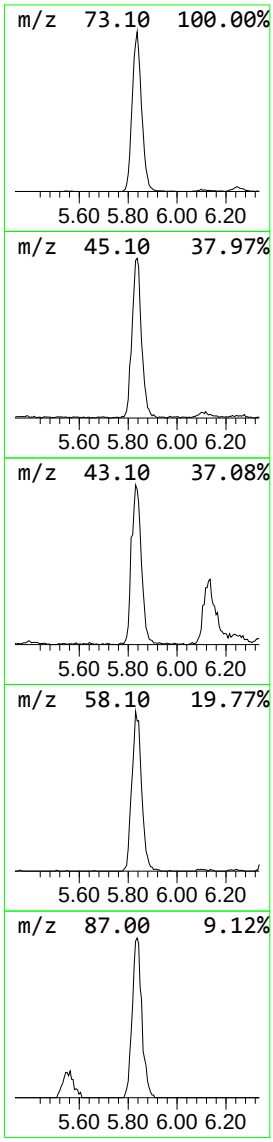
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	29.76 ug/l	375653	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

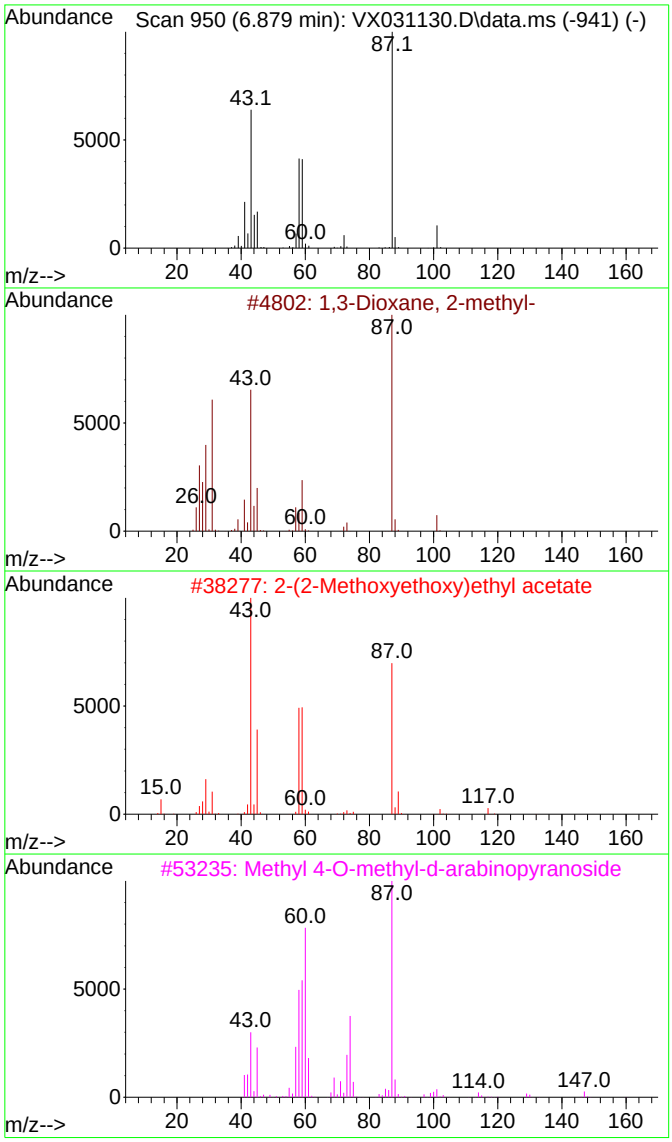
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

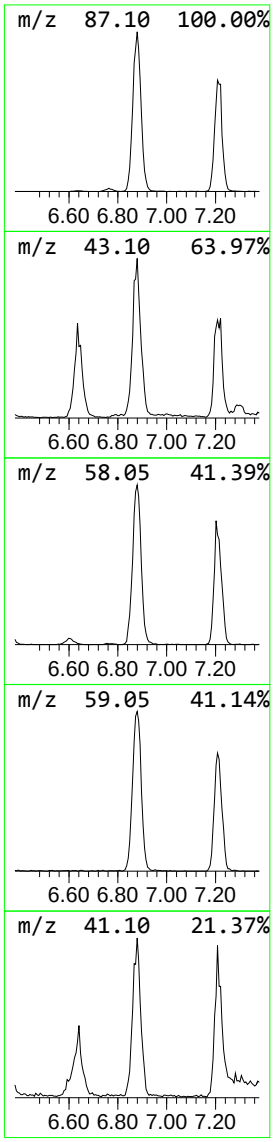
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown6.879 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	47.77 ug/l	747997	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	40
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	40
4	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

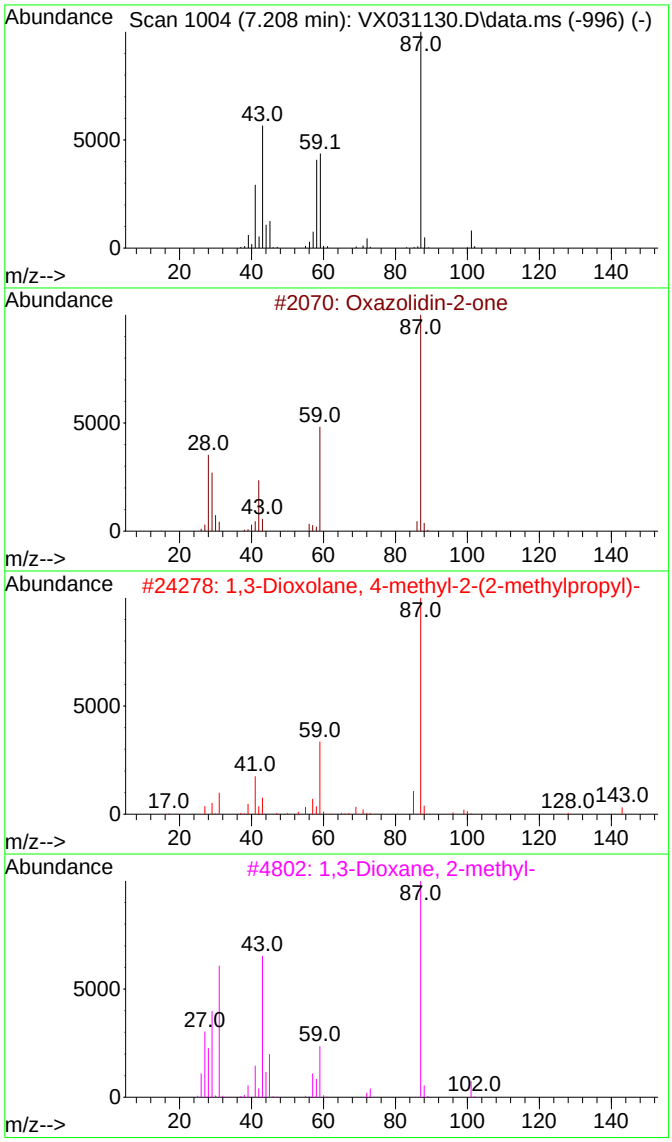
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

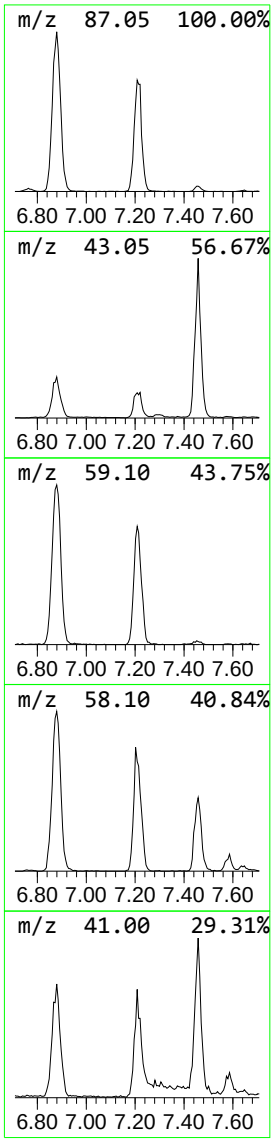
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown7.208 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	31.22 ug/l	488776	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
2	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
3	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	38
4	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
5	Diazene, butyl[1-(2,2-dimethylhy...	172	C8H20N4	061940-95-2	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

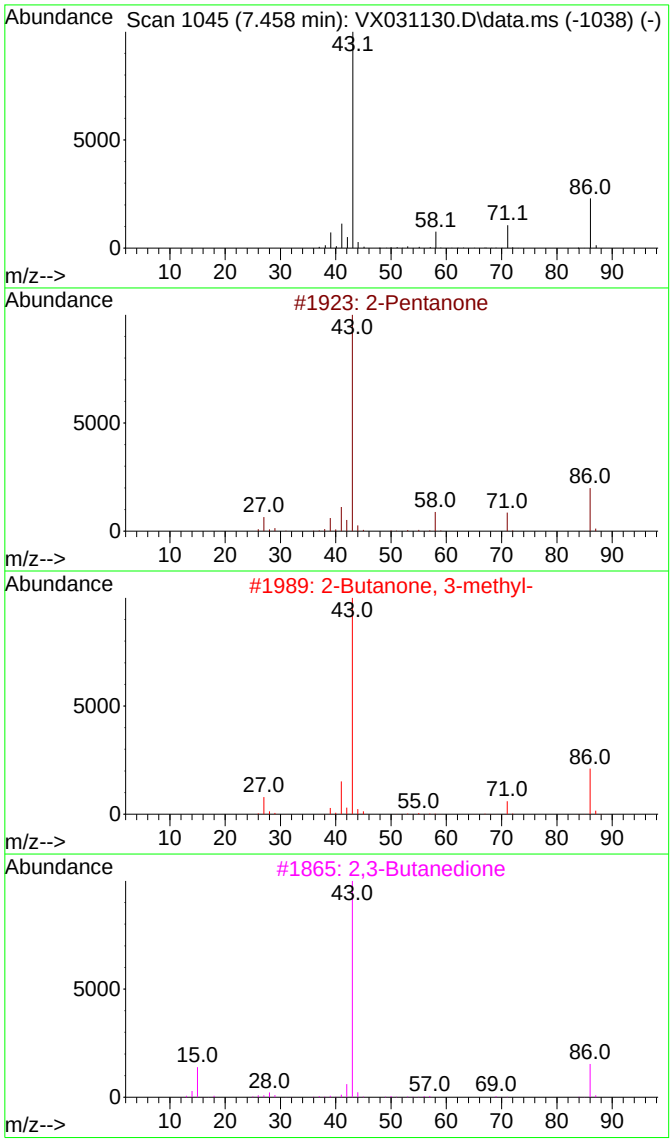
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

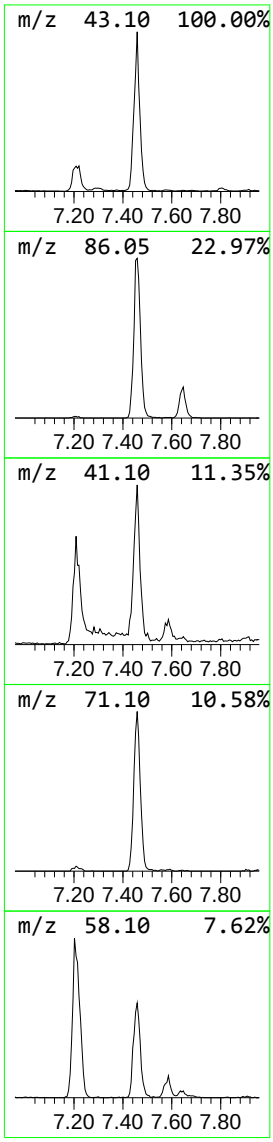
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	44.58 ug/l	697973	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	87
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	9
4	Butane	58	C4H10	000106-97-8	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

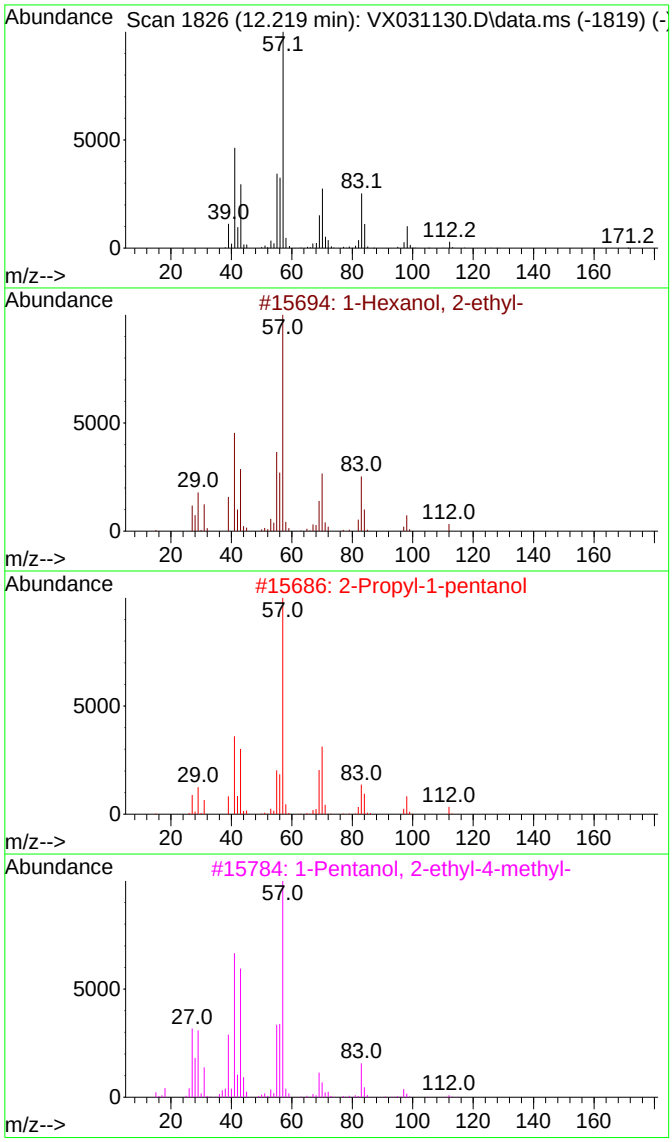
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

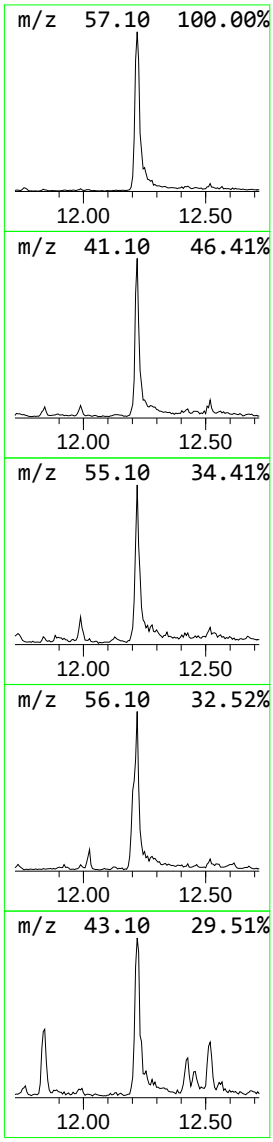
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	62.86 ug/l	1086120	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	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031130.D
Acq On : 06 Sep 2022 16:02
Operator : JC/MD
Sample : N4489-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0044

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.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
Ethanol	2.118	565.4	ug/l	7135800	1	5.556	631042	50.0
Propanal	2.294	82.5	ug/l	1041310	1	5.556	631042	50.0
1-Propanol	3.879	64.3	ug/l	810992	1	5.556	631042	50.0
Butanal	4.233	32.0	ug/l	403980	1	5.556	631042	50.0
1,3-Dioxolane, ...	5.836	29.8	ug/l	375653	1	5.556	631042	50.0
unknown6.879	6.879	47.8	ug/l	747997	2	6.763	782851	50.0
unknown7.208	7.208	31.2	ug/l	488776	2	6.763	782851	50.0
2-Pentanone	7.458	44.6	ug/l	697973	2	6.763	782851	50.0
1-Hexanol, 2-et...	12.219	62.9	ug/l	1086120	4	12.024	863969	50.0