

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
 Data File : VX022542.D
 Acq On : 07 Jun 2021 18:27
 Operator : JC/MD
 Sample : M2583-22 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 54-57

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\82X060721W.M
 Title : SW846 8260

Signal : TIC: VX022542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.569	69	79	82	rVB5	4603	9076	2.17%	0.351%
2	2.386	208	213	218	rBV	7323	11619	2.78%	0.449%
3	2.550	232	240	250	rBV	8697	15118	3.62%	0.584%
4	4.580	565	573	581	rBV4	2545	7797	1.87%	0.301%
5	5.397	694	707	721	rBV2	43252	125644	30.08%	4.855%
6	5.556	724	733	745	rBV2	73084	202425	48.47%	7.822%
7	5.964	790	800	812	rBV2	55098	147366	35.28%	5.694%
8	6.769	922	932	946	rBV2	124987	298172	71.39%	11.521%
9	8.580	1224	1229	1234	rBV3	4051	6411	1.53%	0.248%
10	8.653	1234	1241	1249	rVV	262040	417661	100.00%	16.138%
11	8.720	1249	1252	1263	rVB3	3780	6508	1.56%	0.251%
12	10.055	1465	1471	1485	rVB	243746	347409	83.18%	13.424%
13	11.085	1634	1640	1653	rBV	189104	237109	56.77%	9.162%
14	11.360	1680	1685	1692	rBV	3965	5563	1.33%	0.215%
15	12.024	1789	1794	1803	rVB	224521	274387	65.70%	10.602%
16	12.103	1803	1807	1812	rBV2	15951	21503	5.15%	0.831%
17	12.219	1819	1826	1837	rBV2	10656	19816	4.74%	0.766%
18	12.768	1912	1916	1918	rBV4	3142	4635	1.11%	0.179%
19	12.792	1918	1920	1926	rVB3	3349	4697	1.12%	0.181%
20	12.859	1926	1931	1941	rBV	25057	45726	10.95%	1.767%
21	12.975	1945	1950	1953	rBV	9920	14641	3.51%	0.566%
22	13.073	1961	1966	1968	rBV3	10448	17336	4.15%	0.670%
23	13.103	1968	1971	1975	rVV	35256	59607	14.27%	2.303%
24	13.140	1975	1977	1988	rVV3	22380	45992	11.01%	1.777%
25	13.213	1988	1989	1996	rVB5	3060	4890	1.17%	0.189%
26	13.402	2018	2020	2022	rBV3	3552	4536	1.09%	0.175%
27	13.530	2031	2041	2043	rBV6	8433	20718	4.96%	0.801%
28	13.591	2048	2051	2054	rVV4	15061	24199	5.79%	0.935%
29	13.627	2054	2057	2063	rVV6	11687	27986	6.70%	1.081%
30	13.695	2064	2068	2071	rVV3	12637	23090	5.53%	0.892%
31	13.731	2071	2074	2084	rVV4	26883	63083	15.10%	2.437%
32	13.835	2087	2091	2093	rVV3	12758	22148	5.30%	0.856%
33	13.859	2093	2095	2098	rVV3	11279	17577	4.21%	0.679%
34	13.896	2098	2101	2113	rVB7	13371	33593	8.04%	1.298%

Sum of corrected areas: 2588038

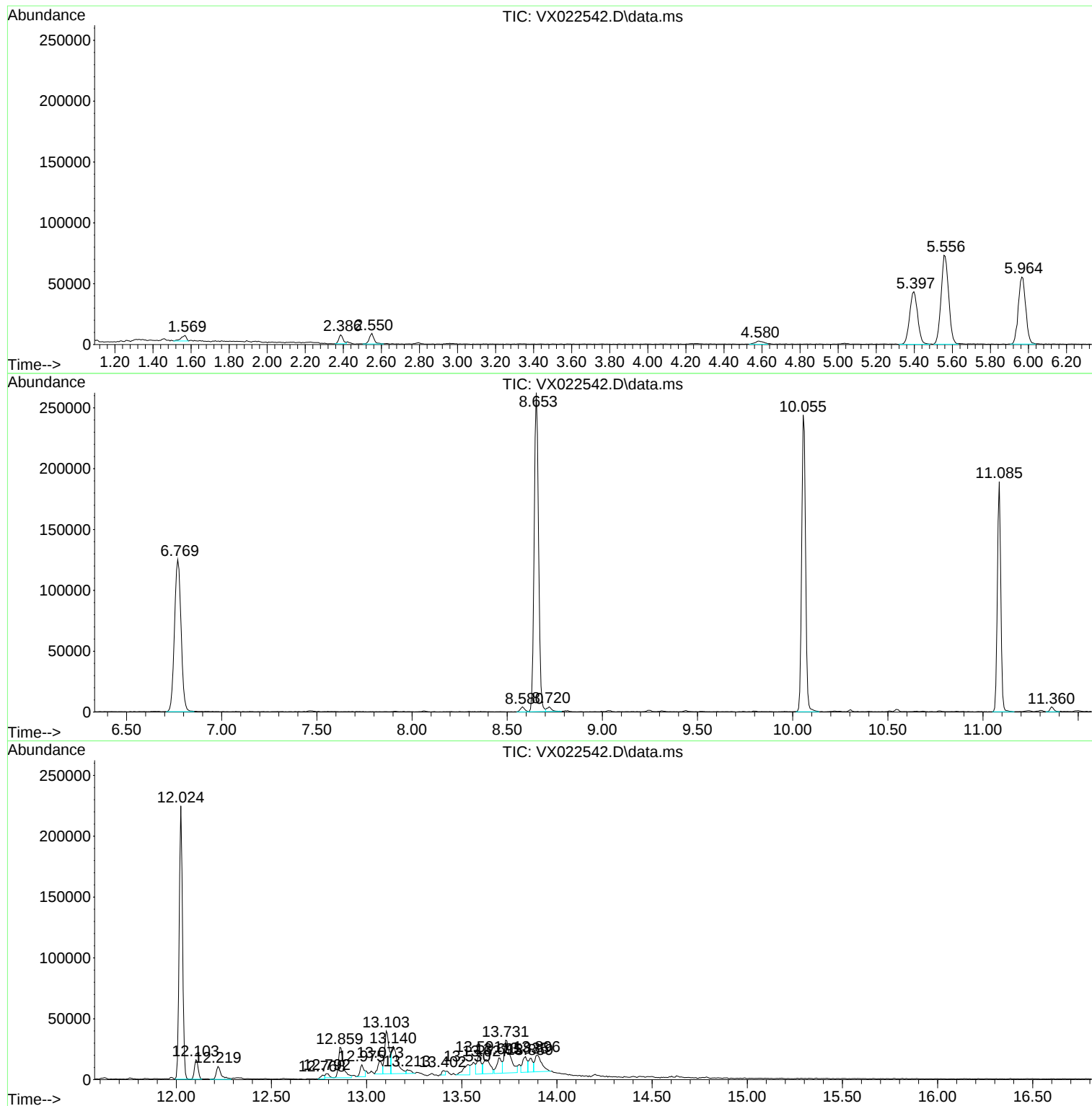
Instrument :
MSVOA_X
ClientSampleId :
54-57

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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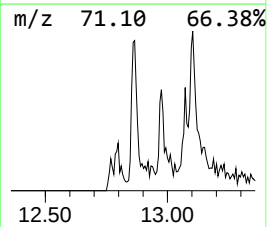
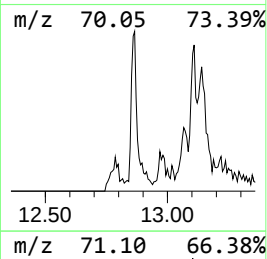
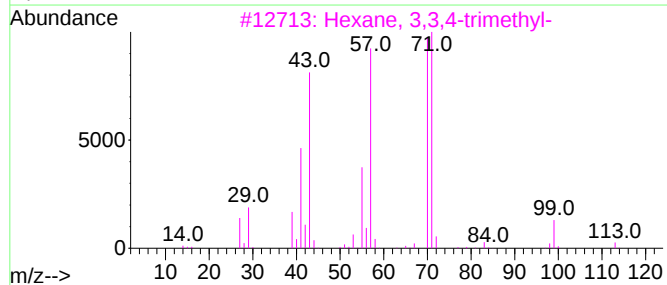
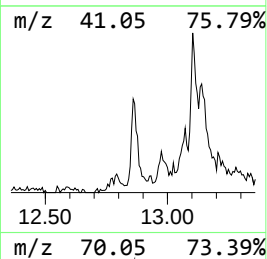
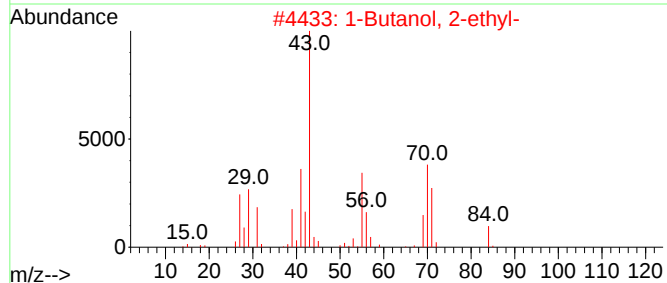
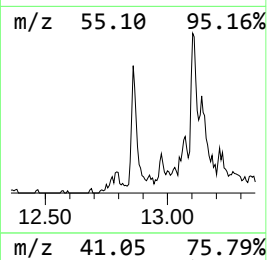
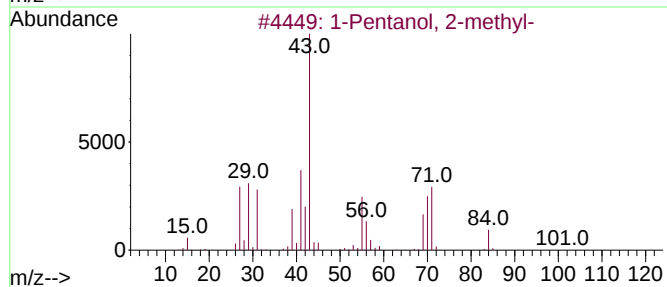
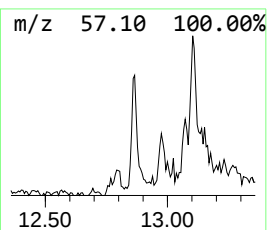
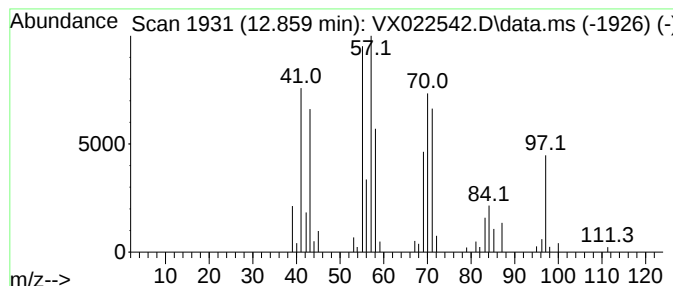
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown12.859 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	8.33 ug/l	45726	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	47
2		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47
3		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	38
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	38
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	35



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Instrument :
MSVOA_X
ClientSampled :
54-57

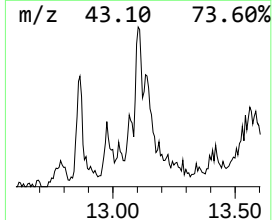
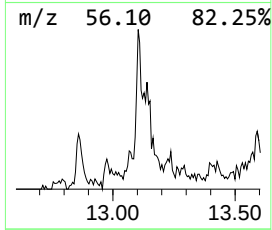
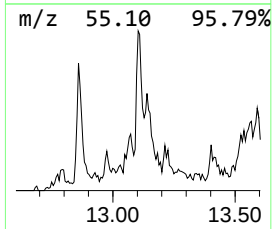
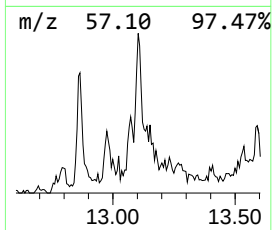
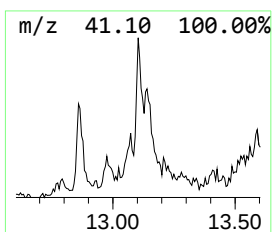
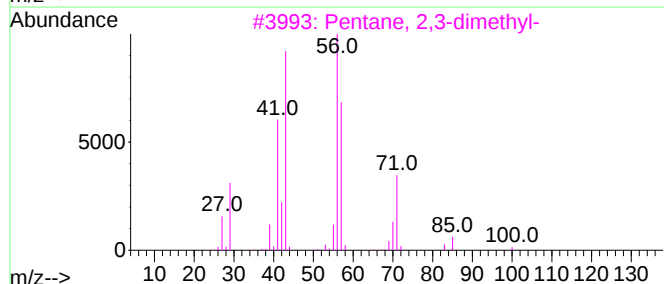
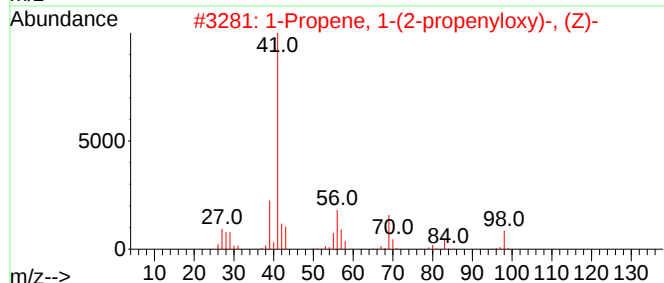
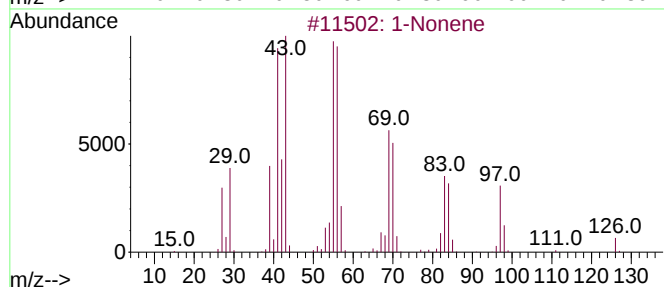
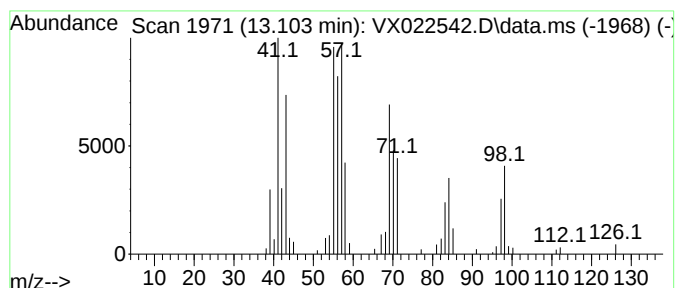
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Nonene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	10.86 ug/l	59607	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene		126	C9H18	000124-11-8	55
2	1-Propene, 1-(2-propenyloxy)-, (Z)-		98	C6H10O	061142-12-9	43
3	Pentane, 2,3-dimethyl-		100	C7H16	000565-59-3	38
4	Cycloheptane		98	C7H14	000291-64-5	38
5	Cyclobutane, 1,2-diethyl-		112	C8H16	061141-83-1	35



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Instrument :
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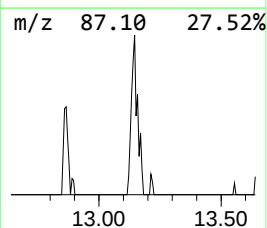
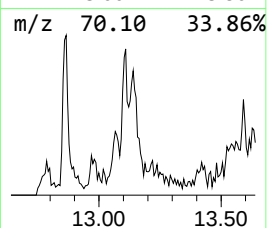
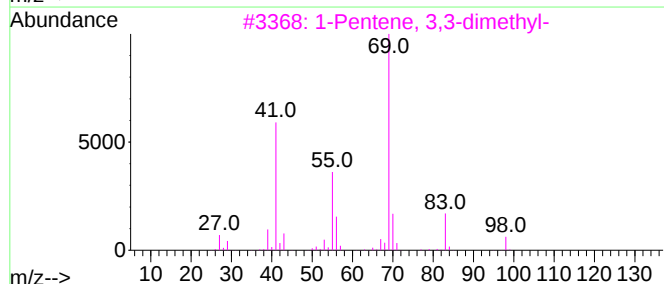
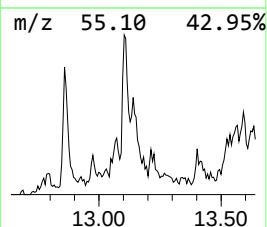
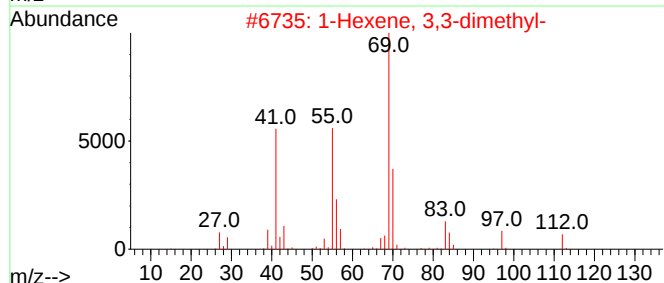
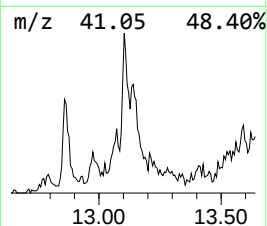
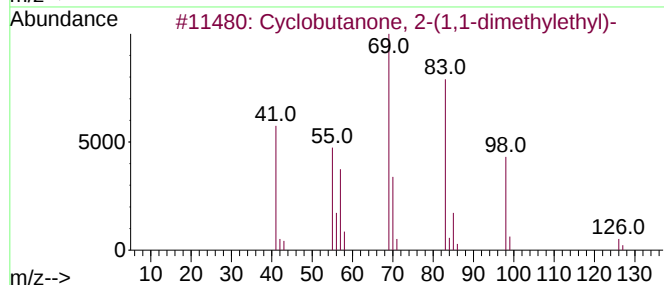
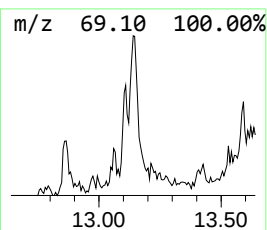
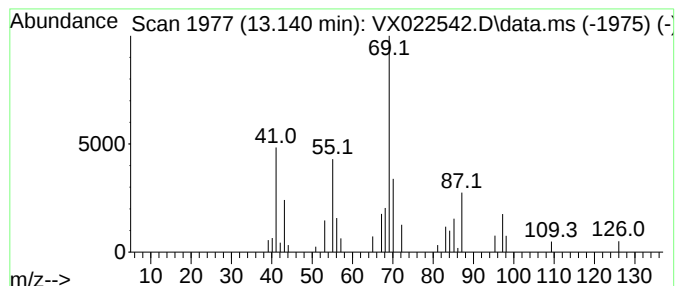
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclobutanone, 2-(1,1-dimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	8.38 ug/l	45992	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutanone, 2-(1,1-dimethylet...	126	C8H14O	004579-31-1	52
2			1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	50
3			1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	38
4			2-Hexene, 4-methyl-, (E)-	98	C7H14	003683-22-5	38
5			(Z)-4-Methyl-2-hexene	98	C7H14	003683-19-0	38



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Instrument :
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54-57

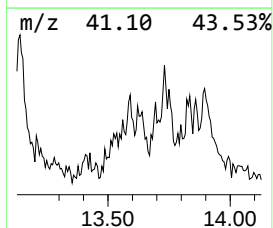
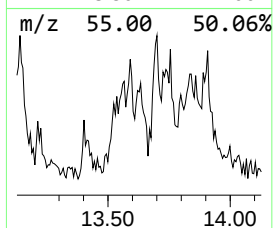
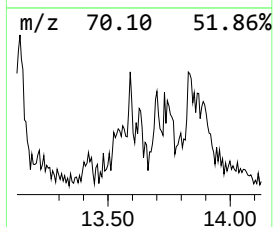
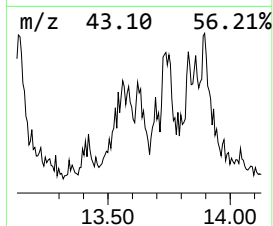
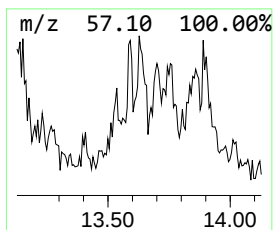
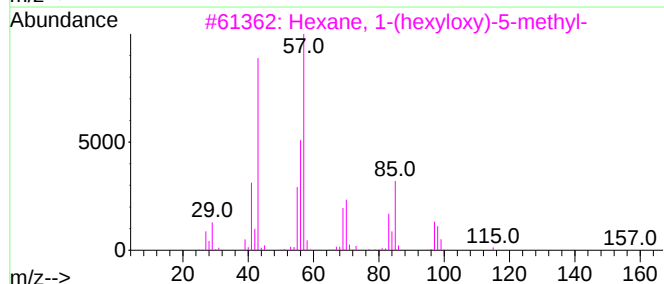
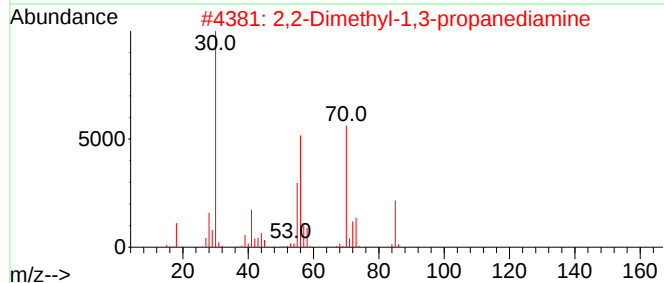
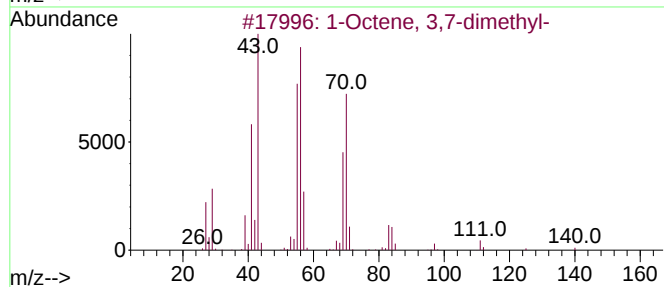
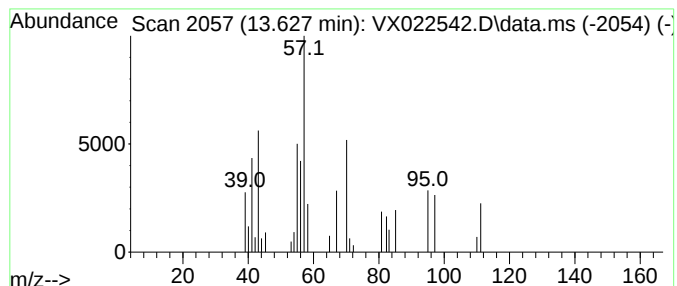
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.628 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.628	5.10 ug/l	27986	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octene, 3,7-dimethyl-	140	C10H20	004984-01-4	27
2			2,2-Dimethyl-1,3-propanediamine	102	C5H14N2	007328-91-8	17
3			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	16
4			2-Methylpyrrolidine	85	C5H11N	000765-38-8	12
5			1-Hexanol, 5-methyl-	116	C7H16O	000627-98-5	12



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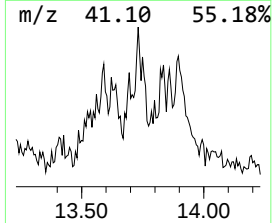
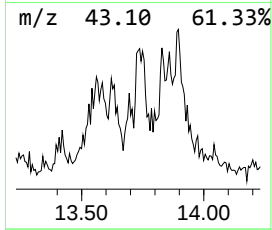
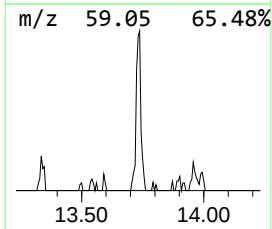
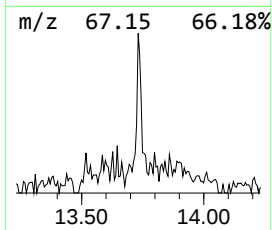
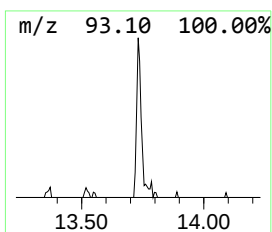
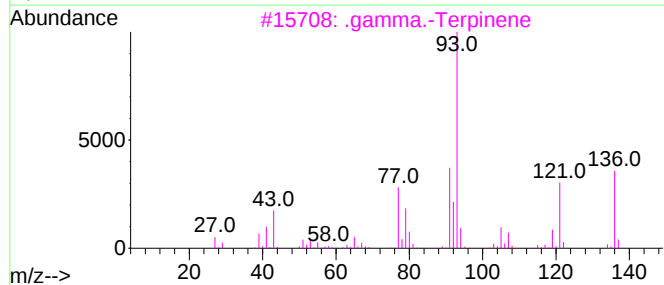
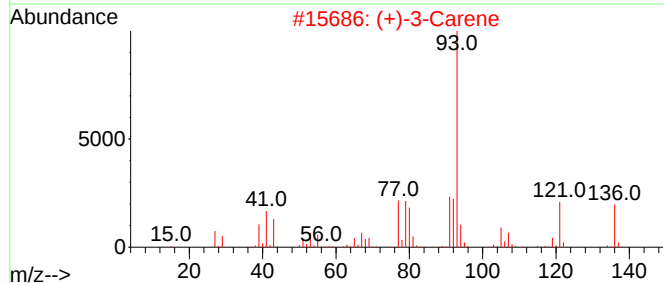
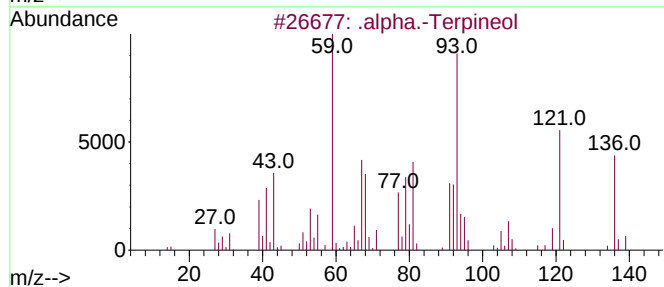
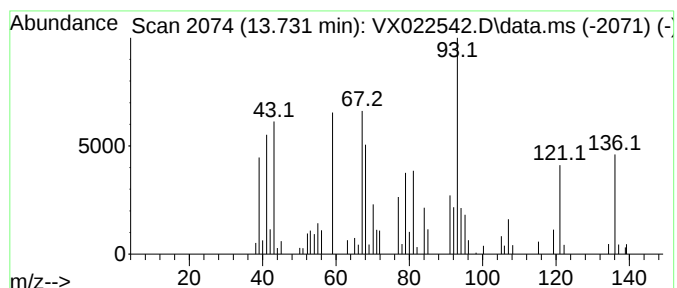
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.731 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.731	11.50 ug/l	63083	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	alpha.-	Terpineol	154	C10H18O	000098-55-5	47
2	(+)-	3-Carene		136	C10H16	000498-15-7	43
3	.	gamma.-	Terpinene	136	C10H16	000099-85-4	43
4	3-	Carene		136	C10H16	013466-78-9	43
5	.	alpha.-	Phellandrene	136	C10H16	000099-83-2	38



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54-57

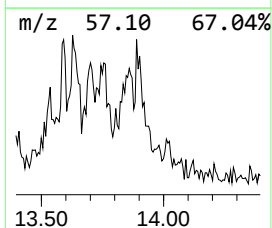
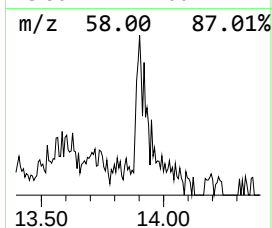
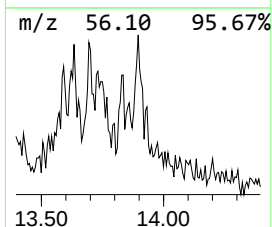
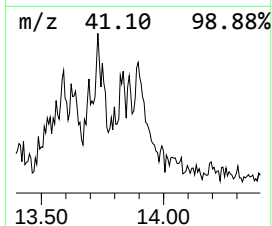
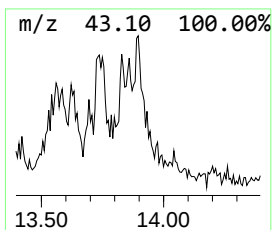
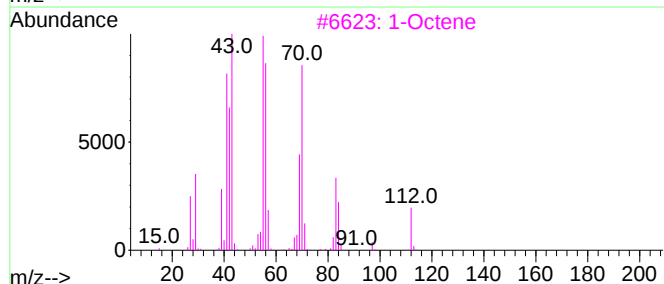
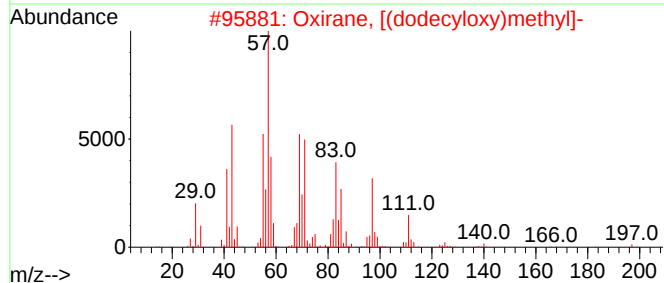
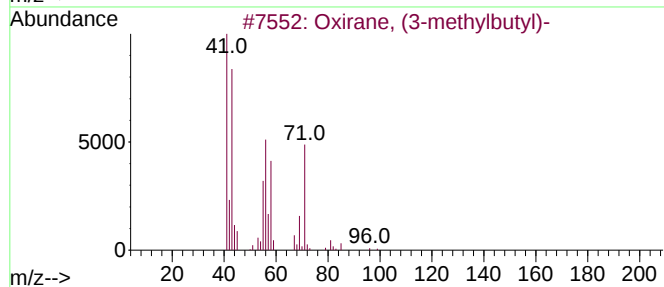
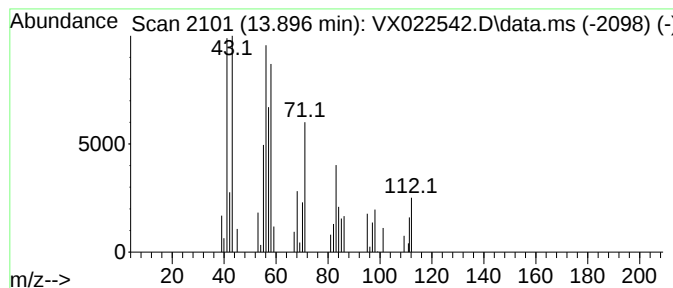
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.896 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	6.12 ug/l	33593	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, (3-methylbutyl)-	114	C7H14O	053229-41-7	46
2		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	32
3		1-Octene	112	C8H16	000111-66-0	27
4		1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	27
5		1-Nonanol	144	C9H20O	000143-08-8	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060721\
Data File : VX022542.D
Acq On : 07 Jun 2021 18:27
Operator : JC/MD
Sample : M2583-22 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
54-57

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.859	12.859	8.3	ug/l	45726	4	12.024	274387	50.0
1-Nonene	13.103	10.9	ug/l	59607	4	12.024	274387	50.0
Cyclobutanone, ...	13.140	8.4	ug/l	45992	4	12.024	274387	50.0
unknown13.628	13.628	5.1	ug/l	27986	4	12.024	274387	50.0
unknown13.731	13.731	11.5	ug/l	63083	4	12.024	274387	50.0
unknown13.896	13.896	6.1	ug/l	33593	4	12.024	274387	50.0