LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040222\
Data File : VX027940.D
Acq On : 02 Apr 2022 17:51
Operator : JC/MD
Sample : N2249-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 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\82X032922W.M
Title : SW846 8260

Signal : TIC: VX027940.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	20	26	27	rBV	4725	5650	1.23%	0.189%
2	1.264	27	29	41	rVV3	14067	26529	5.79%	0.888%
3	1.374	43	47	51	rVV	21780	23663	5.16%	0.792%
4	1.752	104	109	116	rVB	22783	31277	6.82%	1.046%
5	1.959	139	143	149	rVB3	2693	4764	1.04%	0.159%
6	2.130	166	171	181	rVV4	3561	7430	1.62%	0.249%
7	2.337	199	205	219	rVB	8094	16990	3.71%	0.568%
8	2.782	271	278	288	rBV2	30774	70763	15.43%	2.367%
9	2.873	288	293	301	rVB3	7143	15842	3.45%	0.530%
10	3.105	322	331	341	rVB	20855	44909	9.79%	1.503%
11	3.843	444	452	459	rBV3	2524	6489	1.42%	0.217%
12	4.215	502	513	521	rBV2	5230	14661	3.20%	0.491%
13	4.306	521	528	540	rVB6	2526	7520	1.64%	0.252%
14	4.434	540	549	555	rBV7	2642	8470	1.85%	0.283%
15	5.391	694	706	717	rBV	55923	160614	35.03%	5.374%
16	5.556	723	733	742	rBV2	87957	255554	55.73%	8.550%
17	5.958	790	799	810	rBV	62732	162976	35.54%	5.453%
18	6.159	825	832	837	rBV7	2703	7550	1.65%	0.253%
19	6.251	838	847	858	rVB2	20599	64188	14.00%	2.148%
20	6.763	922	931	943	rBV	143446	339879	74.12%	11.371%
21	7.988	1123	1132	1141	rBV2	8442	16876	3.68%	0.565%
22	8.110	1145	1152	1163	rVB2	10046	20381	4.44%	0.682%
23	8.653	1230	1241	1249	rBV	288211	458526	100.00%	15.341%
24	10.055	1466	1471	1482	rVB	304286	411783	89.81%	13.777%
25	10.195	1490	1494	1499	rBV	5045	6384	1.39%	0.214%
26	10.305	1507	1512	1521	rVB	16463	23084	5.03%	0.772%
27	10.646	1563	1568	1573	rBV	4586	5945	1.30%	0.199%
28	11.085	1634	1640	1652	rVB	240821	316619	69.05%	10.593%
29	11.756	1746	1750	1755	rVB	6451	7522	1.64%	0.252%
30	12.024	1789	1794	1802	rBV	315122	378131	82.47%	12.651%
31	12.244	1823	1830	1837	rBV	37698	49018	10.69%	1.640%
32	12.701	1900	1905	1911	rVB	15283	18947	4.13%	0.634%

Sum of corrected areas: 2988934

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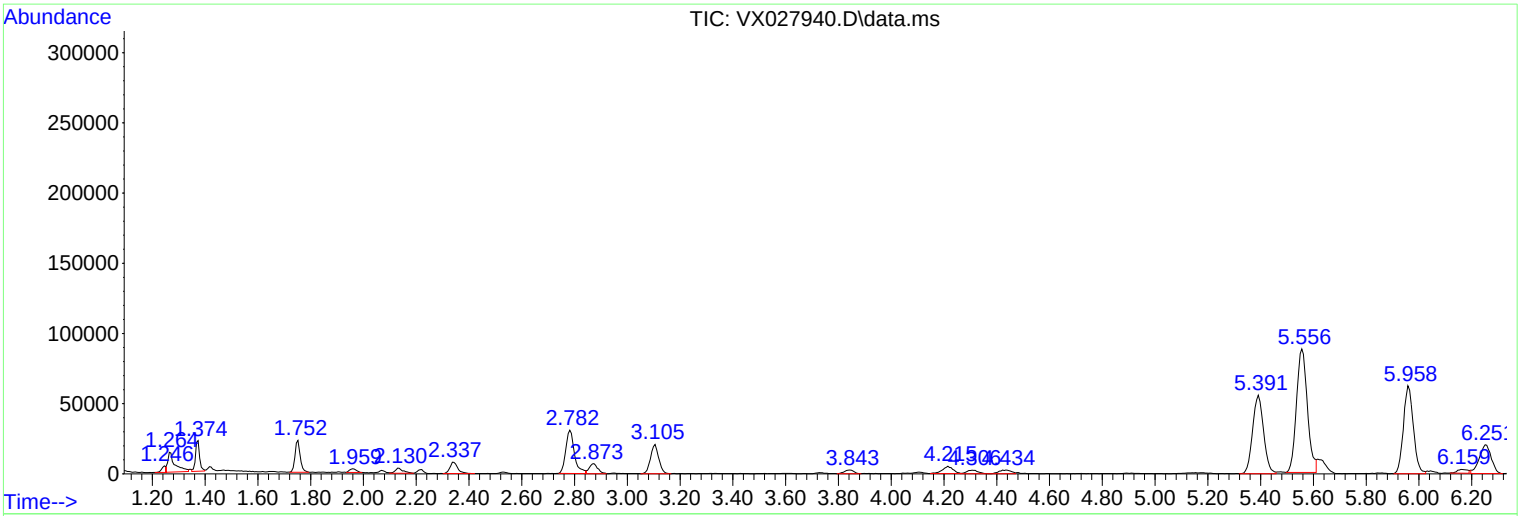
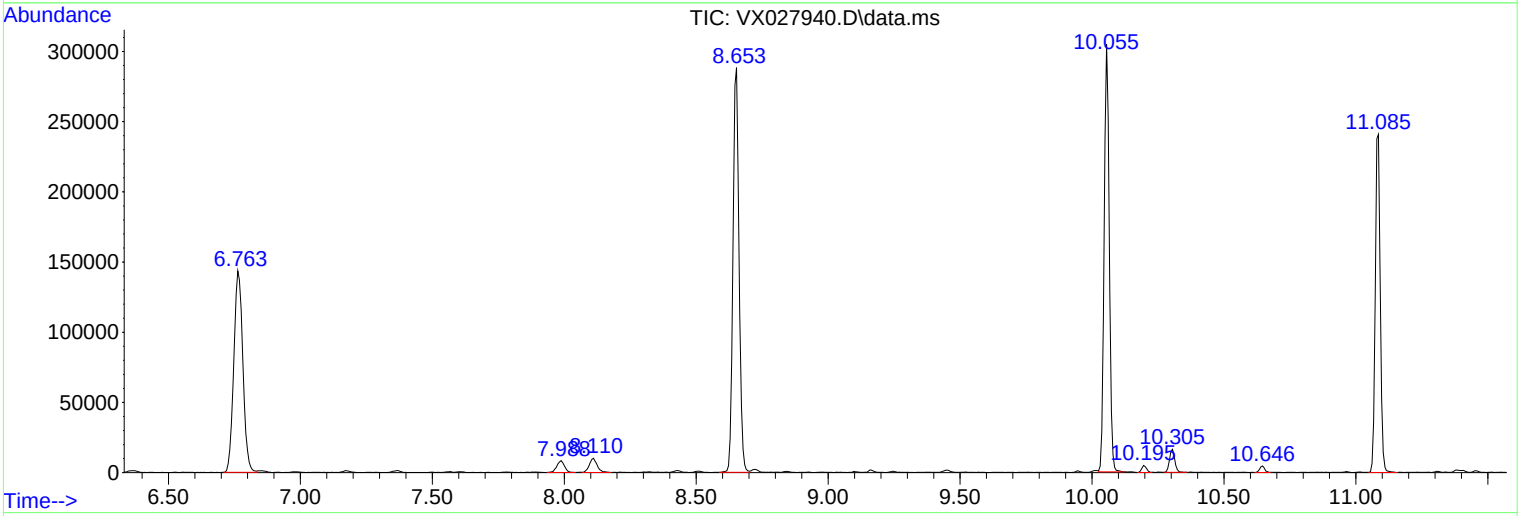
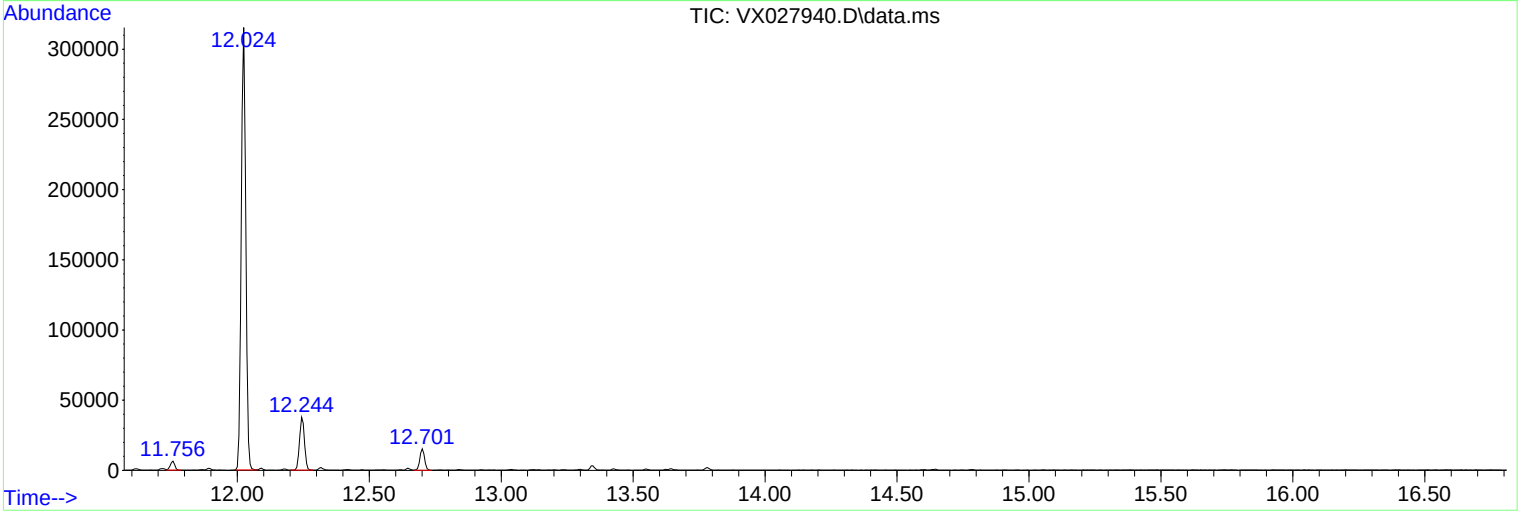
Instrument :
MSVOA_X
ClientSampleId :
MW-6S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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







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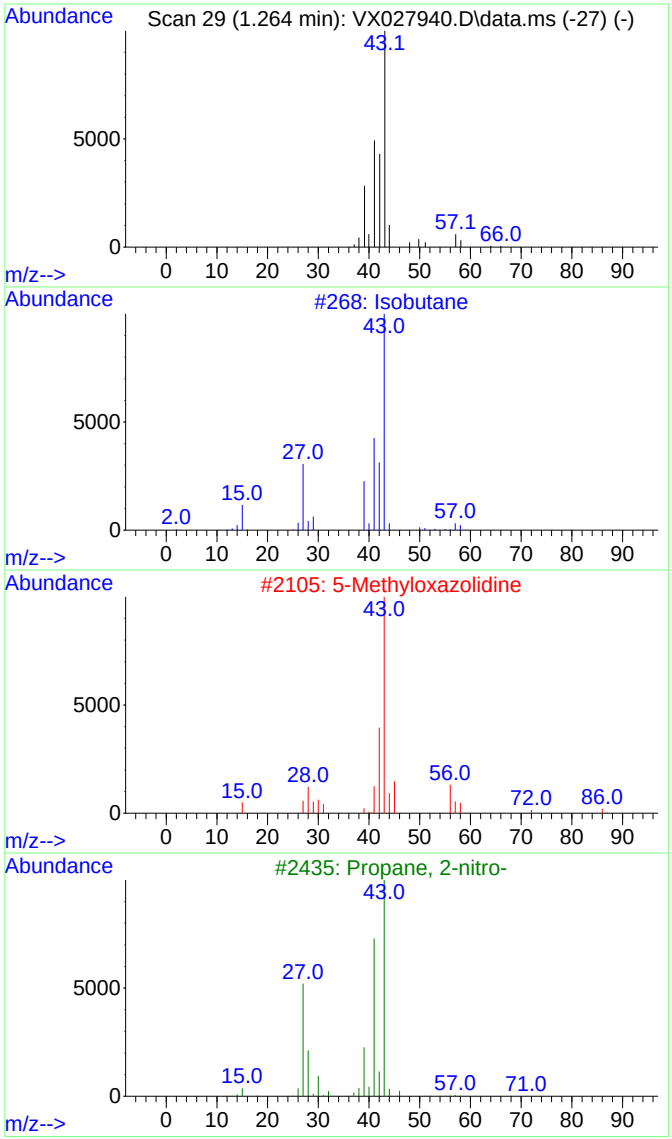
Quant Title : SW846 8260

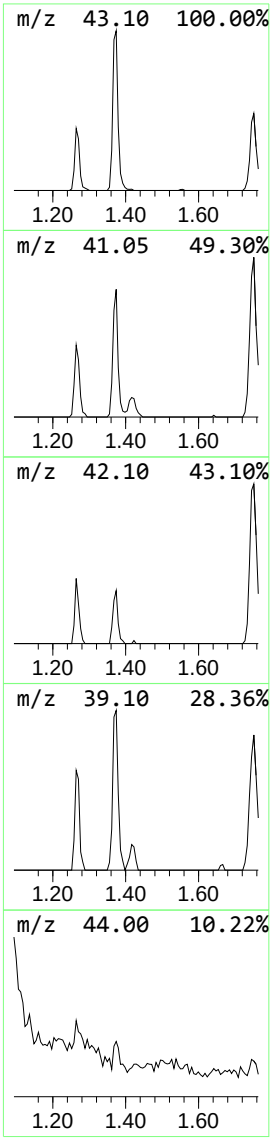
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown1.264 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.19 ug/l	26529	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	45
2	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	4





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Data File : VX027940.D
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Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

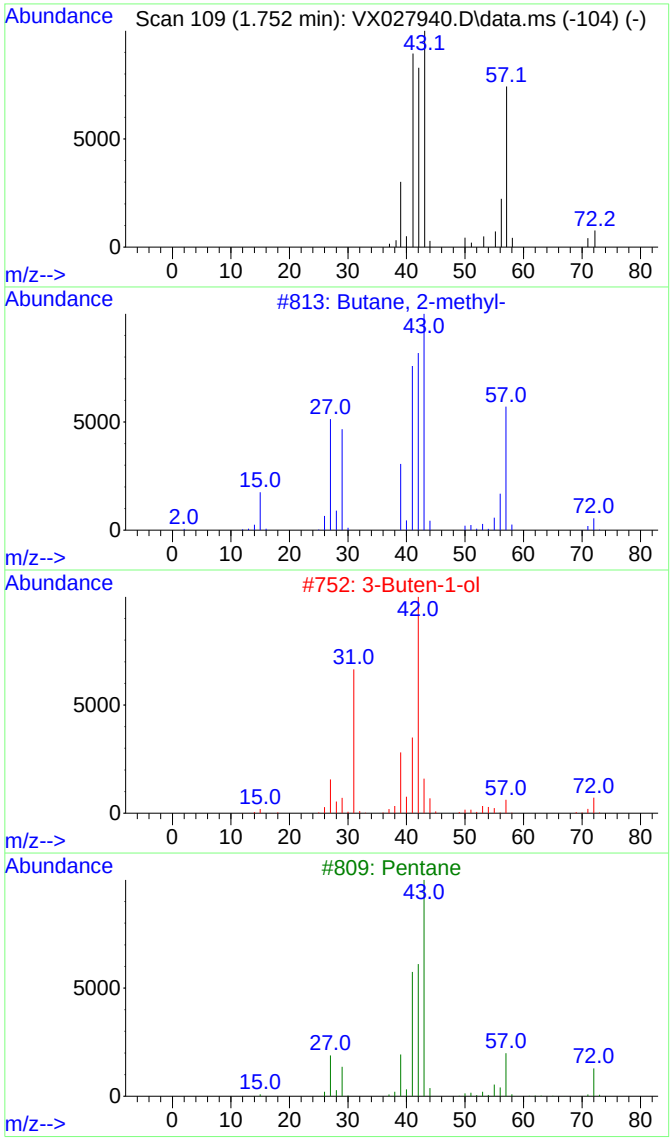
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

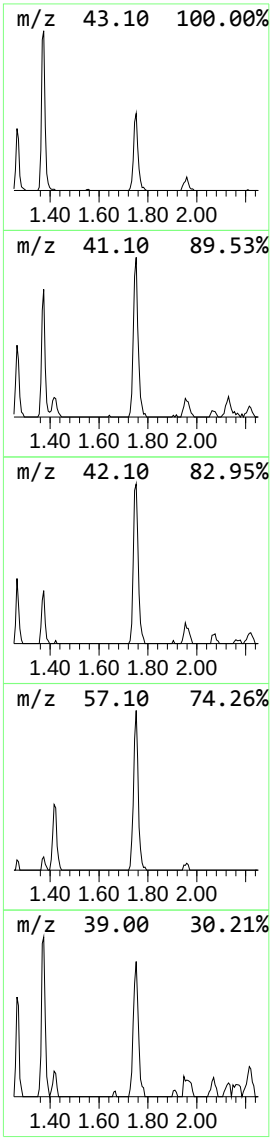
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	6.12 ug/l	31277	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	37
3	Pentane	72	C5H12	000109-66-0	33
4	3-Buten-2-ol	72	C4H8O	000598-32-3	9
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	9





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Sample : N2249-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

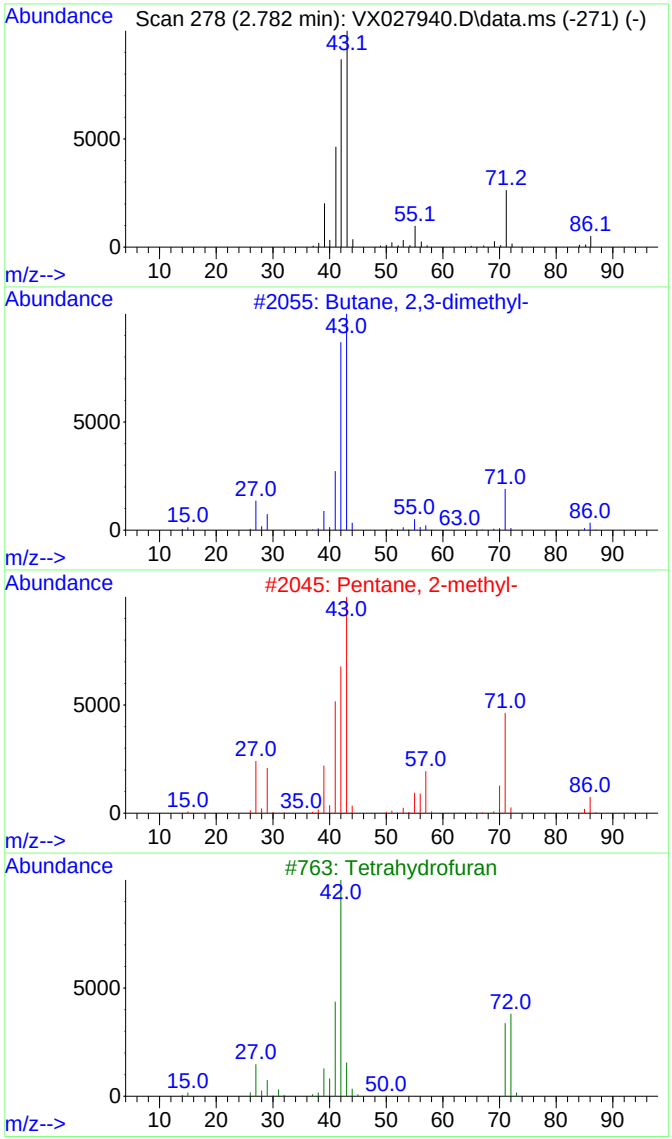
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

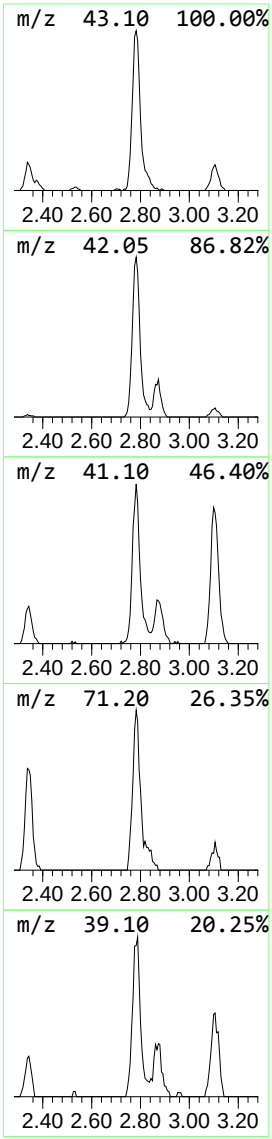
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	13.85 ug/l	70763	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12
5	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	10





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6S

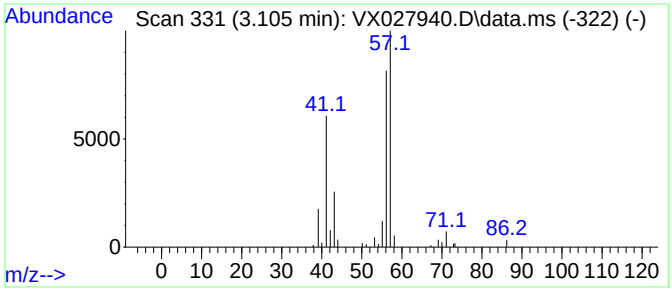
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

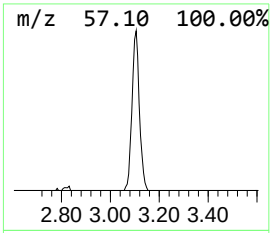
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

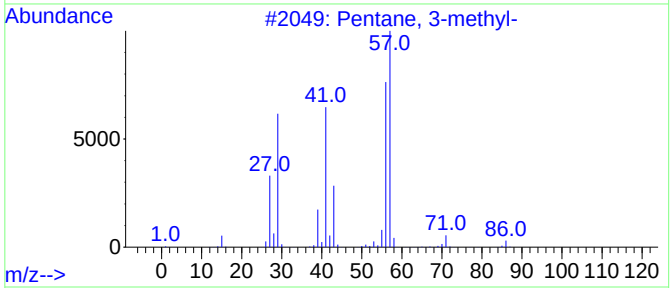
****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 3

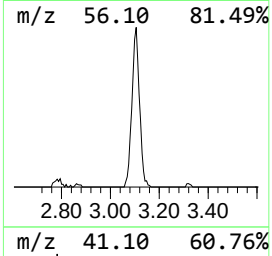
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	8.79 ug/l	44909	Pentafluorobenzene	5.556

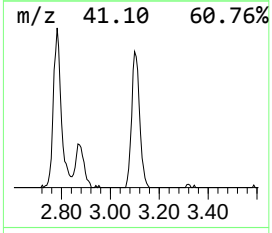
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	72
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	43
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42

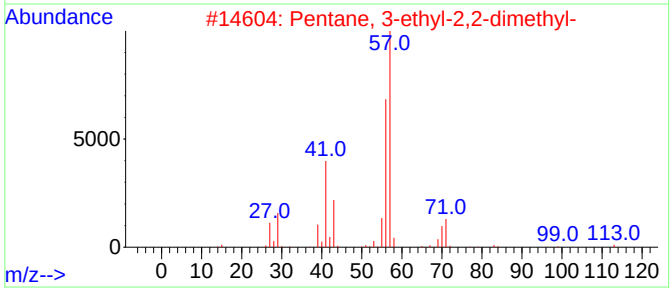


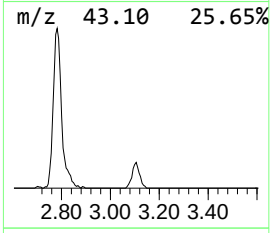


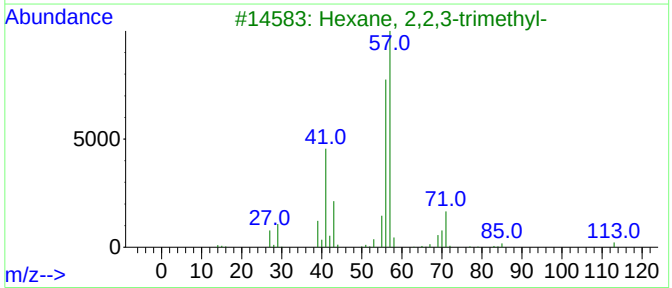


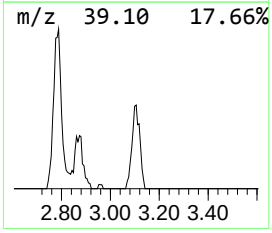












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ClientSampleId :
MW-6S

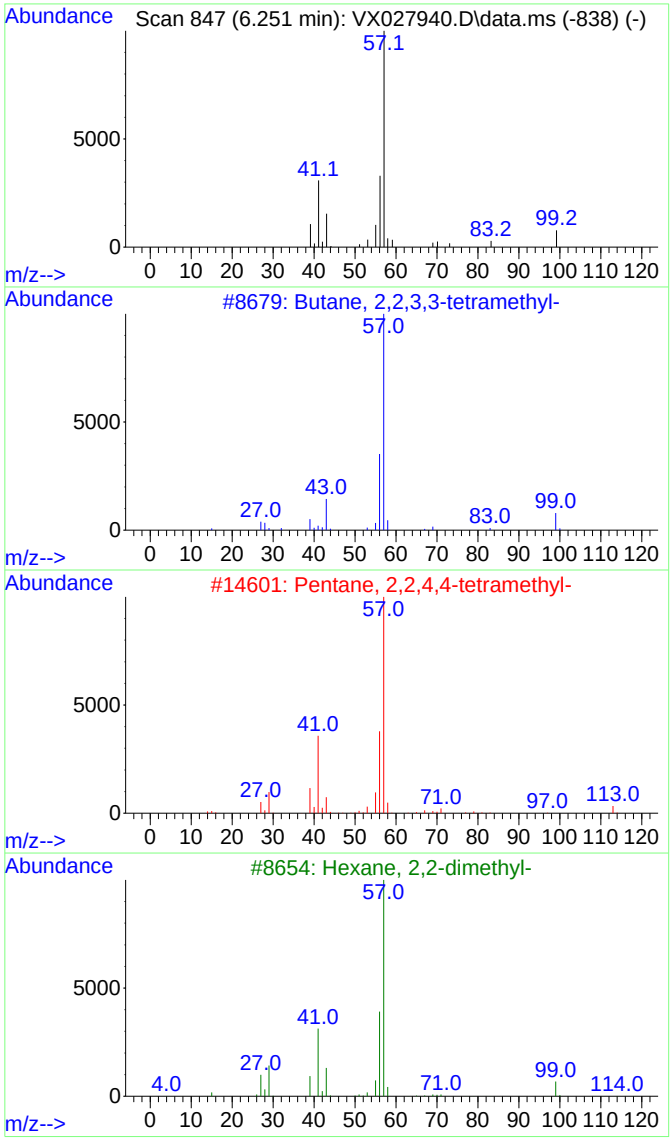
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

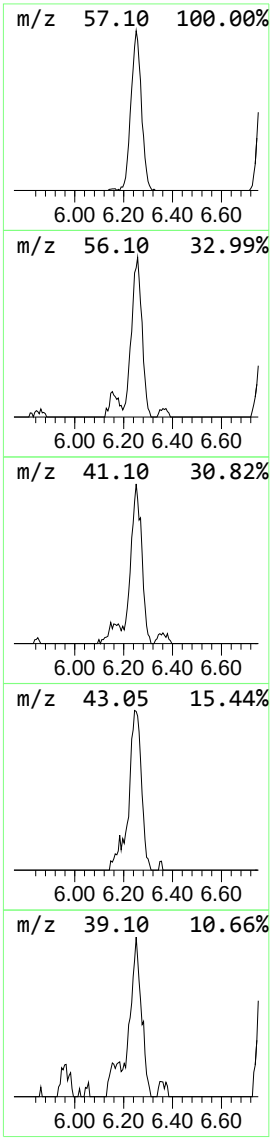
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	9.44 ug/l	64188	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	45
5	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	45





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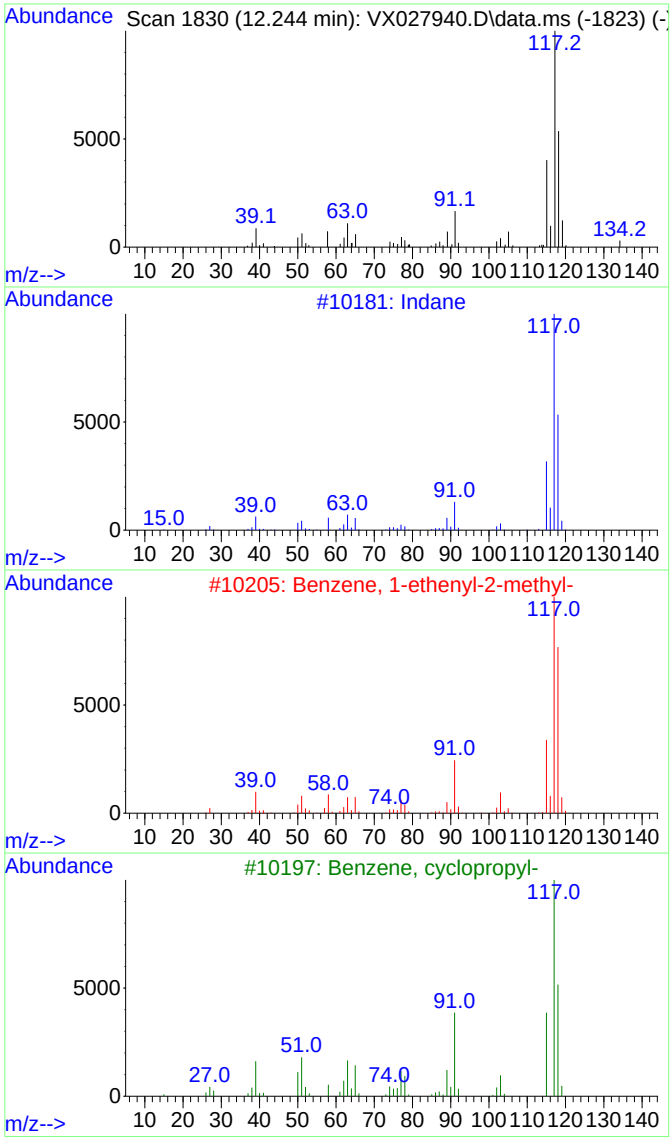
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

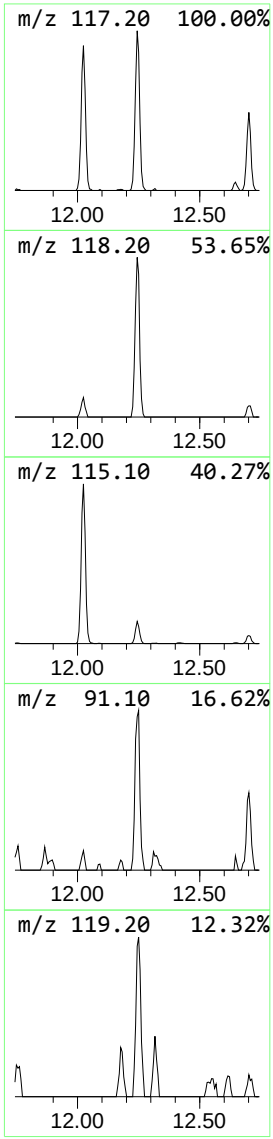
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	6.48 ug/l	49018	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	53





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	5.2	ug/l	26529	1	5.556	255554	50.0
Butane, 2-methyl-	1.752	6.1	ug/l	31277	1	5.556	255554	50.0
Butane, 2,3-dim...	2.782	13.9	ug/l	70763	1	5.556	255554	50.0
Pentane, 3-methyl-	3.105	8.8	ug/l	44909	1	5.556	255554	50.0
Butane, 2,2,3,3...	6.251	9.4	ug/l	64188	2	6.763	339879	50.0
Indane	12.244	6.5	ug/l	49018	4	12.024	378131	50.0