

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
 Data File : VX017538.D
 Acq On : 24 Jul 2020 13:28
 Operator : JC/SP
 Sample : L3362-05 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1754

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X072320W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.776	108	113	121	rVB	239299	327064	1.10%	0.355%
2	1.989	143	148	156	rVB3	178552	347317	1.17%	0.377%
3	2.093	159	165	174	rBV	875934	1496777	5.02%	1.626%
4	2.251	186	191	200	rVB	292941	450630	1.51%	0.490%
5	2.422	212	219	233	rVB	2386537	4037897	13.55%	4.387%
6	3.166	329	341	352	rBV4	184180	495106	1.66%	0.538%
7	3.922	457	465	478	rBV	274038	704540	2.36%	0.765%
8	4.373	530	539	551	rVB2	190529	529945	1.78%	0.576%
9	5.470	709	719	726	rBV	313349	866498	2.91%	0.941%
10	5.556	726	733	735	rVV3	124320	311715	1.05%	0.339%
11	5.629	738	745	766	rVB	478428	1485914	4.99%	1.614%
12	5.903	779	790	801	rBV3	110035	308303	1.03%	0.335%
13	6.037	803	812	817	rBV	314629	811004	2.72%	0.881%
14	6.116	817	825	837	rVB	2176966	5543688	18.61%	6.023%
15	6.830	933	942	953	rBV	728857	1768005	5.93%	1.921%
16	7.439	1028	1042	1051	rBV2	178538	431754	1.45%	0.469%
17	8.695	1242	1248	1254	rBV	1609705	2415228	8.11%	2.624%
18	8.768	1254	1260	1274	rVB	19346078	29793274	100.00%	32.368%
19	10.097	1472	1478	1487	rVB	1780481	2398650	8.05%	2.606%
20	10.238	1494	1501	1510	rBV	2474982	3303717	11.09%	3.589%
21	10.341	1510	1518	1525	rBV	7693030	10090769	33.87%	10.963%
22	10.683	1568	1574	1585	rVB	4084568	5093825	17.10%	5.534%
23	11.122	1640	1646	1652	rBV	1658482	2048525	6.88%	2.226%
24	11.347	1677	1683	1687	rBV	349503	454591	1.53%	0.494%
25	11.420	1689	1695	1702	rVV	1528281	2639125	8.86%	2.867%
26	11.487	1702	1706	1717	rVB	640062	852390	2.86%	0.926%
27	11.652	1728	1733	1740	rBV	728662	856058	2.87%	0.930%
28	11.792	1747	1756	1762	rBV	2982690	3512017	11.79%	3.816%
29	12.060	1795	1800	1806	rBV	2147236	2669377	8.96%	2.900%
30	12.128	1806	1811	1815	rBV	916277	1057081	3.55%	1.148%
31	12.280	1828	1836	1844	rBV3	783375	1405835	4.72%	1.527%
32	12.359	1844	1849	1855	rVB3	315646	492223	1.65%	0.535%
33	12.652	1893	1897	1900	rBV	295973	339244	1.14%	0.369%
34	12.737	1907	1911	1919	rBV2	233369	348191	1.17%	0.378%

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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

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35	12.999	1951	1954	1961	rVB	262620	312741	1.05%	0.340%
36	13.335	2004	2009	2014	rVB2	466475	585819	1.97%	0.636%
37	13.816	2081	2088	2095	rVB	795664	980460	3.29%	1.065%
38	14.676	2221	2229	2234	rBV	360356	479730	1.61%	0.521%

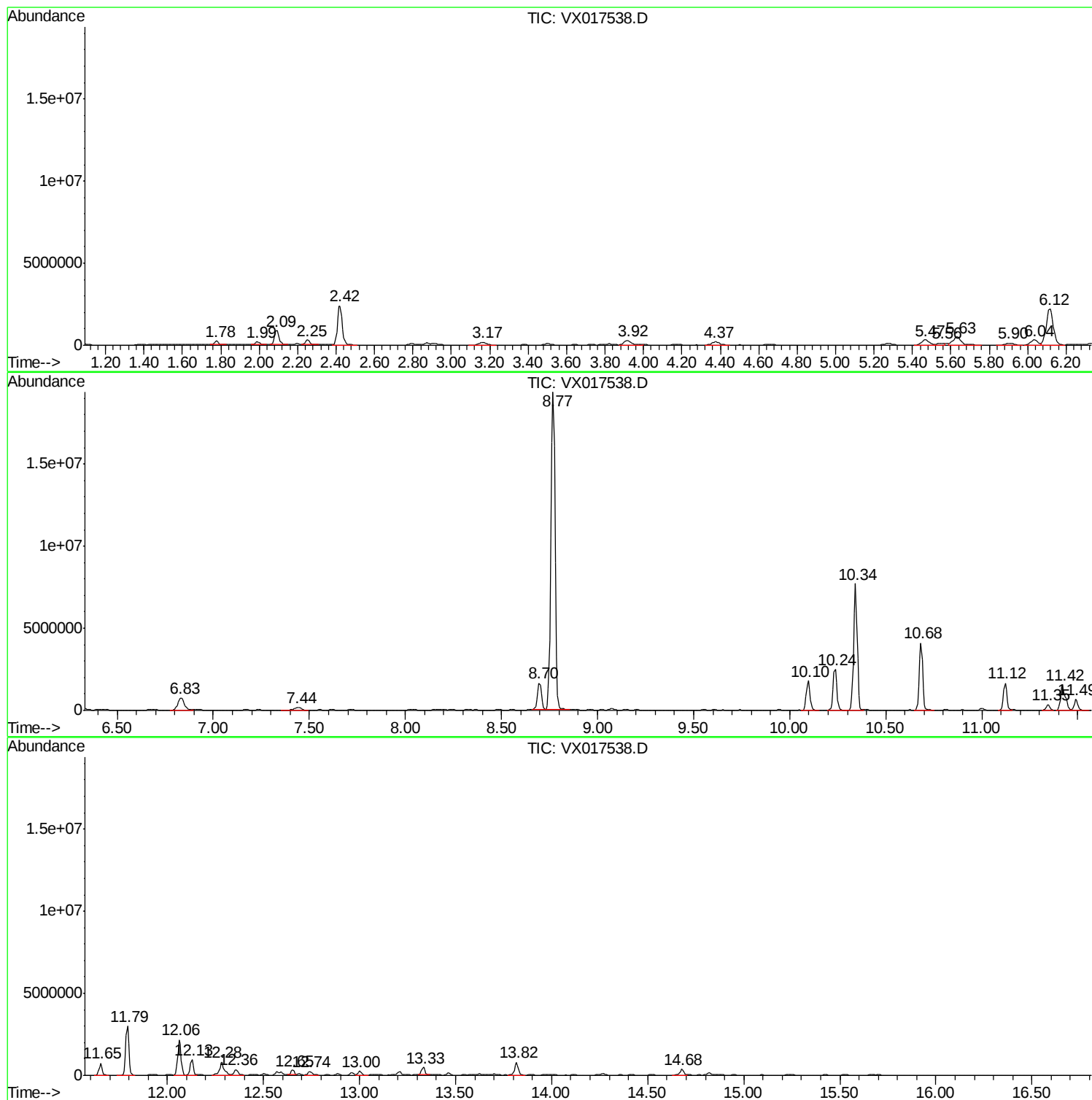
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Quant Title : SW846 8260

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



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1754

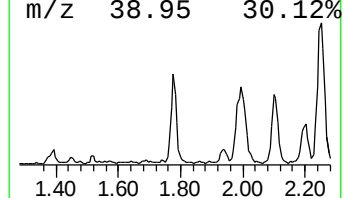
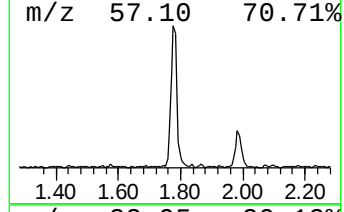
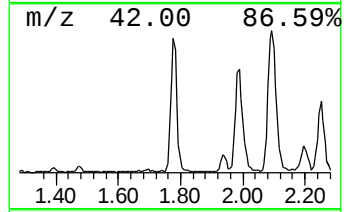
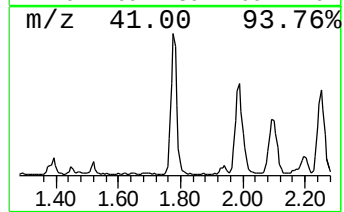
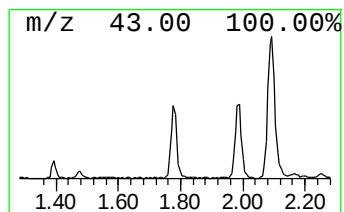
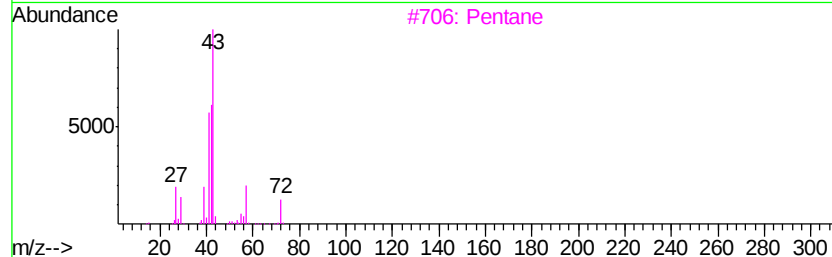
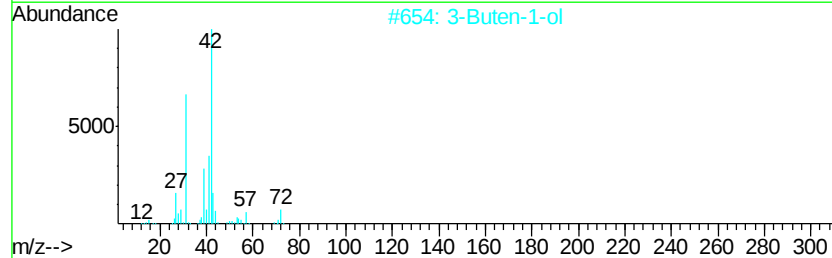
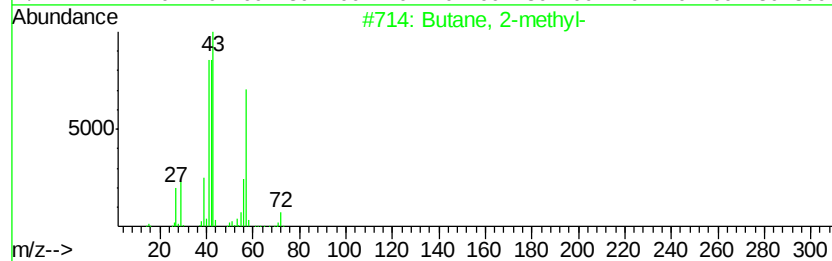
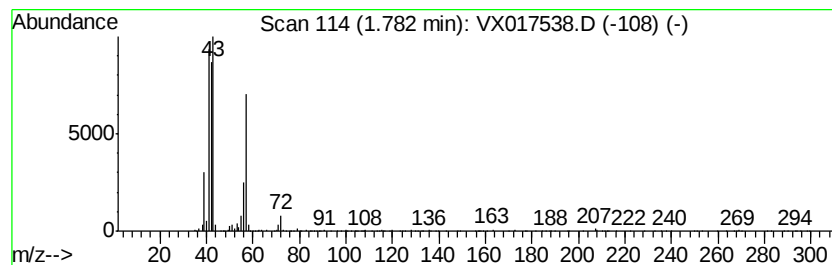
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X072320W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	11.01 ug/l	327064	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		3-Buten-1-ol	72	C4H8O	000627-27-0	43
3		Pentane	72	C5H12	000109-66-0	33
4		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5		1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	9



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Instrument :
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ClientSampleId :
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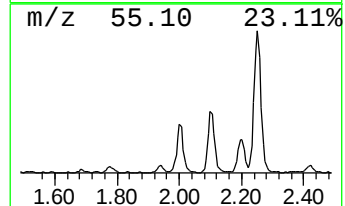
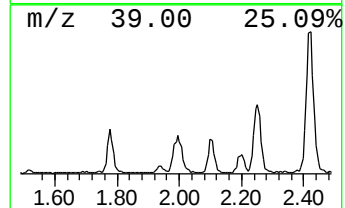
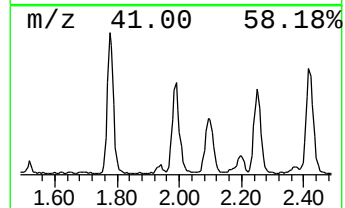
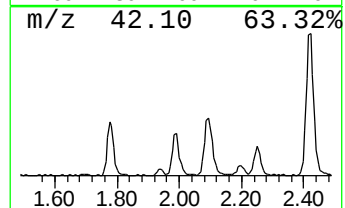
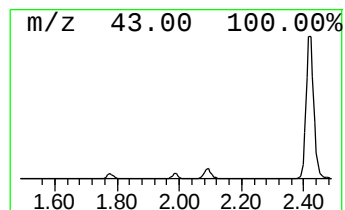
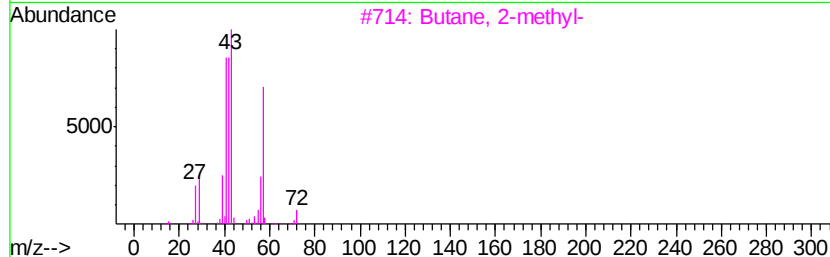
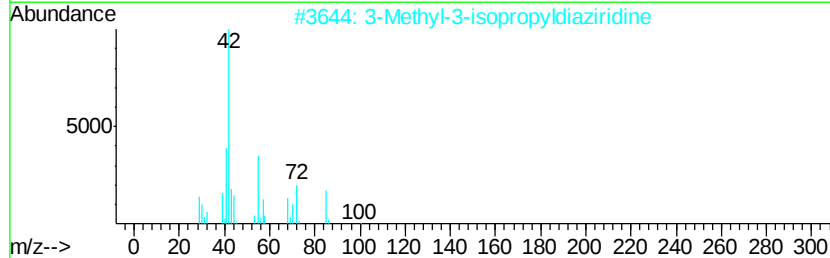
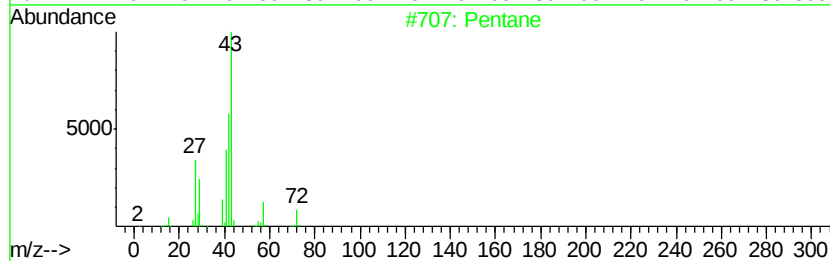
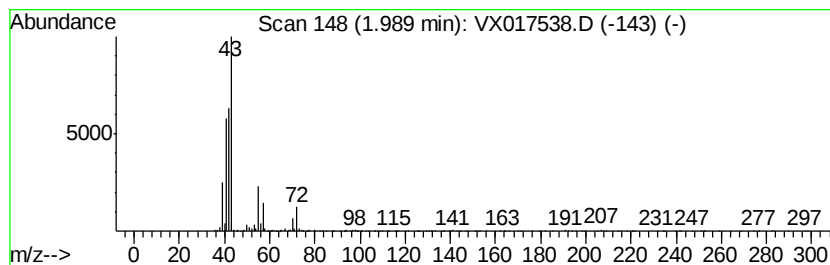
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	11.69 ug/l	347317	Pentafluorobenzene	5.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	80
2	3-Methyl-3-isopropyldiaziridine		100	C5H12N2	024476-95-7	53
3	Butane, 2-methyl-		72	C5H12	000078-78-4	50
4	1-Butanol		74	C4H10O	000071-36-3	36
5	1-Pentene		70	C5H10	000109-67-1	12



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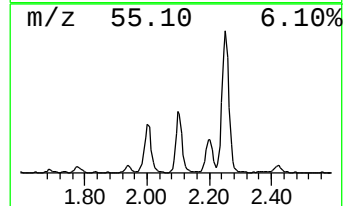
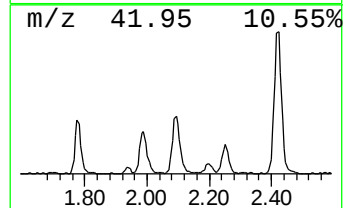
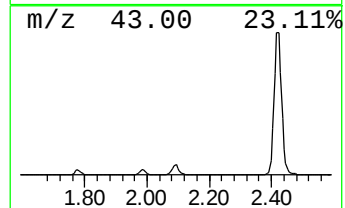
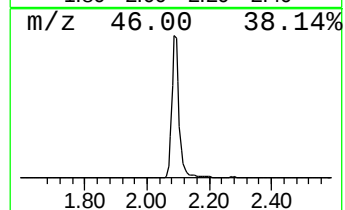
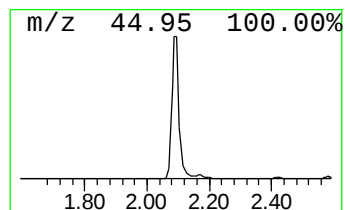
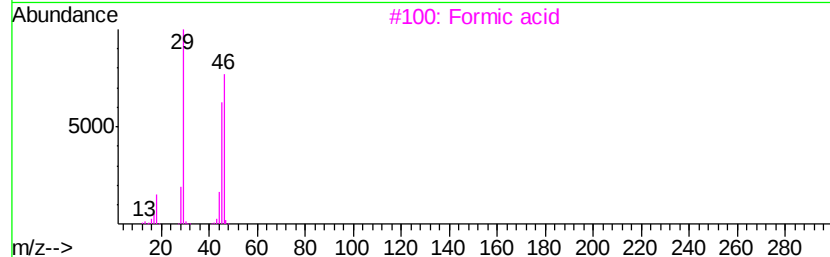
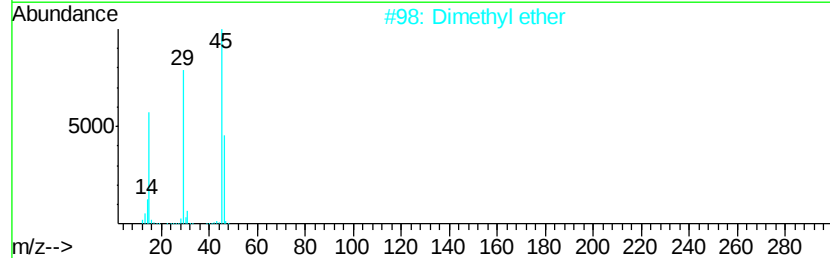
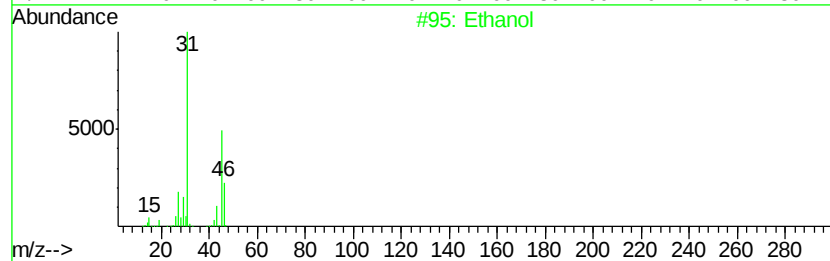
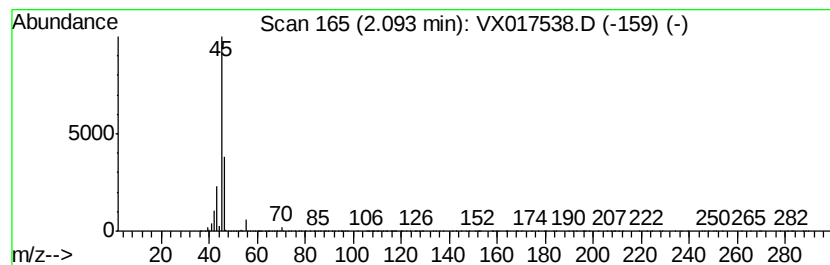
Instrument :
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Quant Title : SW846 8260

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

Peak Number 3 unknown2.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	50.37 ug/l	1496780	Pentafluorobenzene	5.63
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ethanol	46 C2H6O	000064-17-5	43
2	Dimethyl ether	46 C2H6O	000115-10-6	9
3	Formic acid	46 CH2O2	000064-18-6	4
4	Methane, nitroso-	45 CH3NO	000865-40-7	3
5	4-Penten-2-ol	86 C5H10O	000625-31-0	2



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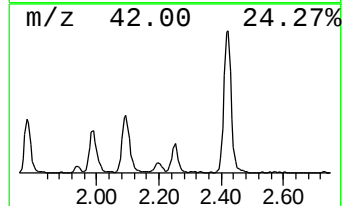
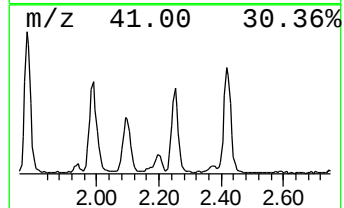
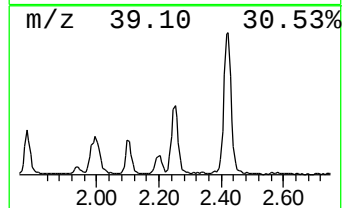
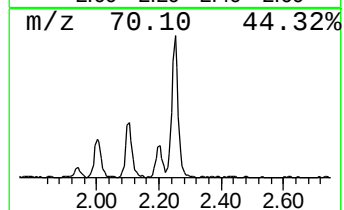
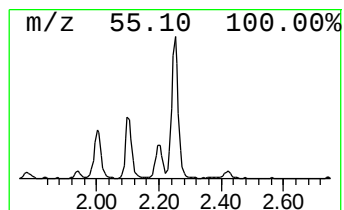
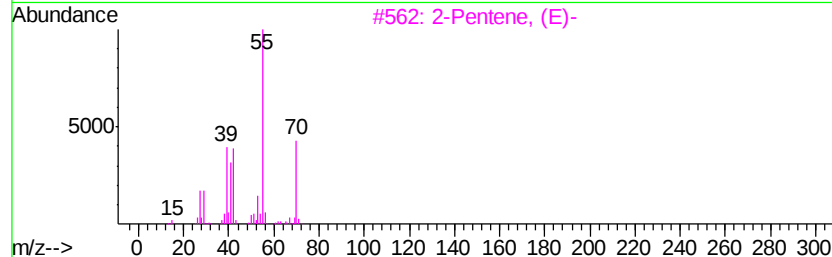
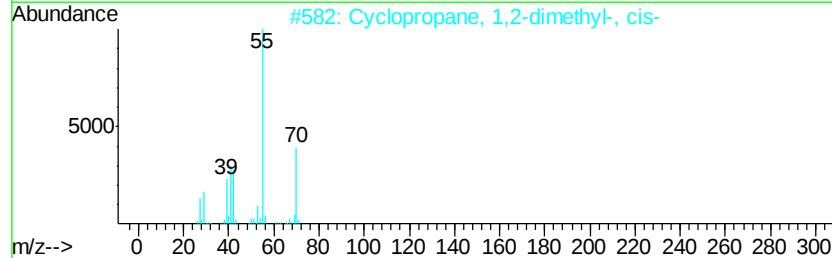
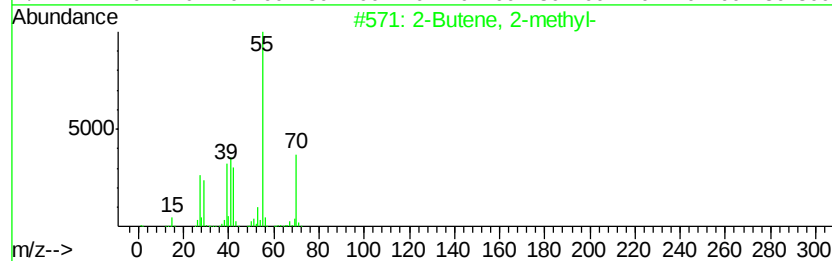
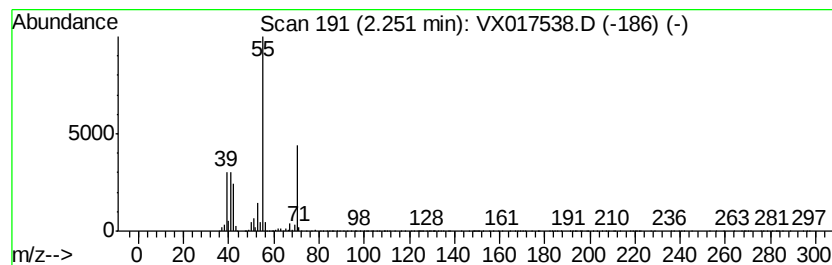
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Butene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	15.16 ug/l	450630	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
2		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3		2-Pentene, (E)-	70	C5H10	000646-04-8	87
4		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86
5		1-Butene, 3-methyl-	70	C5H10	000563-45-1	86



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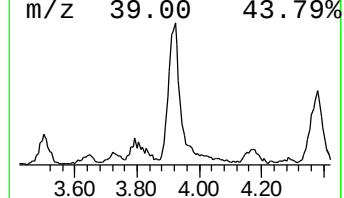
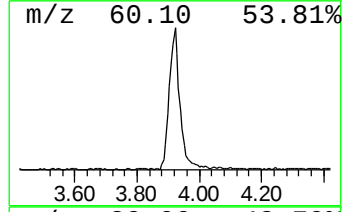
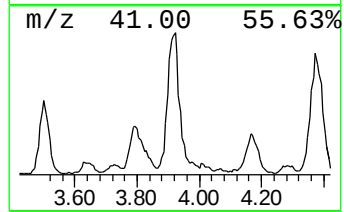
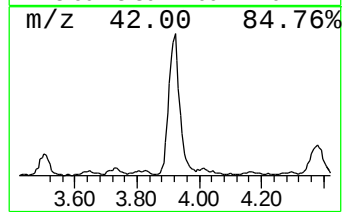
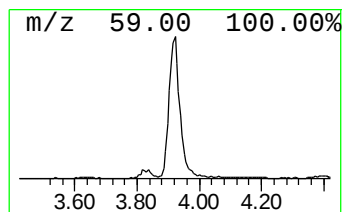
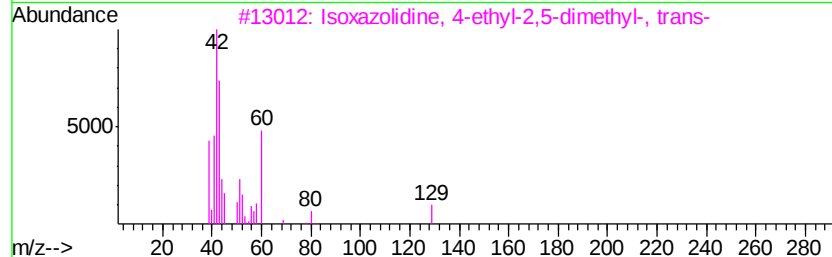
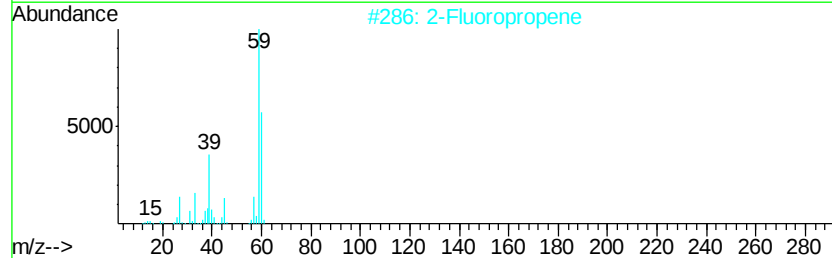
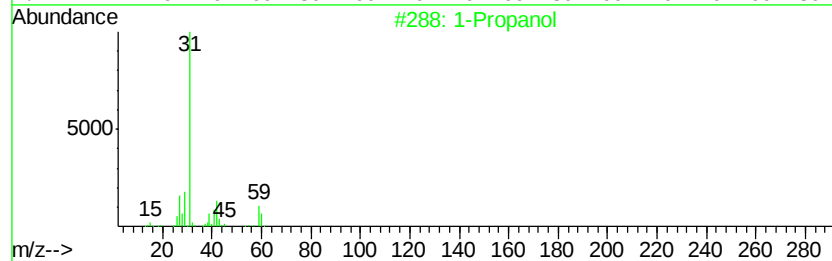
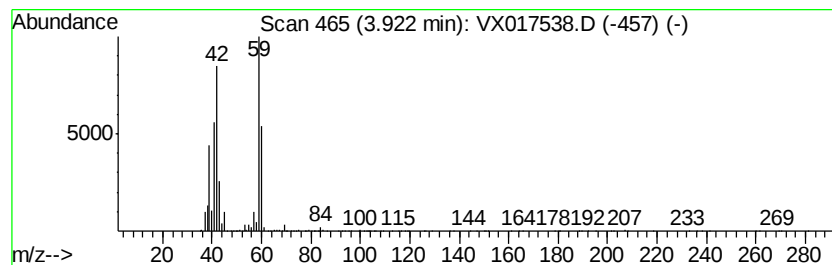
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	23.71 ug/l	704540	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	58
2		2-Fluoropropene	60	C3H5F	001184-60-7	38
3		Isoxazolidine, 4-ethyl-2,5-dimet...	129	C7H15NO	056728-13-3	33
4		Cyclopropane	42	C3H6	000075-19-4	32
5		3-Buten-1-ol	72	C4H8O	000627-27-0	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
Data File : VX017538.D
Acq On : 24 Jul 2020 13:28
Operator : JC/SP
Sample : L3362-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1754

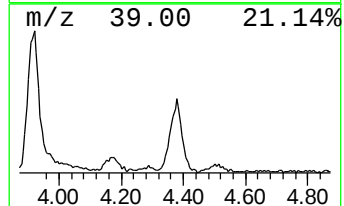
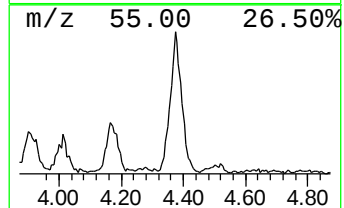
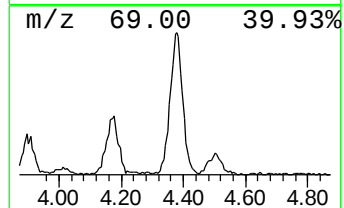
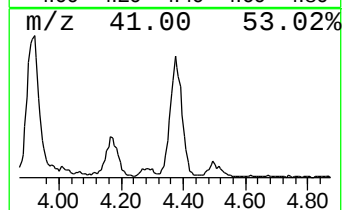
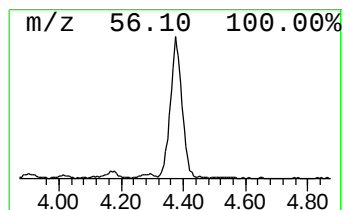
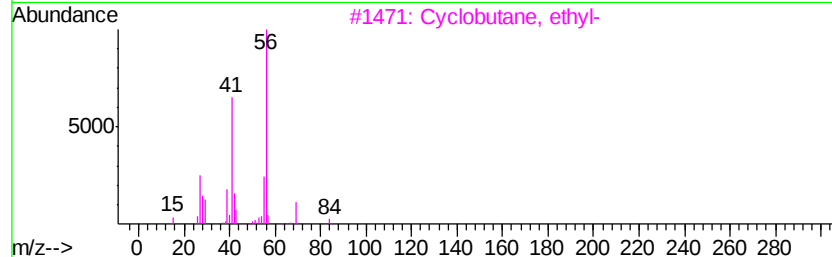
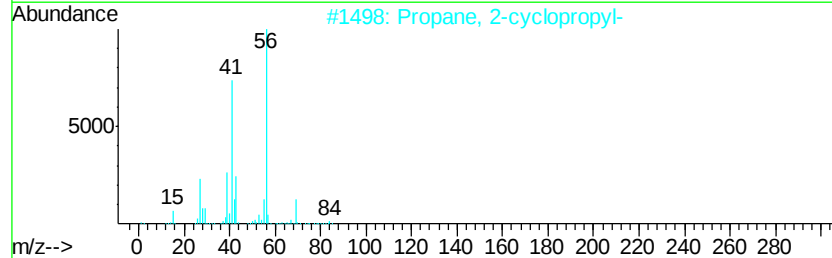
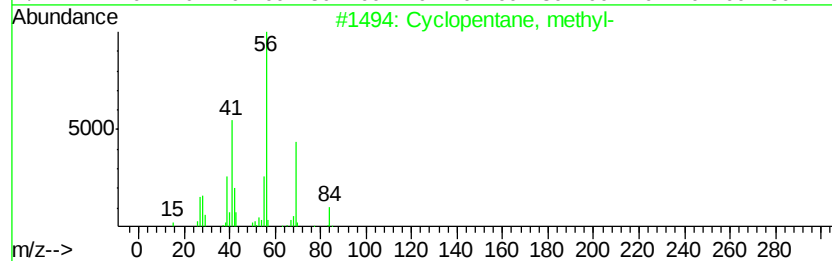
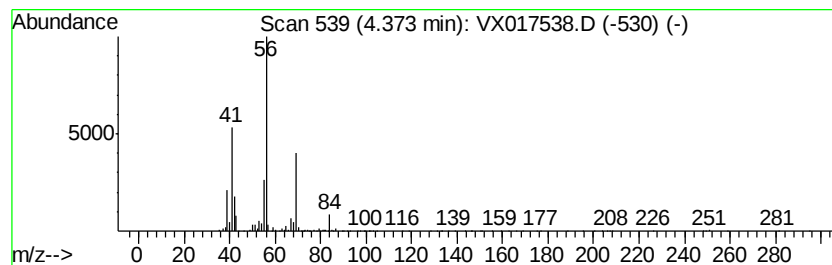
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	17.83 ug/l	529945	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
5		Cyclohexane	84	C6H12	000110-82-7	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
Data File : VX017538.D
Acq On : 24 Jul 2020 13:28
Operator : JC/SP
Sample : L3362-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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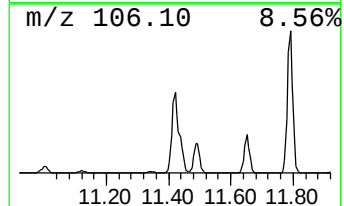
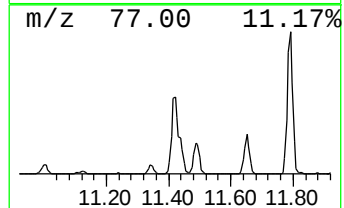
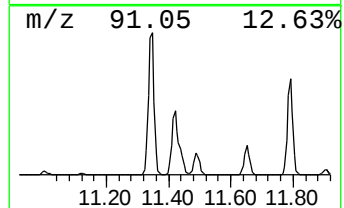
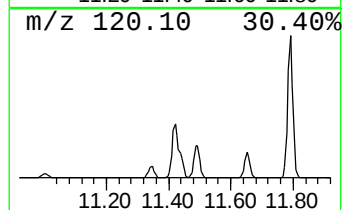
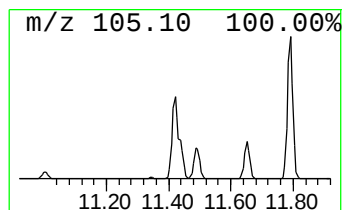
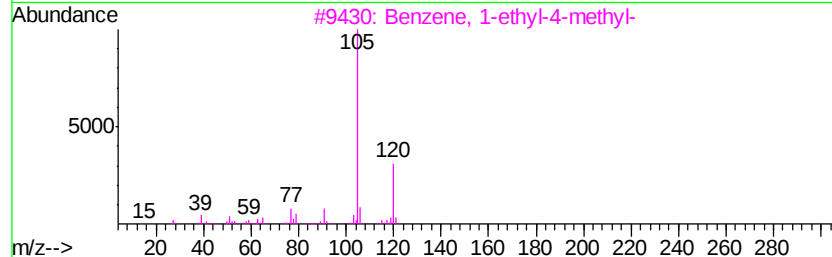
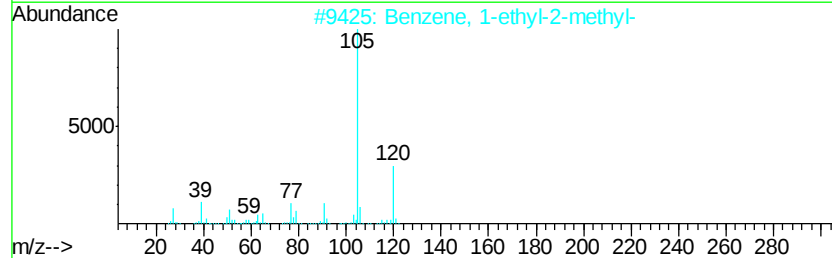
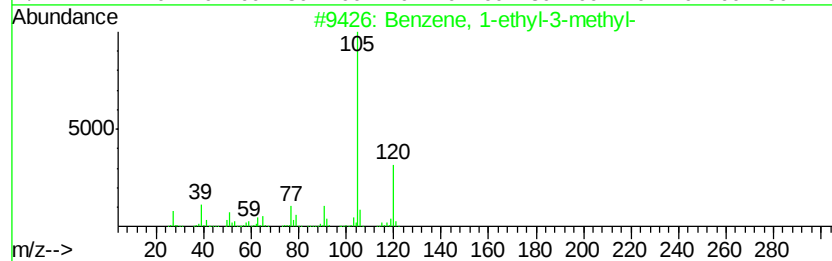
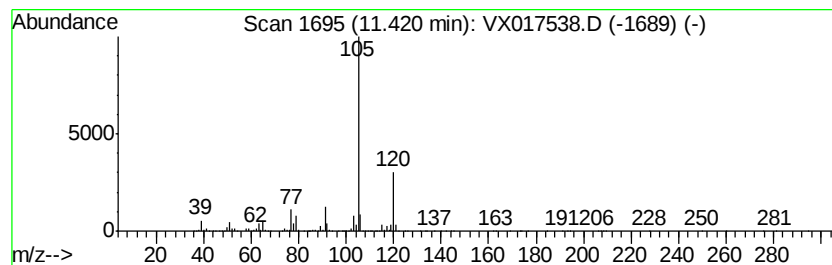
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	49.43 ug/l	2639130	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
Data File : VX017538.D
Acq On : 24 Jul 2020 13:28
Operator : JC/SP
Sample : L3362-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1754

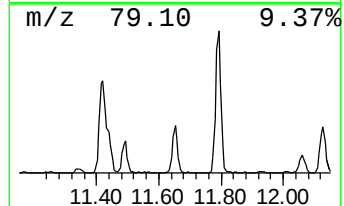
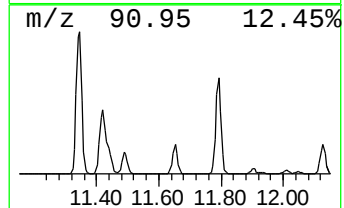
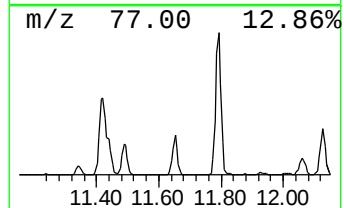
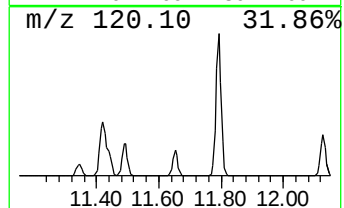
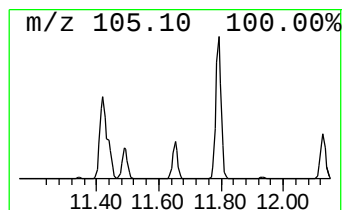
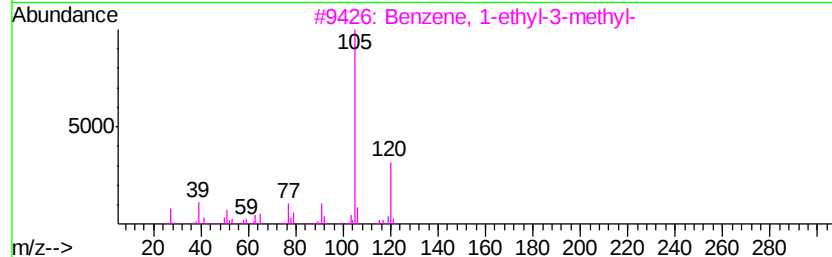
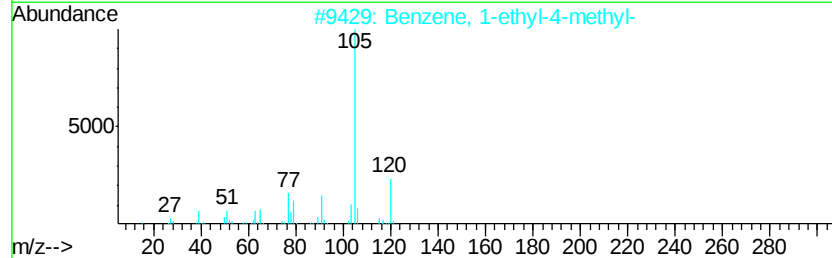
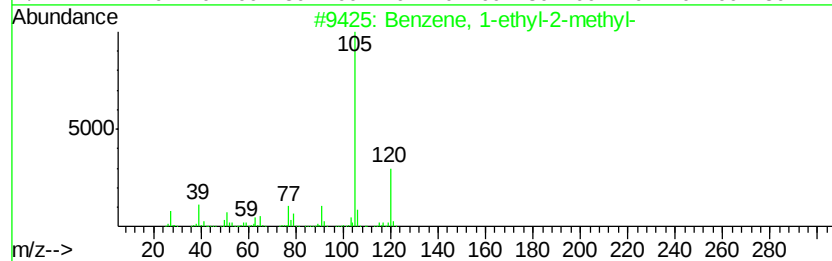
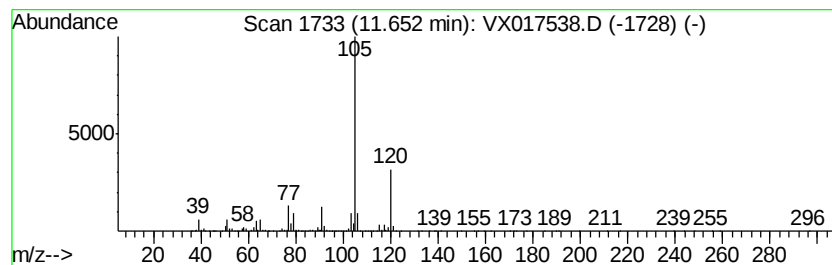
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	16.03 ug/l	856058	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
Data File : VX017538.D
Acq On : 24 Jul 2020 13:28
Operator : JC/SP
Sample : L3362-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1754

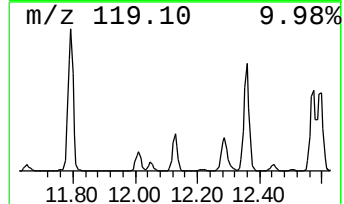
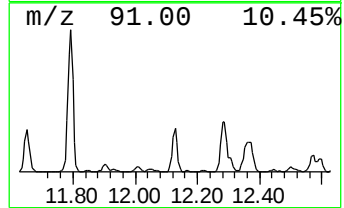
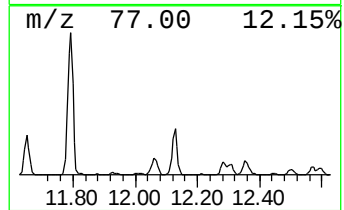
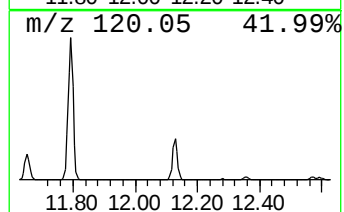
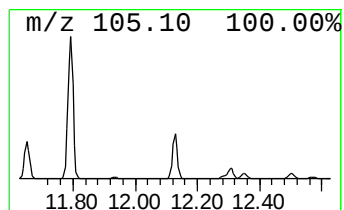
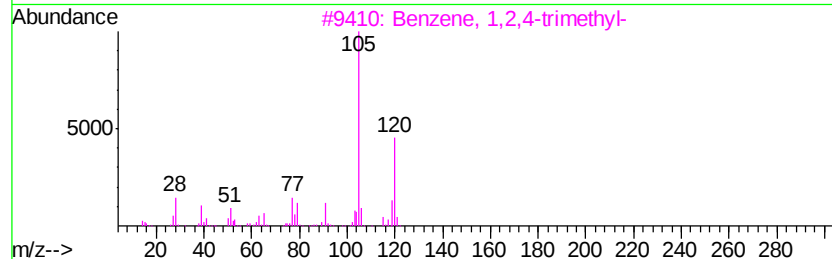
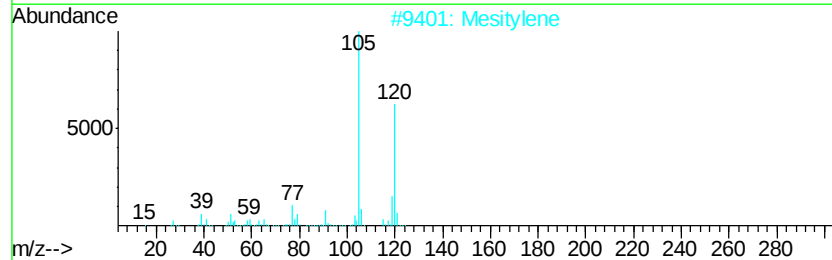
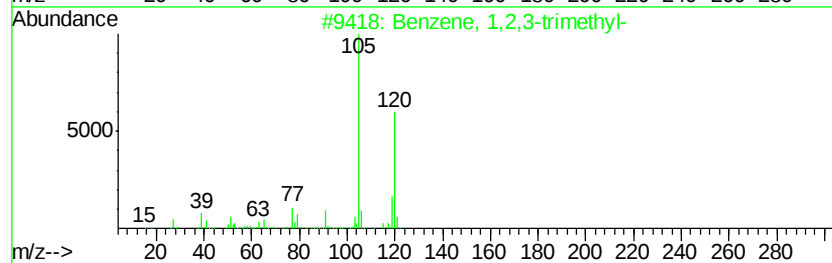
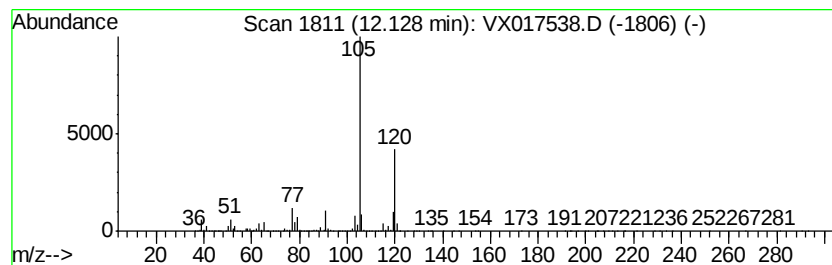
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	19.80 ug/l	1057080	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Mesitylene	120	C9H12	000108-67-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
Data File : VX017538.D
Acq On : 24 Jul 2020 13:28
Operator : JC/SP
Sample : L3362-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

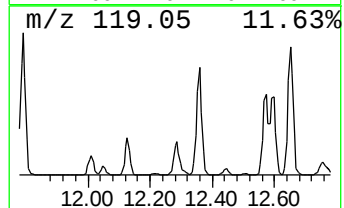
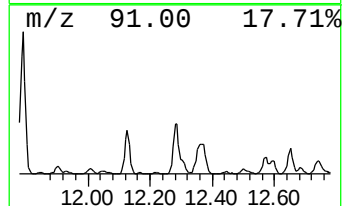
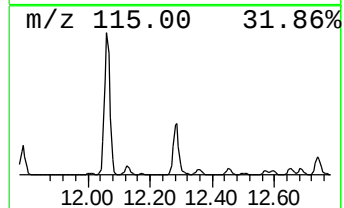
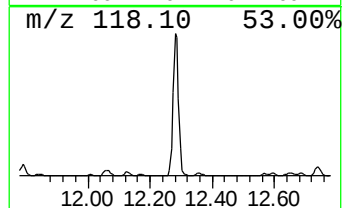
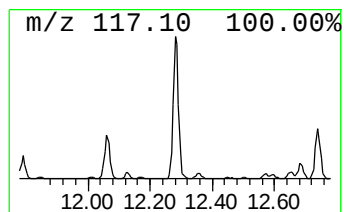
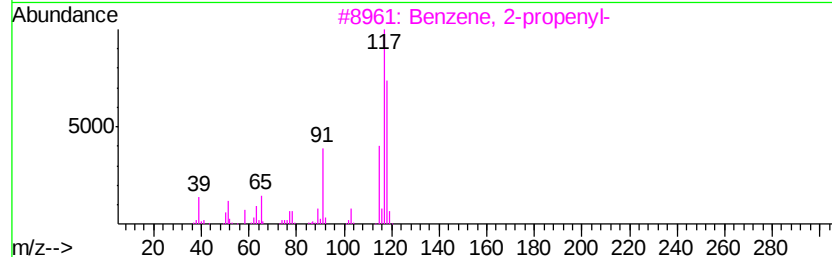
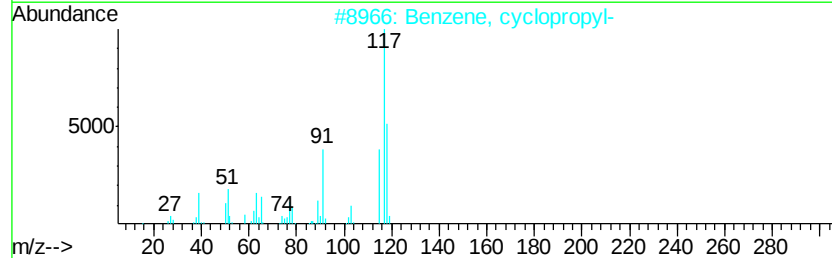
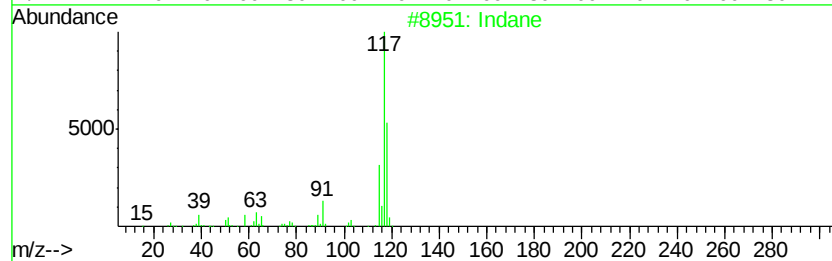
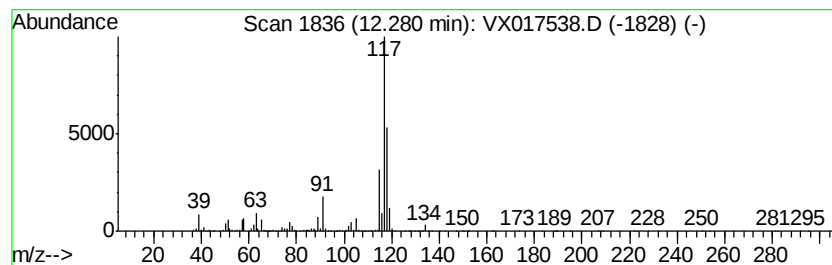
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X072320W.M
Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	26.33 ug/l	1405840	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indane	118 C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118 C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118 C9H10	000300-57-2	72
4	trans-Cinnamyl bromide	196 C9H9Br	026146-77-0	53
5	Deltacyclene	118 C9H10	007785-10-6	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX072420\
Data File : VX017538.D
Acq On : 24 Jul 2020 13:28
Operator : JC/SP
Sample : L3362-05 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1754

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X072320W.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
Butane, 2-methyl-	1.78	11.0	ug/l	327064	1	5.63	1485910	50.0
Pentane	1.99	11.7	ug/l	347317	1	5.63	1485910	50.0
unknown2.09	2.09	50.4	ug/l	1496780	1	5.63	1485910	50.0
2-Butene, 2-methyl-	2.25	15.2	ug/l	450630	1	5.63	1485910	50.0
1-Propanol	3.92	23.7	ug/l	704540	1	5.63	1485910	50.0
Cyclopentane, met...	4.37	17.8	ug/l	529945	1	5.63	1485910	50.0
Benzene, 1-ethyl-...	11.42	49.4	ug/l	2639130	4	12.06	2669380	50.0
Benzene, 1-ethyl-...	11.65	16.0	ug/l	856058	4	12.06	2669380	50.0
Benzene, 1,2,3-tr...	12.13	19.8	ug/l	1057080	4	12.06	2669380	50.0
Indane	12.28	26.3	ug/l	1405840	4	12.06	2669380	50.0