LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025380.D
Acq On : 29 Nov 2021 19:18
Operator : JC/MD
Sample : M4837-19 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20936

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\82X111721W.M
Title : SW846 8260

Signal : TIC: VX025380.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	68	rVB	51400	55347	3.04%	0.941%
2	2.294	193	198	206	rBV	16290	25372	1.39%	0.432%
3	2.380	206	212	228	rVB	142401	228373	12.55%	3.885%
4	3.867	448	456	467	rBV2	7692	22497	1.24%	0.383%
5	5.391	694	706	721	rBV2	71000	203376	11.18%	3.460%
6	5.556	721	733	749	rVB	119405	336982	18.52%	5.732%
7	5.958	789	799	816	rBV2	71533	193505	10.64%	3.292%
8	6.763	921	931	942	rBV	183792	438591	24.11%	7.461%
9	6.873	944	949	960	rVB2	10156	23438	1.29%	0.399%
10	8.653	1234	1241	1250	rBV	378019	600617	33.01%	10.217%
11	8.994	1290	1297	1309	rBV	69667	106446	5.85%	1.811%
12	9.573	1381	1392	1411	rBV	579056	1819297	100.00%	30.948%
13	10.055	1465	1471	1484	rBV	388832	531165	29.20%	9.036%
14	11.085	1634	1640	1650	rVB	304917	403941	22.20%	6.871%
15	11.890	1765	1772	1780	rBV	66659	110101	6.05%	1.873%
16	12.024	1789	1794	1801	rVB	420713	509935	28.03%	8.674%
17	12.219	1822	1826	1831	rBV	38037	52319	2.88%	0.890%
18	12.286	1831	1837	1838	rVV3	47539	79119	4.35%	1.346%
19	12.311	1838	1841	1846	rVV3	53812	81218	4.46%	1.382%
20	12.359	1846	1849	1857	rVB2	9788	20029	1.10%	0.341%
21	13.780	2077	2082	2088	rVB	27524	36933	2.03%	0.628%

Sum of corrected areas: 5878601

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
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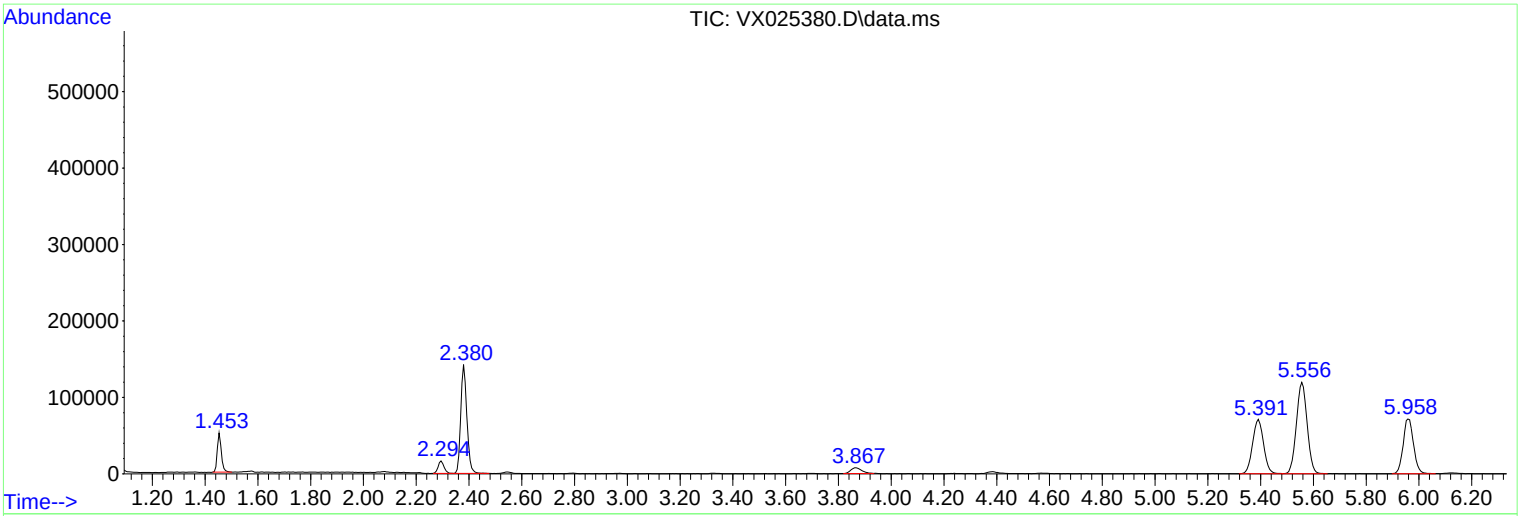
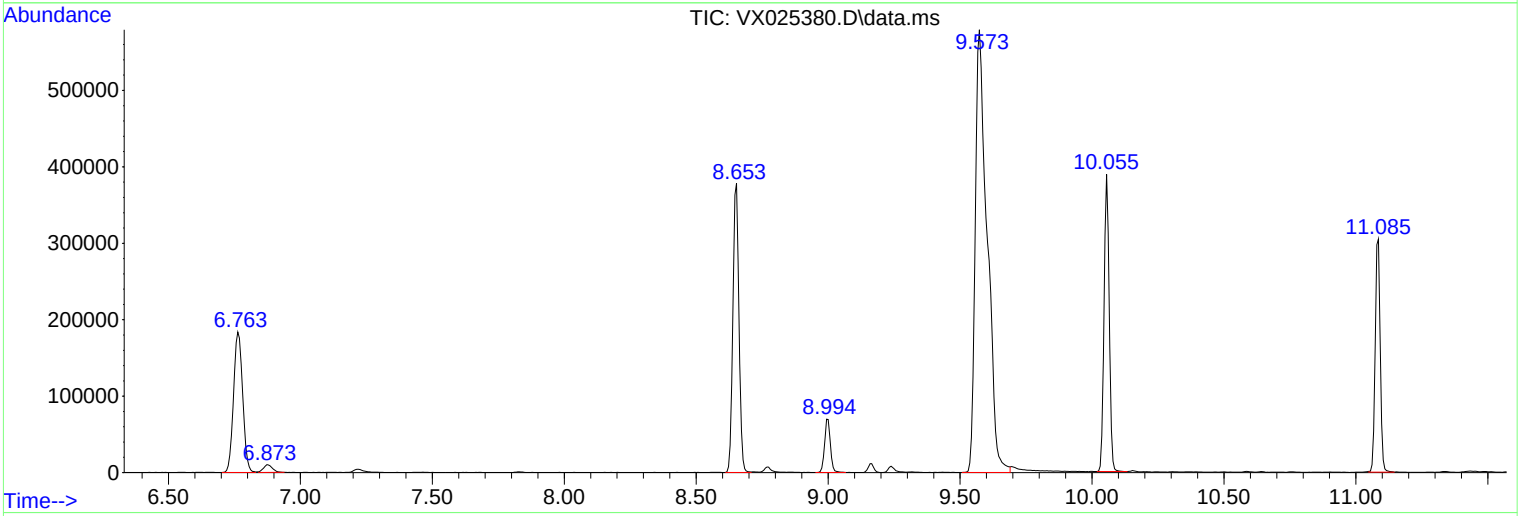
ALS Vial : 24 Sample Multiplier: 1

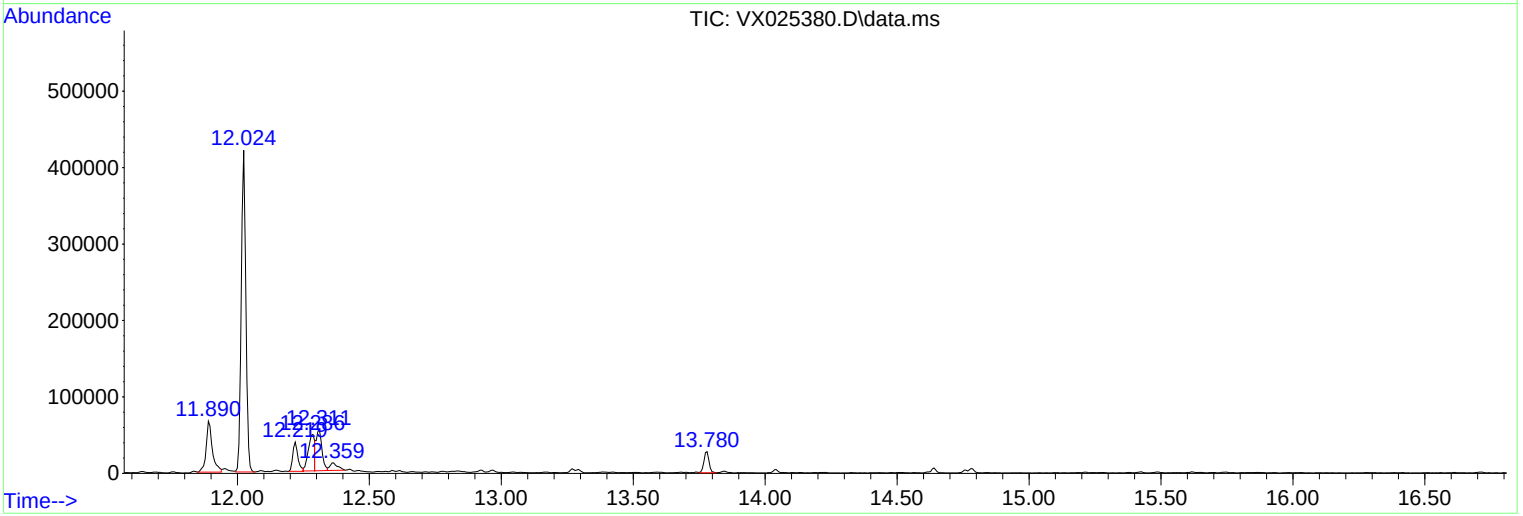
Instrument :
MSVOA_X
ClientSampleId :
20936

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

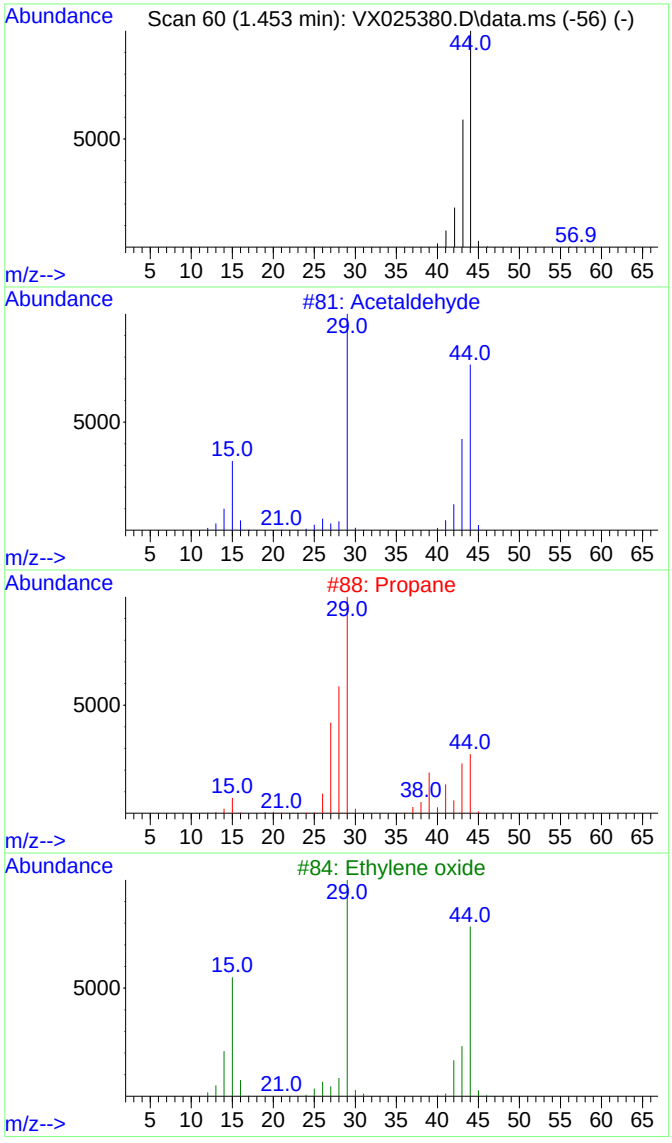
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

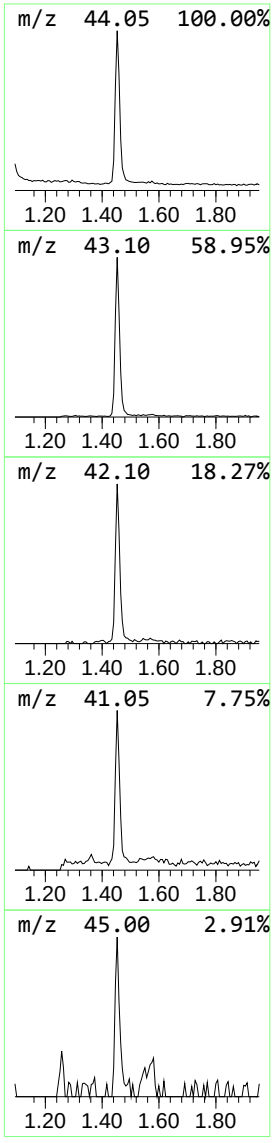
****

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	8.21 ug/l	55347	Pentafluorobenzene	5.556

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	1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5	Alanine	89	C3H7NO2	000056-41-7	4





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Instrument :
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ClientSampleId :
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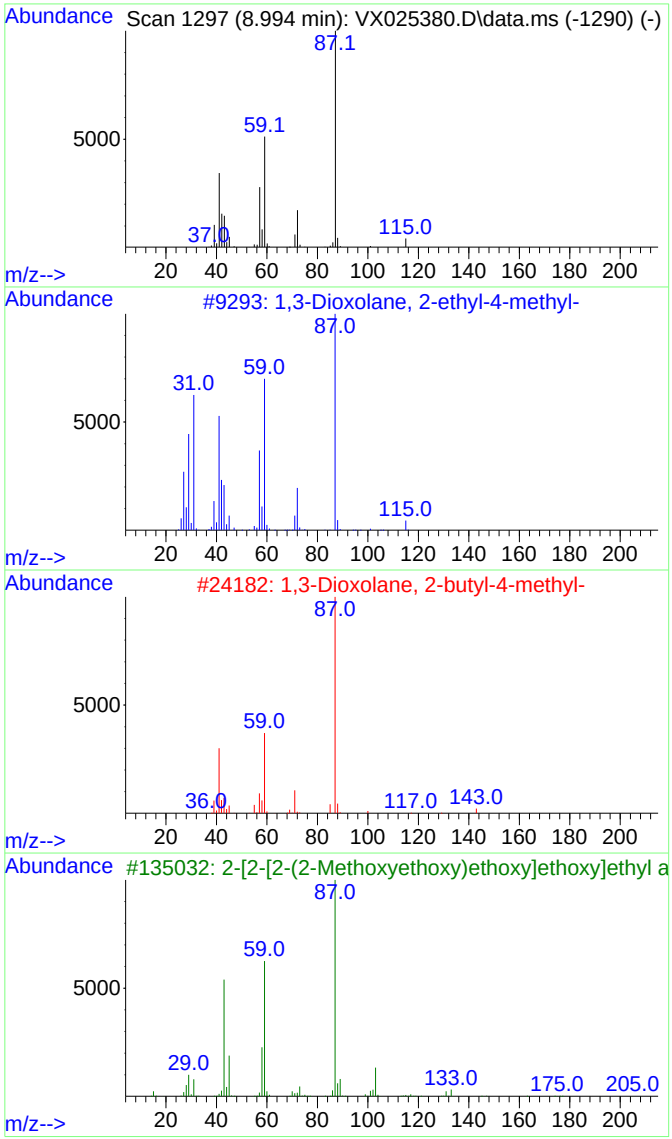
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

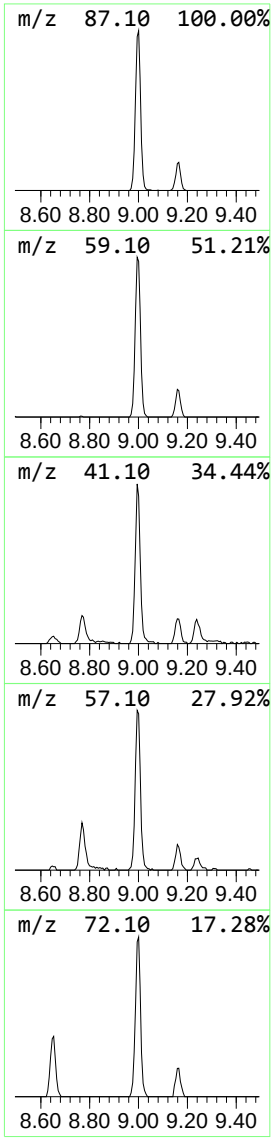
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.994	10.02 ug/l	106446	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	64
3	2-[2-[2-(2-Methoxyethoxy)ethoxy]...	250	C11H22O6	1000351-91-4	64
4	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
5	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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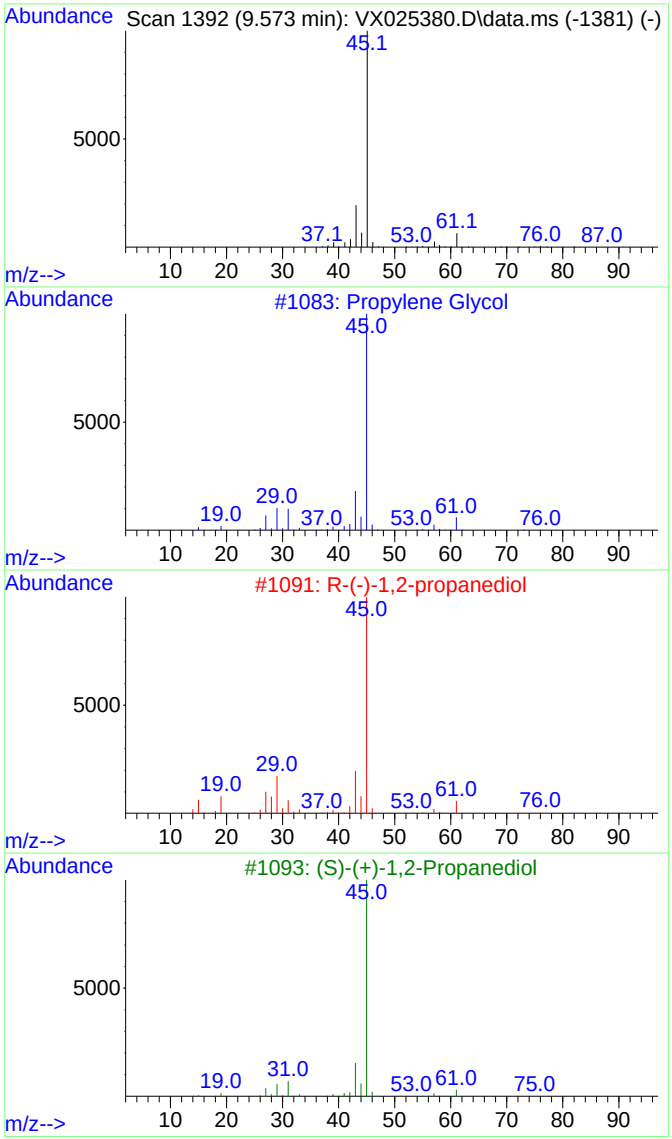
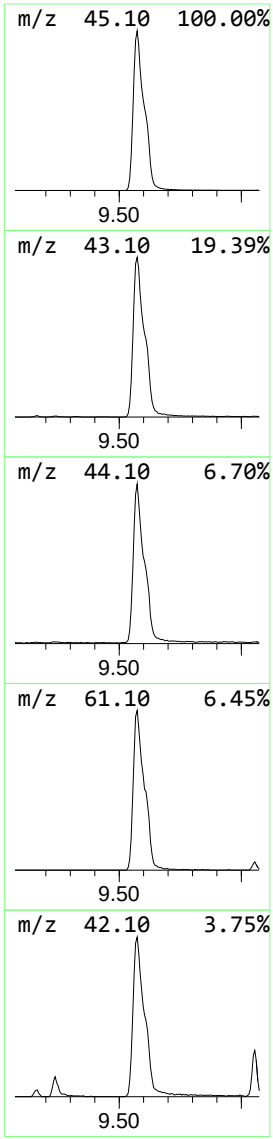
****
Peak Number 3 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.573	171.26 ug/l	1819300	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40





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Instrument :
MSVOA_X
ClientSampleId :
20936

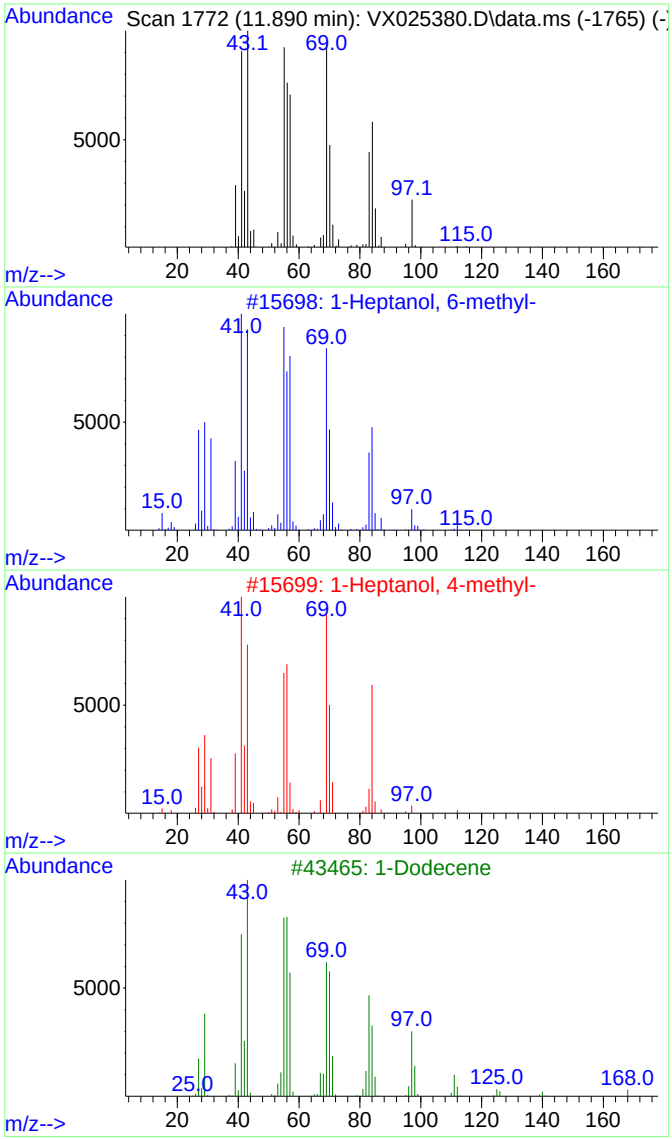
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

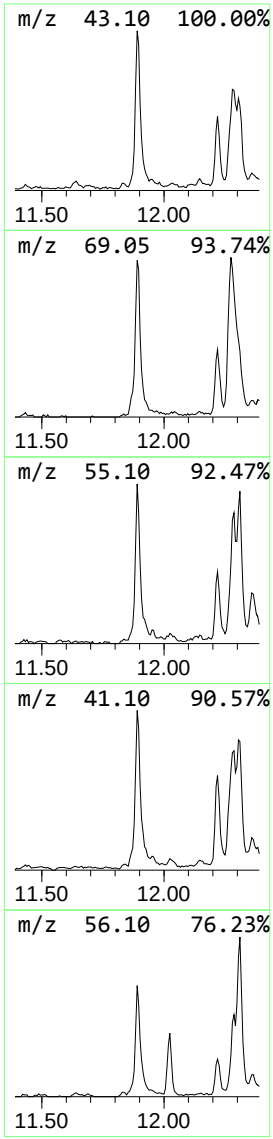
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heptanol, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.890	10.80 ug/l	110101	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	64
3	1-Dodecene	168	C12H24	000112-41-4	53
4	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	38
5	Pentane, 3-methylene-	84	C6H12	000760-21-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20936

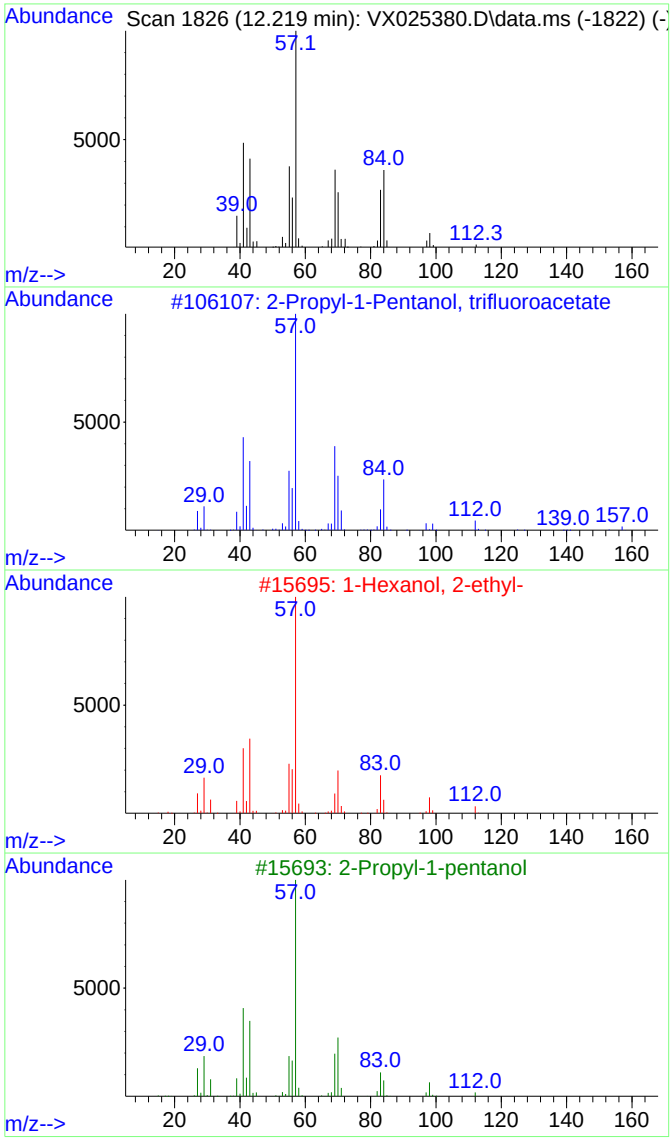
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

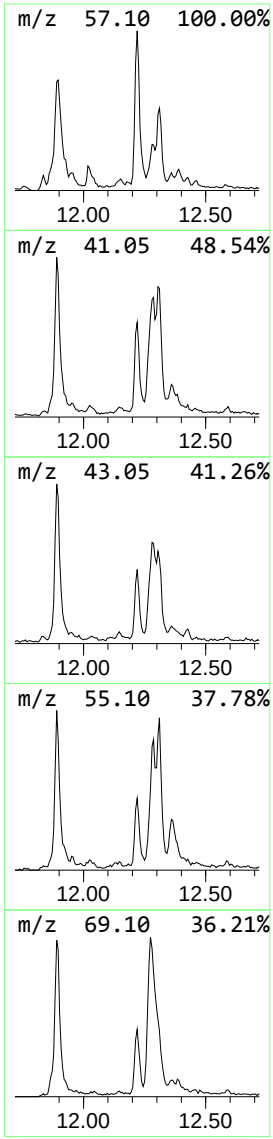
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propyl-1-Pentanol, triflu... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	5.13 ug/l	52319	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	56
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	50
5	Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	45





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20936

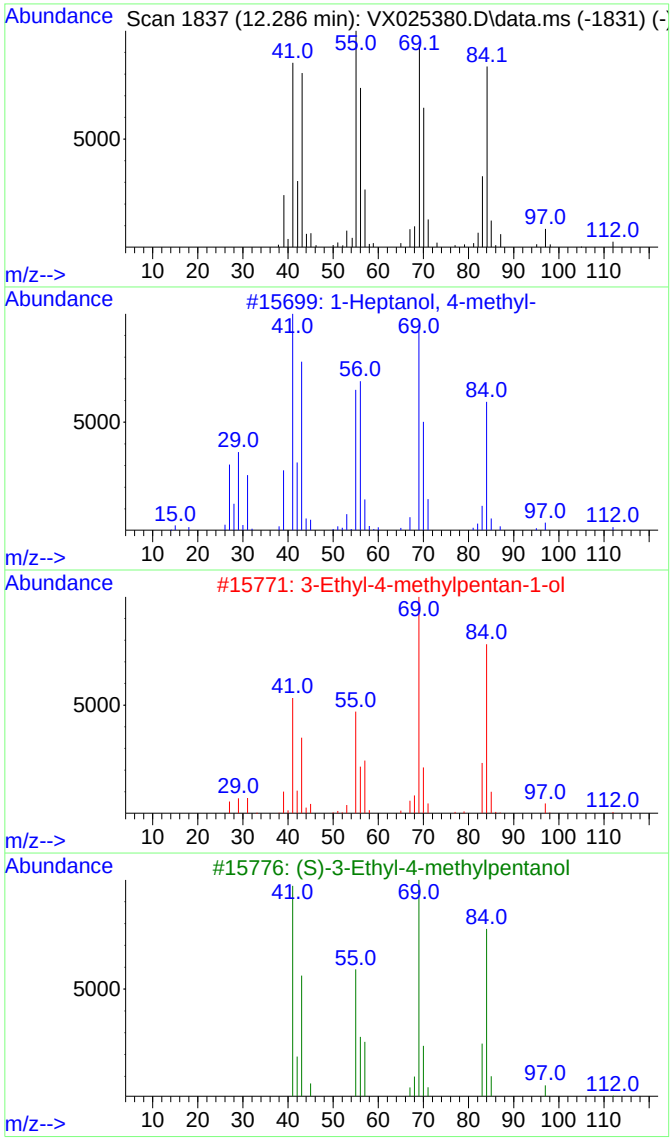
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

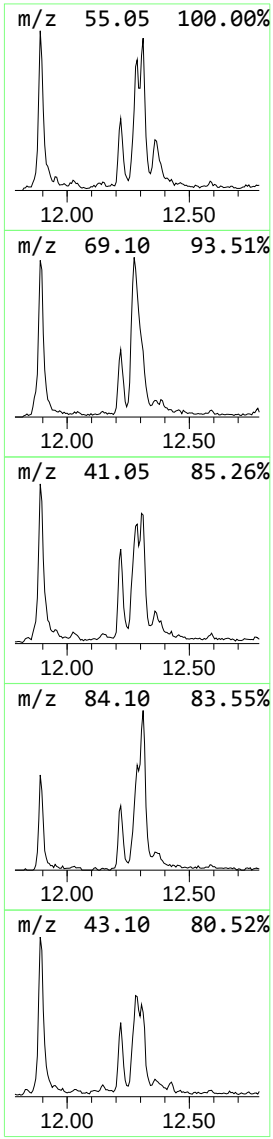
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Heptanol, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.286	7.76 ug/l	79119	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	64
2	3-Ethyl-4-methylpentan-1-ol	130	C8H18O	038514-13-5	53
3	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	53
4	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	50
5	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	47





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Instrument :
MSVOA_X
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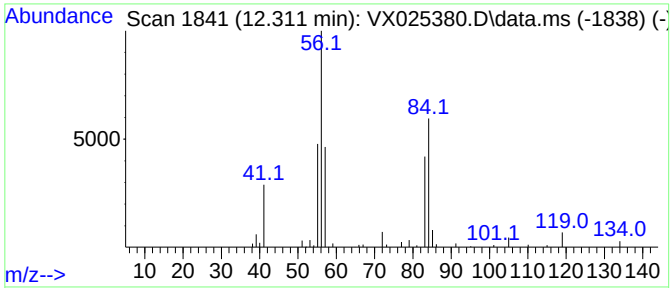
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

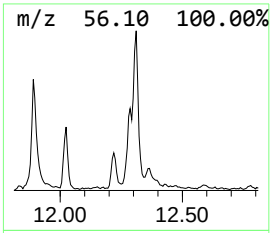
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

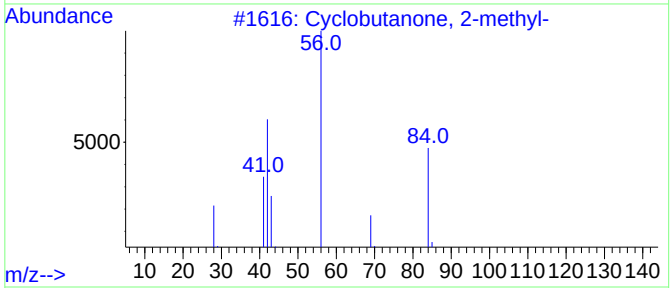
****
Peak Number 7 unknown12.311 Concentration Rank 5

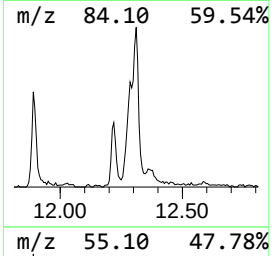
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.311	7.96 ug/l	81218	1,4-Dichlorobenzene-d4	12.024

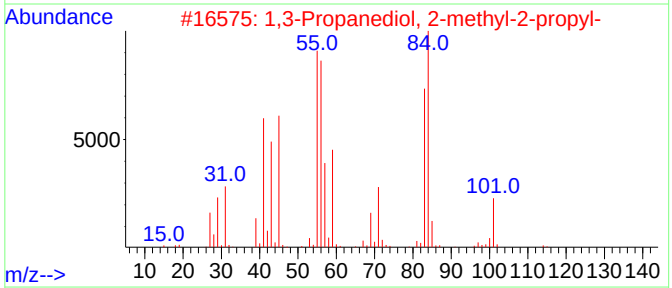
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanone, 2-methyl-	84	C5H8O	001517-15-3	38
2	1,3-Propanediol, 2-methyl-2-propyl-	132	C7H16O2	000078-26-2	36
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	32
4	Cyclopentane-1,2-diol	102	C5H10O2	1010194-24-0	28
5	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	12

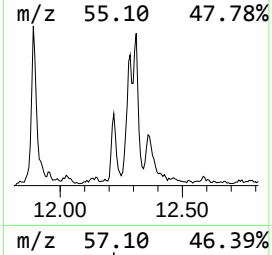


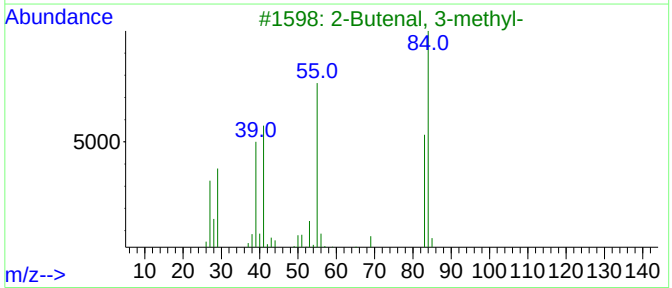


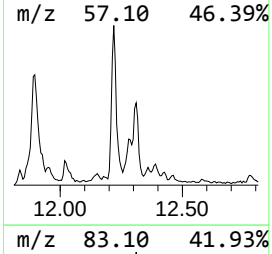


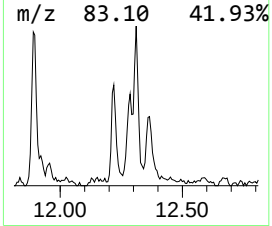












Tentatively Identified Compound (LSC) summary

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ALS Vial : 24 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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	8.2	ug/l	55347	1	5.556	336982	50.0
1,3-Dioxolane, ...	8.994	10.0	ug/l	106446	3	10.055	531165	50.0
Propylene Glycol	9.573	171.3	ug/l	1819300	3	10.055	531165	50.0
1-Heptanol, 6-m...	11.890	10.8	ug/l	110101	4	12.024	509935	50.0
2-Propyl-1-Pent...	12.219	5.1	ug/l	52319	4	12.024	509935	50.0
1-Heptanol, 4-m...	12.286	7.8	ug/l	79119	4	12.024	509935	50.0
unknown12.311	12.311	8.0	ug/l	81218	4	12.024	509935	50.0