LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
Data File : VX029691.D
Acq On : 22 Jun 2022 12:07
Operator : JC/MD
Sample : N3286-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

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\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	43	rBV3	39827	91074	7.01%	1.102%
2	1.368	43	46	51	rVV	68156	72489	5.58%	0.877%
3	1.752	104	109	118	rVB	78632	113252	8.71%	1.370%
4	2.136	166	172	180	rVB4	13125	27990	2.15%	0.339%
5	2.343	198	206	218	rVB2	23003	47804	3.68%	0.578%
6	2.782	269	278	288	rBV	75740	178314	13.72%	2.158%
7	2.867	288	292	303	rVB	21463	40485	3.11%	0.490%
8	3.105	321	331	342	rVB	55131	123326	9.49%	1.492%
9	4.215	501	513	521	rBV5	9260	26286	2.02%	0.318%
10	4.306	521	528	538	rVB2	11460	31545	2.43%	0.382%
11	4.434	541	549	566	rVB10	3235	13189	1.01%	0.160%
12	5.391	692	706	718	rBV2	146115	430898	33.15%	5.214%
13	5.556	723	733	744	rBV	268522	774730	59.60%	9.375%
14	5.958	789	799	809	rBV	153705	407965	31.38%	4.937%
15	6.050	809	814	820	rVV	6612	16602	1.28%	0.201%
16	6.172	824	834	837	rVV3	9155	27113	2.09%	0.328%
17	6.257	838	848	858	rVV2	49726	158687	12.21%	1.920%
18	6.763	921	931	943	rBV	409961	983037	75.62%	11.895%
19	7.360	1022	1029	1040	rVB5	6027	14713	1.13%	0.178%
20	7.988	1122	1132	1142	rVB2	19336	39675	3.05%	0.480%
21	8.110	1144	1152	1163	rVB2	25308	57416	4.42%	0.695%
22	8.427	1199	1204	1210	rVB	8361	13341	1.03%	0.161%
23	8.653	1229	1241	1250	rBV	817028	1299983	100.00%	15.730%
24	9.452	1365	1372	1378	rBV5	8499	17427	1.34%	0.211%
25	10.055	1466	1471	1478	rVV	821742	1094418	84.19%	13.243%
26	10.195	1490	1494	1499	rBV	11215	14298	1.10%	0.173%
27	10.305	1506	1512	1518	rVB	15958	24670	1.90%	0.299%
28	11.085	1634	1640	1650	rBV	609959	814441	62.65%	9.855%
29	11.756	1746	1750	1756	rVB	11593	14603	1.12%	0.177%
30	12.024	1788	1794	1801	rBV	833608	1022537	78.66%	12.373%
31	12.244	1824	1830	1836	rBV	160206	193982	14.92%	2.347%
32	12.701	1900	1905	1912	rVB	60268	77826	5.99%	0.942%

Sum of corrected areas: 8264116

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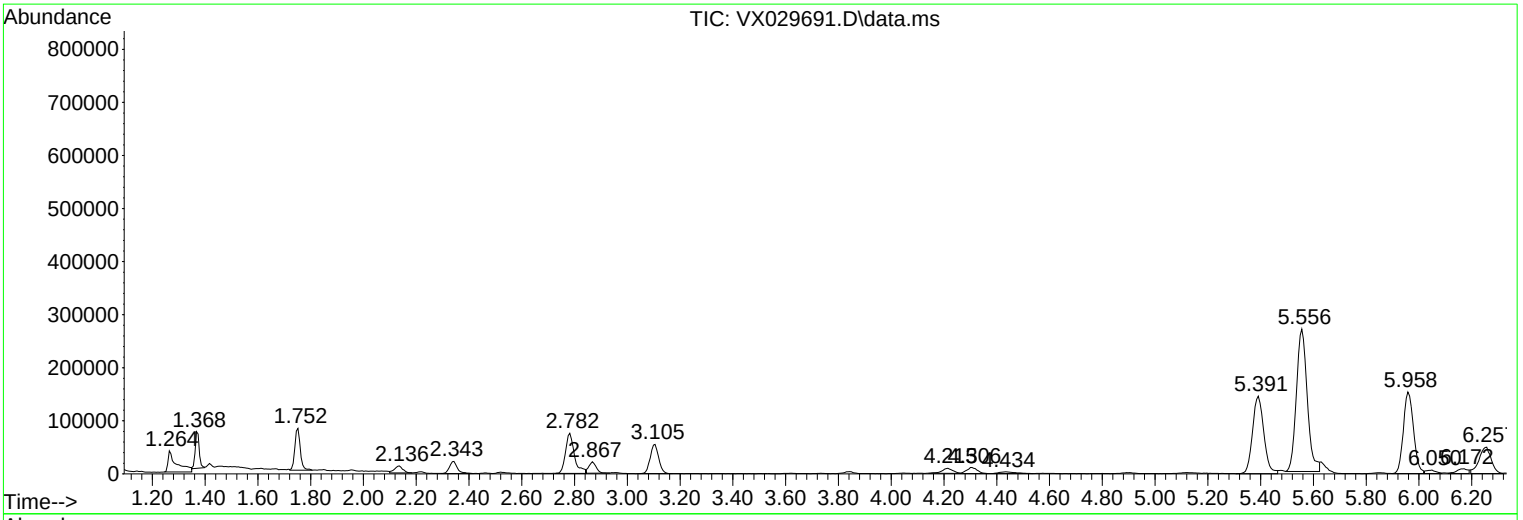
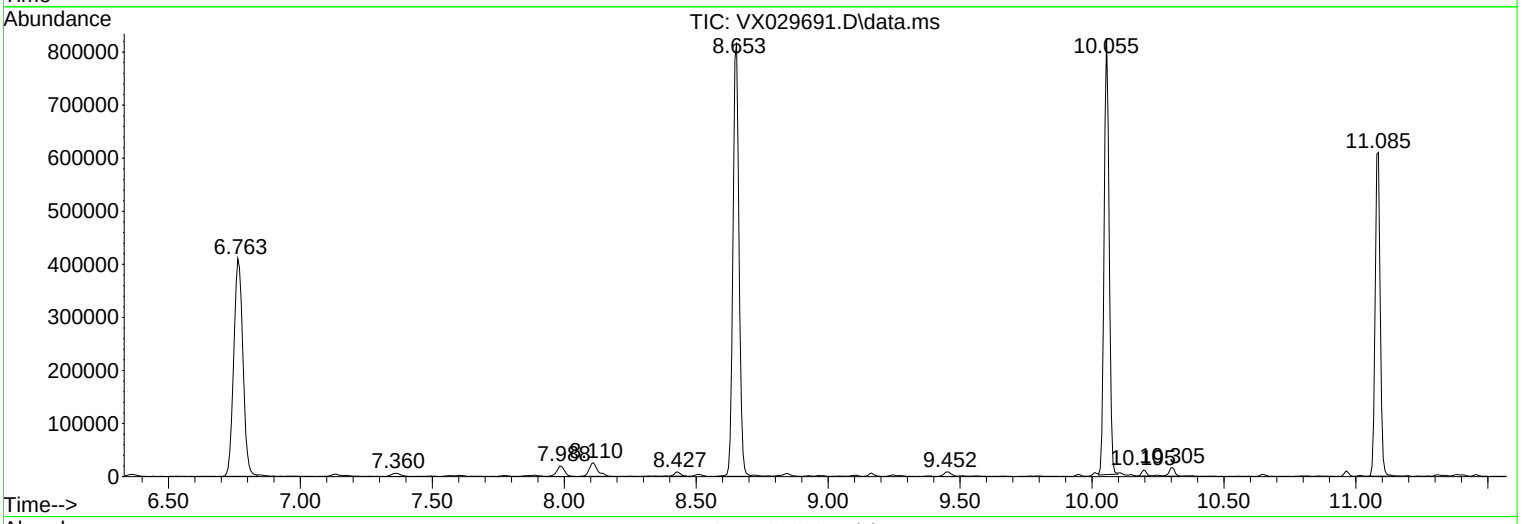
ALS Vial : 8 Sample Multiplier: 1

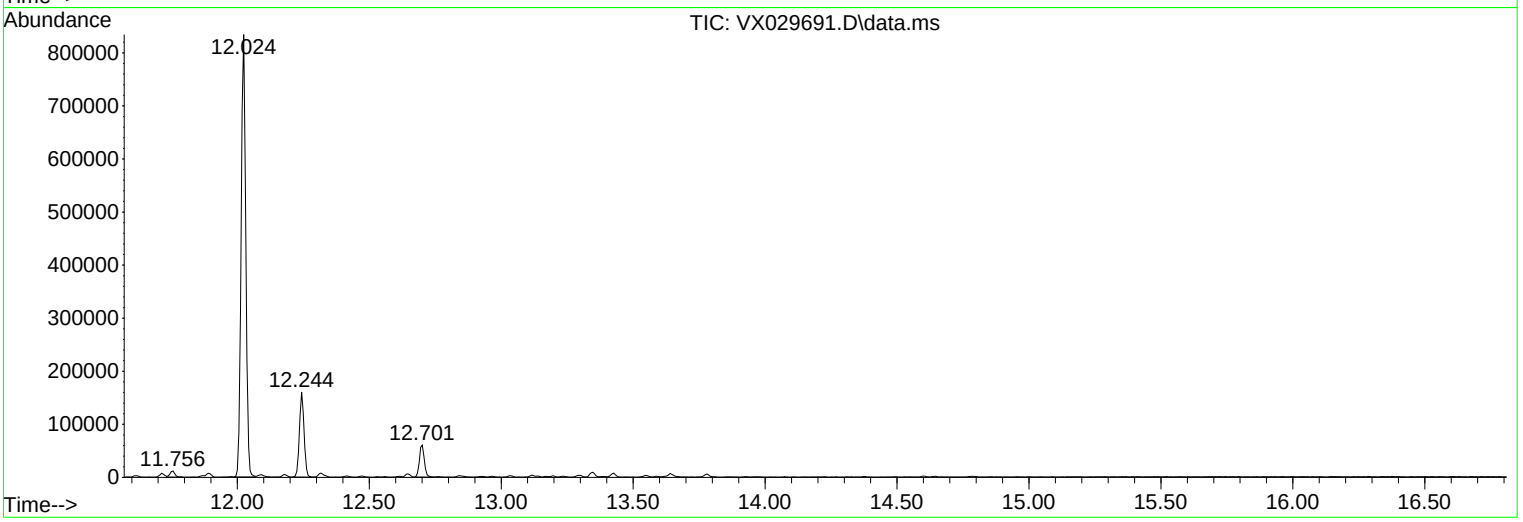
Instrument :
MSVOA_X
ClientSampleId :
MW-6S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

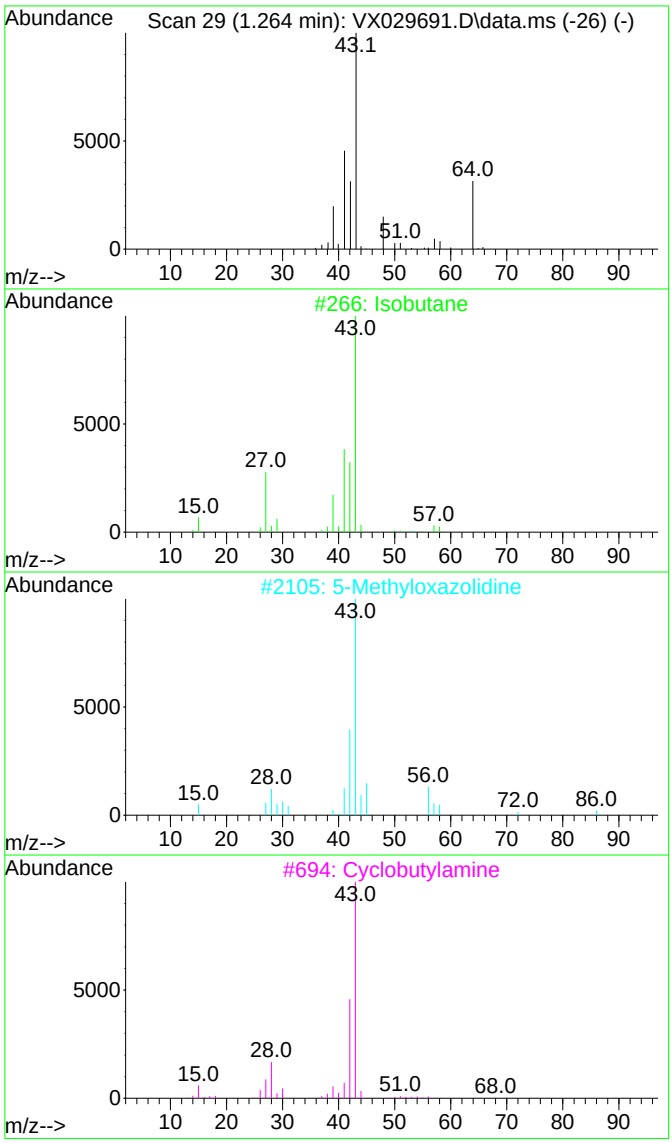
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

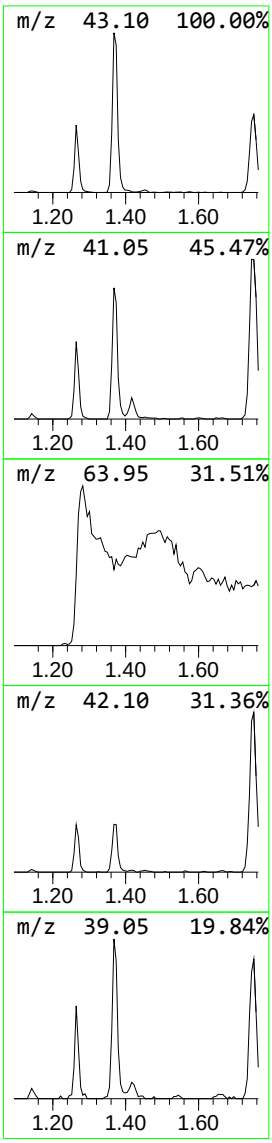
****

Peak Number 1 unknown1.264 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.88 ug/l	91074	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	47
2	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
3	Cyclobutylamine	71	C4H9N	002516-34-9	4
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

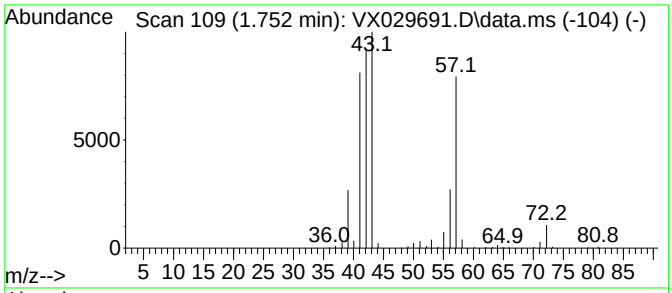
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

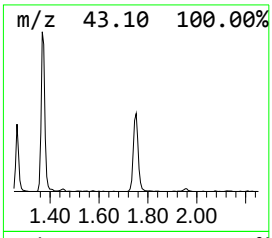
****

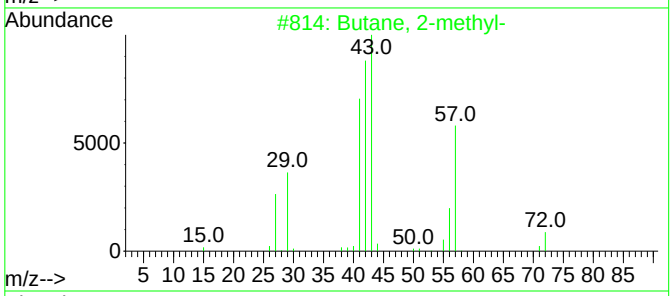
Peak Number 2 Butane, 2-methyl- Concentration Rank 5

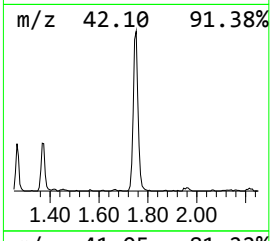
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	7.31 ug/l	113252	Pentafluorobenzene	5.556

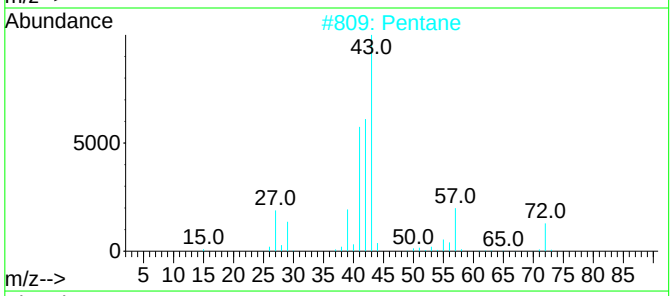
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	37
4	1-Butene	56	C4H8	000106-98-9	10
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10

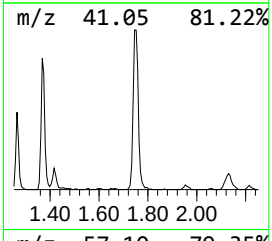


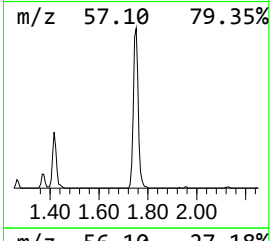


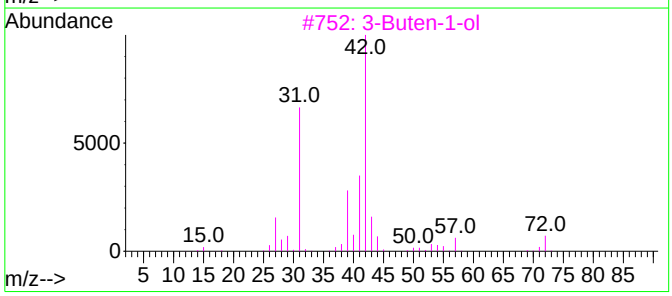


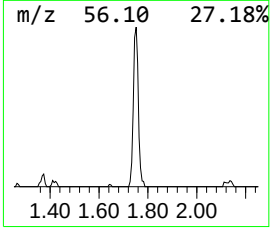












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Instrument :
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ClientSampleId :
MW-6S

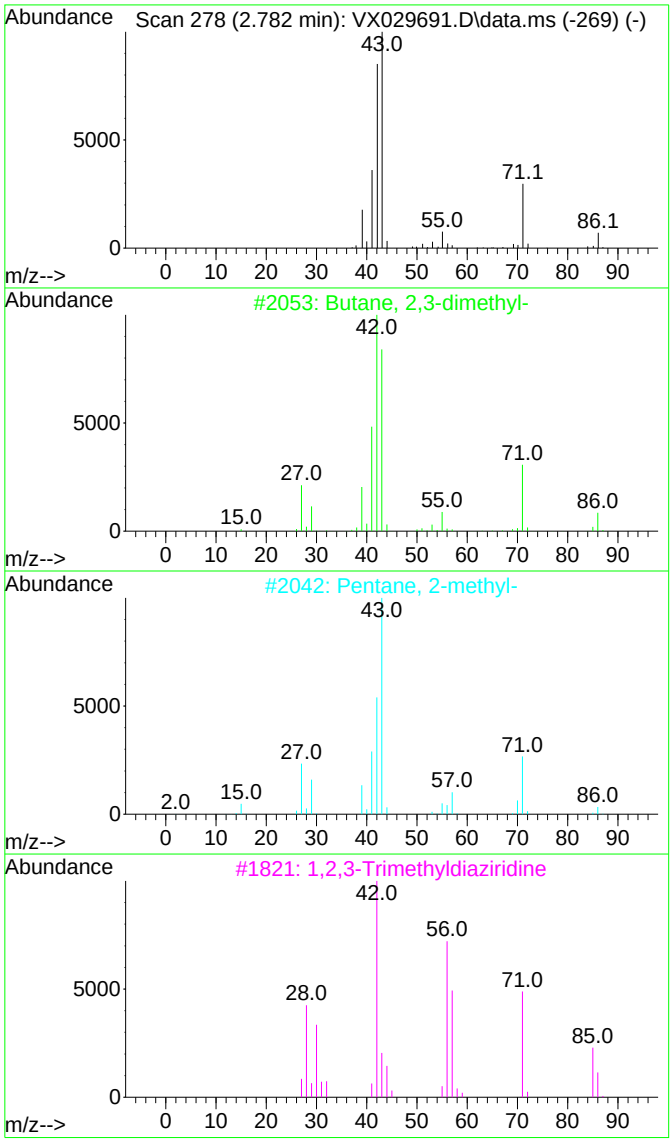
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

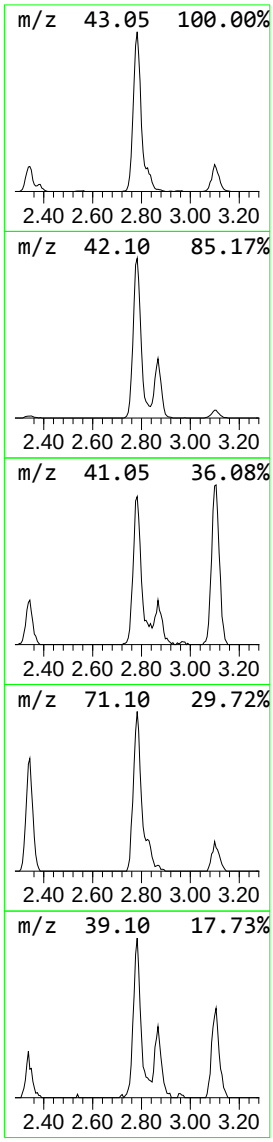
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	11.51 ug/l	178314	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	38
4	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	12
5	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	10





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

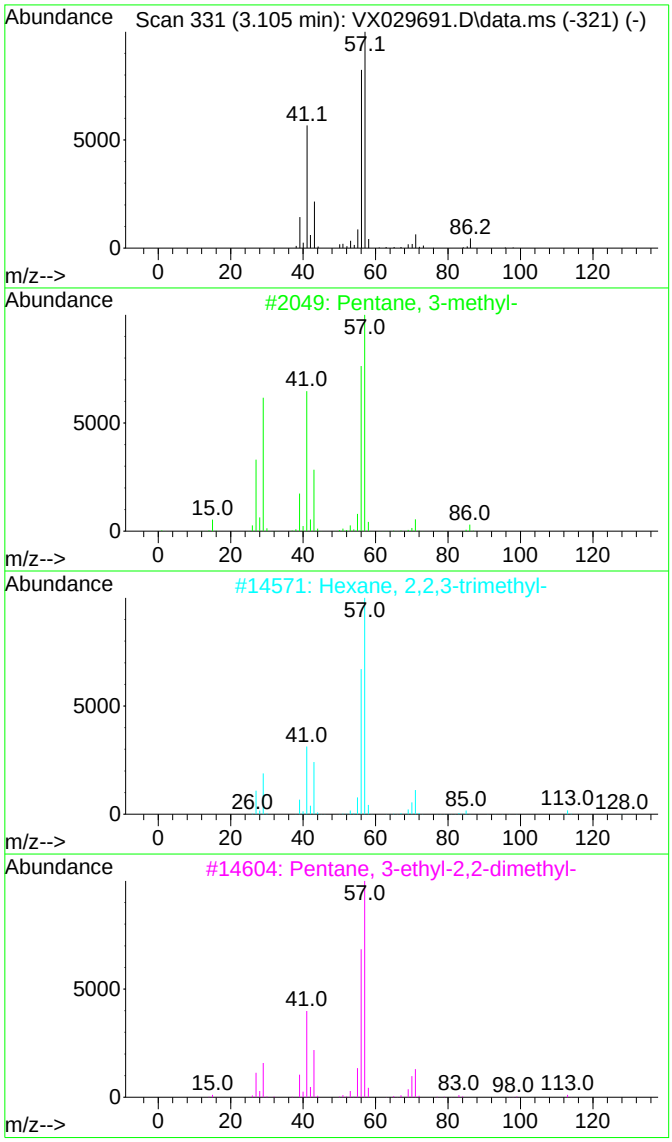
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

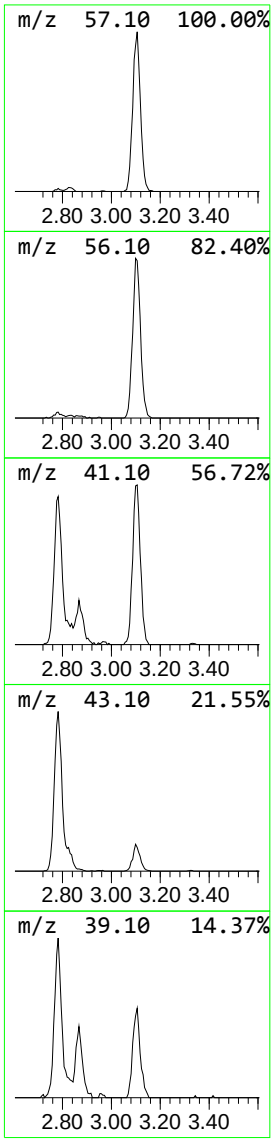
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	7.96 ug/l	123326	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	42





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

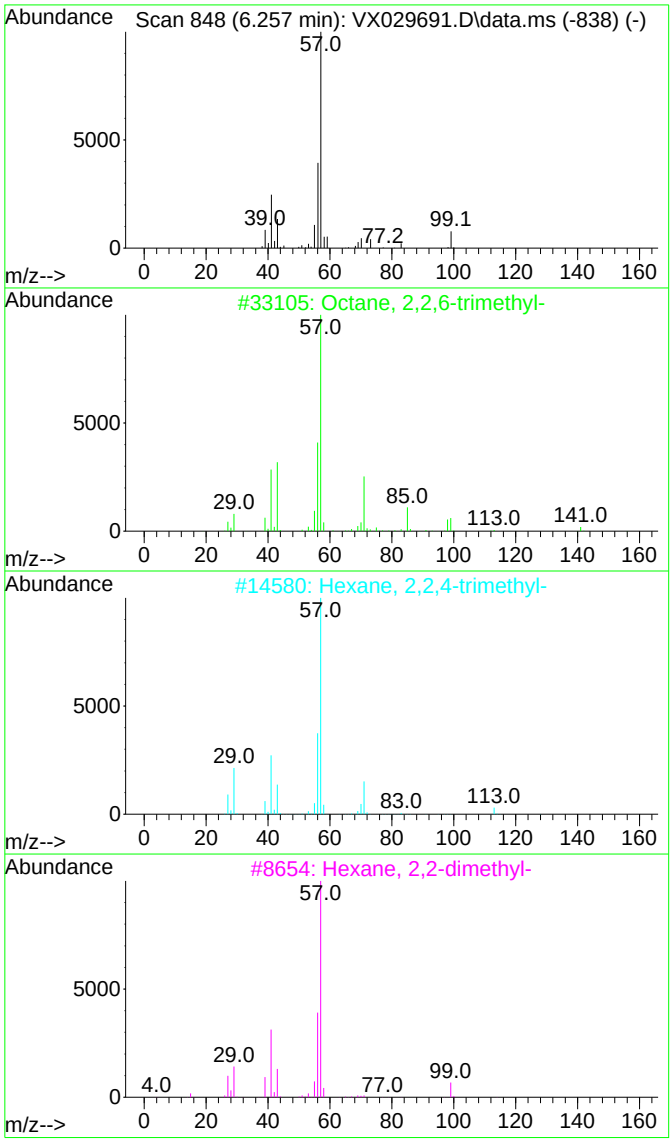
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

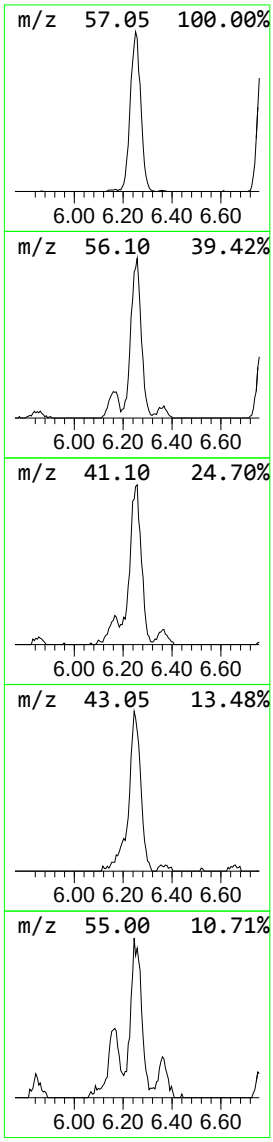
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octane, 2,2,6-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	8.07 ug/l	158687	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
5	Carbonic acid, bis(2-methylpropy...	174	C9H18O3	000539-92-4	50





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MSVOA_X
ClientSampleId :
MW-6S

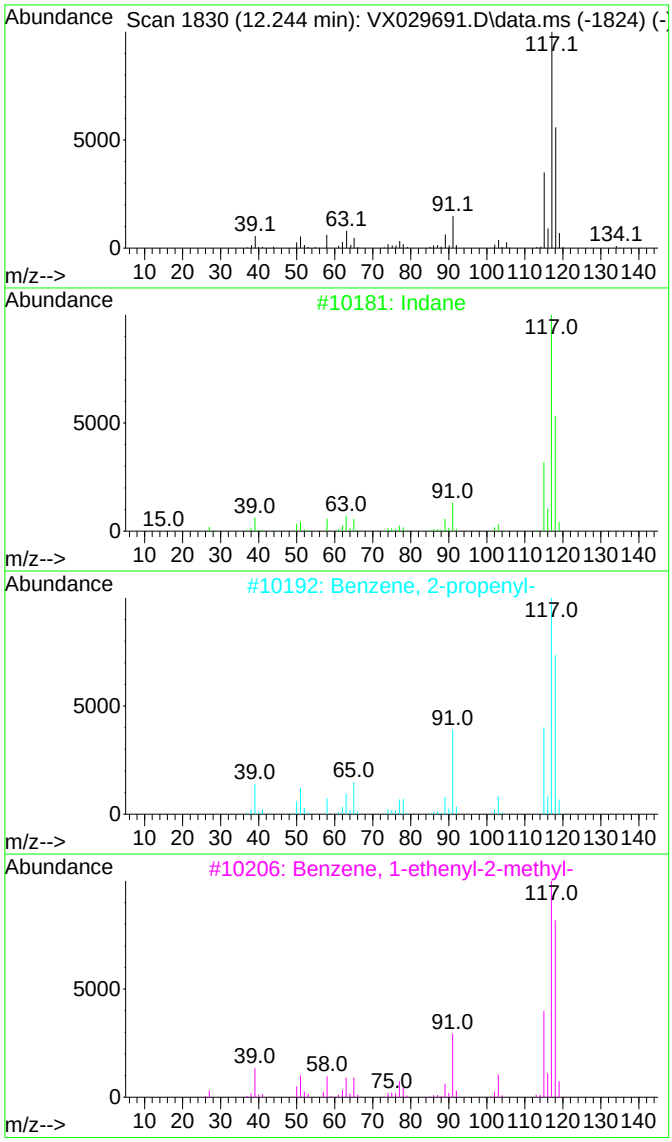
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

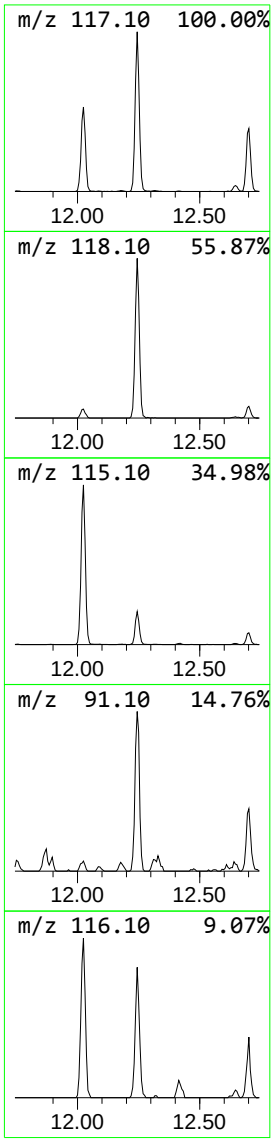
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	9.49 ug/l	193982	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80





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
unknown1.264	1.264	5.9	ug/l	91074	1	5.556	774730	50.0
Butane, 2-methyl-	1.752	7.3	ug/l	113252	1	5.556	774730	50.0
Butane, 2,3-dim...	2.782	11.5	ug/l	178314	1	5.556	774730	50.0
Pentane, 3-methyl-	3.105	8.0	ug/l	123326	1	5.556	774730	50.0
Octane, 2,2,6-t...	6.257	8.1	ug/l	158687	2	6.763	983037	50.0
Indane	12.244	9.5	ug/l	193982	4	12.024	1022540	50.0