

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121919\
 Data File : VX014131.D
 Acq On : 19 Dec 2019 19:20
 Operator : JC/SP
 Sample : K6347-03 50X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

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\82X121319W.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	1.070	26	30	43	rBV	690564	828400	5.75%	1.306%
2	1.296	63	67	77	rBV	417358	419287	2.91%	0.661%
3	1.399	78	84	90	rVV	1205028	1249784	8.67%	1.970%
4	1.454	90	93	101	rVB	393843	368004	2.55%	0.580%
5	1.527	101	105	110	rBV	280800	270605	1.88%	0.427%
6	1.783	142	147	159	rVB	863264	1173776	8.14%	1.850%
7	1.948	169	174	177	rBV	252016	337325	2.34%	0.532%
8	1.991	177	181	189	rVB	458660	653077	4.53%	1.029%
9	2.113	195	201	208	rBV	498864	712572	4.94%	1.123%
10	2.210	211	217	223	rVB	257683	412144	2.86%	0.650%
11	2.808	303	315	323	rBV	183591	435969	3.02%	0.687%
12	2.923	330	334	350	rVB	240150	531318	3.69%	0.837%
13	4.399	565	576	586	rBV	193173	562439	3.90%	0.887%
14	5.490	744	755	762	rBV	299609	851404	5.91%	1.342%
15	5.575	762	769	774	rVV	199745	595810	4.13%	0.939%
16	5.655	774	782	795	rVB	541391	1523561	10.57%	2.401%
17	6.051	839	847	853	rBV	341182	880475	6.11%	1.388%
18	6.136	853	861	875	rVB	2724265	7050628	48.92%	11.113%
19	6.325	883	892	903	rVB3	138386	449132	3.12%	0.708%
20	6.849	968	978	988	rBV	824948	1927041	13.37%	3.037%
21	7.459	1068	1078	1085	rBV2	113164	256930	1.78%	0.405%
22	8.483	1240	1246	1252	rBV	120385	202612	1.41%	0.319%
23	8.563	1252	1259	1267	rBV	380806	607704	4.22%	0.958%
24	8.709	1277	1283	1289	rBV	1716453	2675270	18.56%	4.217%
25	8.782	1289	1295	1307	rVV	9317903	14413992	100.00%	22.719%
26	8.898	1307	1314	1323	rVB	413495	664782	4.61%	1.048%
27	9.495	1405	1412	1419	rBV	194021	290483	2.02%	0.458%
28	10.075	1499	1507	1509	rBV	364268	596750	4.14%	0.941%
29	10.105	1509	1512	1517	rVV	1697104	2284609	15.85%	3.601%
30	10.154	1517	1520	1523	rVV	144890	192173	1.33%	0.303%
31	10.196	1523	1527	1531	rVV	423312	549255	3.81%	0.866%
32	10.245	1531	1535	1540	rVV	1920964	2474103	17.16%	3.900%
33	10.355	1547	1553	1559	rVV	4775903	6290245	43.64%	9.915%
34	10.696	1603	1609	1620	rVB	2078442	2690736	18.67%	4.241%

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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 >
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35	10.843	1626	1633	1639	rBV	158825	273830	1.90%	0.432%
36	11.129	1675	1680	1685	rBV	1375608	1791565	12.43%	2.824%
37	11.221	1689	1695	1701	rVB	216543	310420	2.15%	0.489%
38	11.324	1706	1712	1714	rVV	153736	210831	1.46%	0.332%
39	11.355	1714	1717	1721	rVV	127692	172659	1.20%	0.272%
40	11.428	1725	1729	1736	rVV	439324	770100	5.34%	1.214%
41	11.501	1736	1741	1749	rVB	225146	300487	2.08%	0.474%
42	11.666	1762	1768	1772	rBV	201414	253950	1.76%	0.400%
43	11.800	1786	1790	1794	rBV	698591	849475	5.89%	1.339%
44	11.928	1806	1811	1819	rBV3	130689	249206	1.73%	0.393%
45	12.074	1829	1835	1841	rBV	1752240	2143535	14.87%	3.379%
46	12.141	1841	1846	1852	rVV	244131	360834	2.50%	0.569%
47	12.294	1864	1871	1879	rBV3	219319	334731	2.32%	0.528%

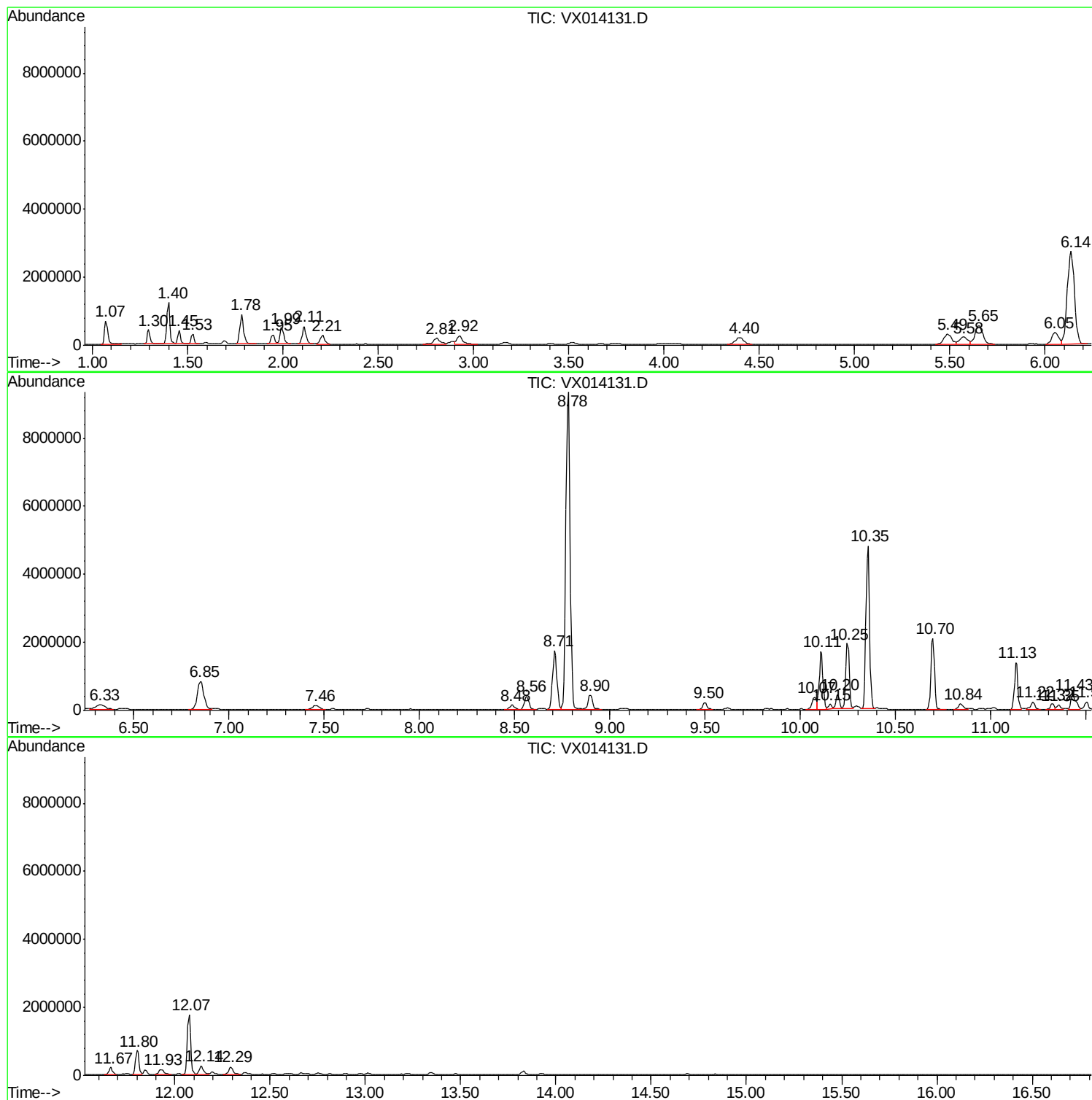
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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



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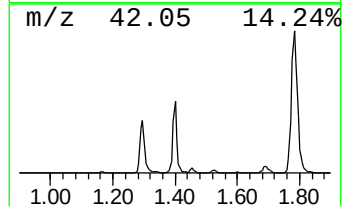
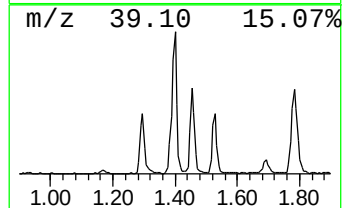
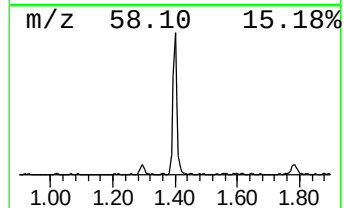
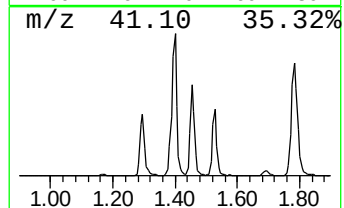
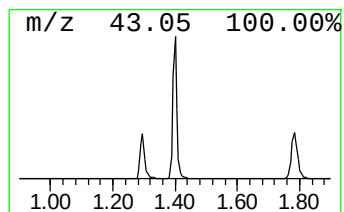
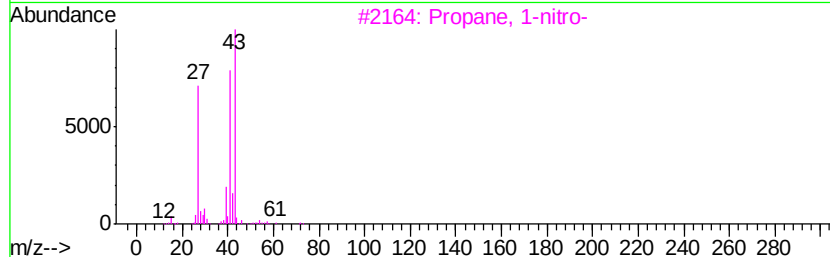
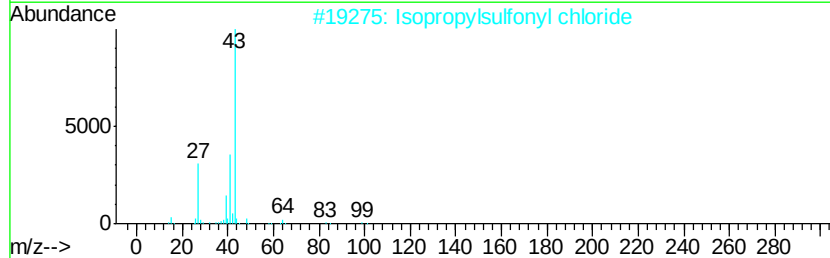
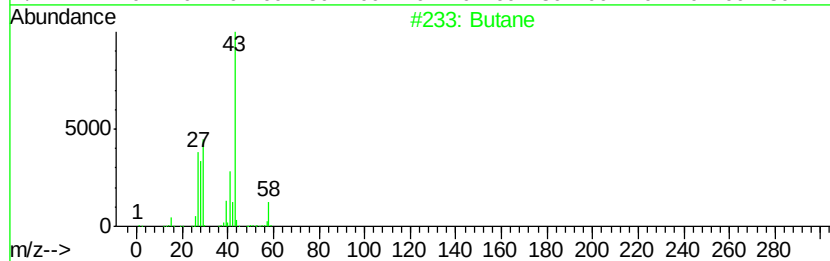
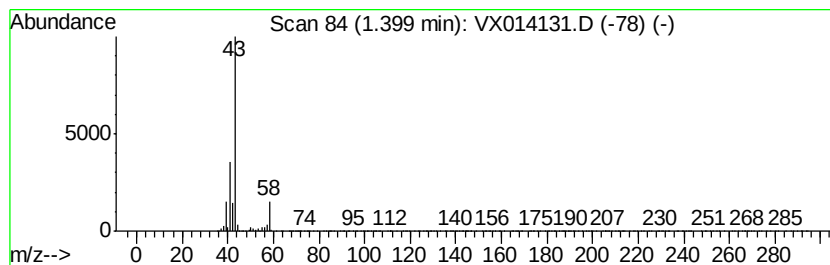
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	41.02 ug/l	1249780	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane	58	C4H10	000106-97-8	72
2		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
4		Isobutane	58	C4H10	000075-28-5	9
5		Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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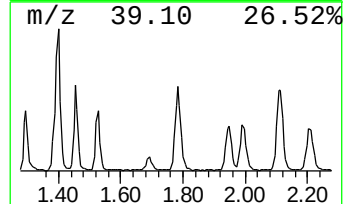
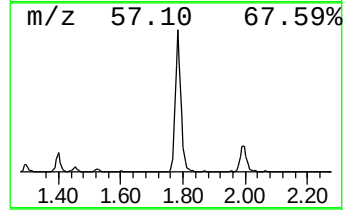
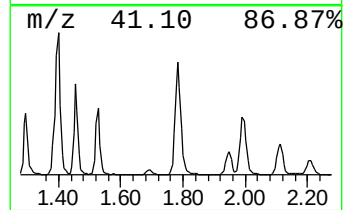
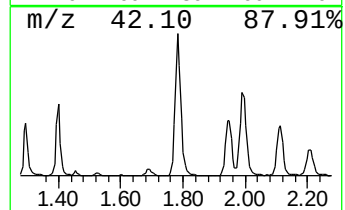
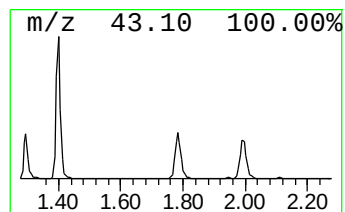
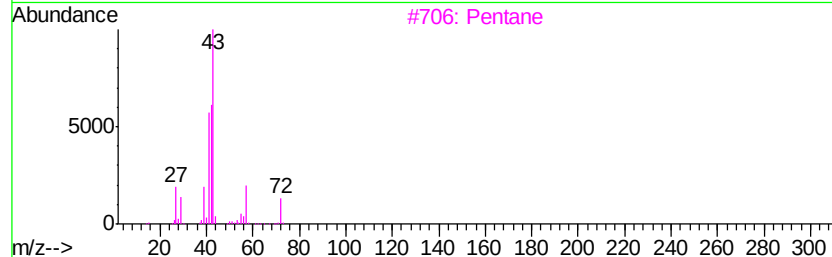
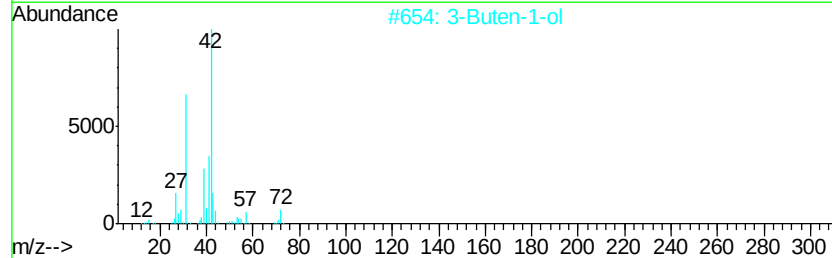
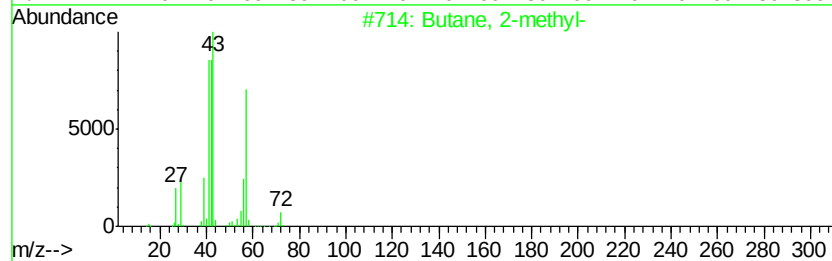
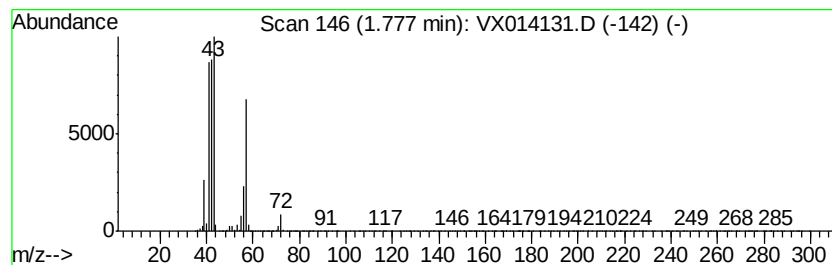
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	38.52 ug/l	1173780	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	40
3		Pentane	72	C5H12	000109-66-0	37
4		1-Butene	56	C4H8	000106-98-9	14
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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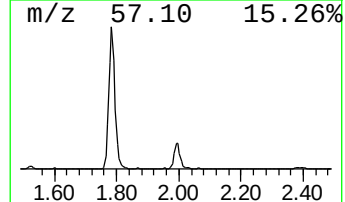
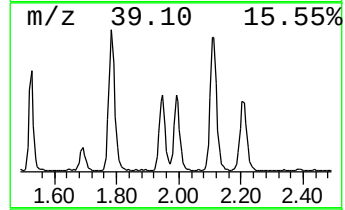
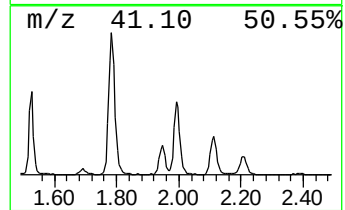
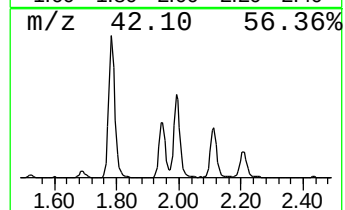
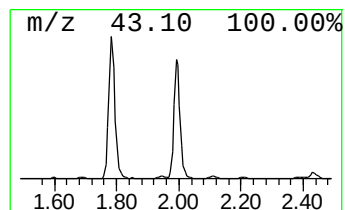
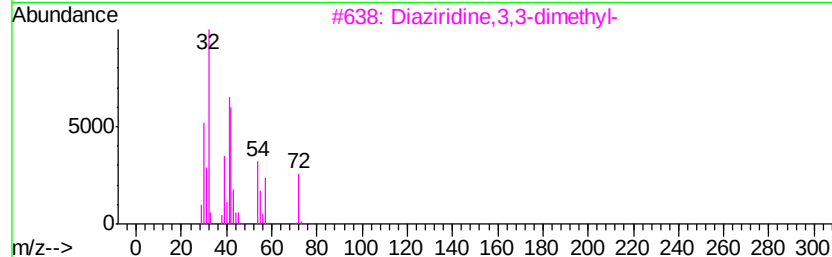
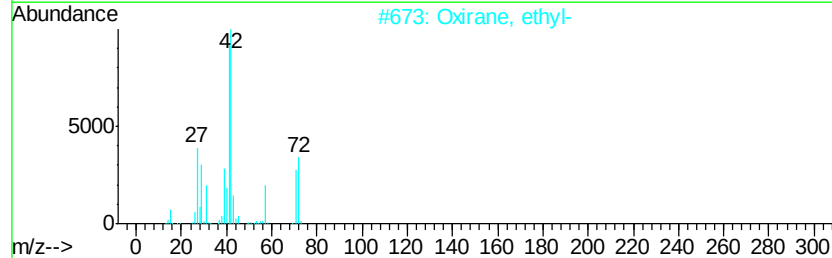
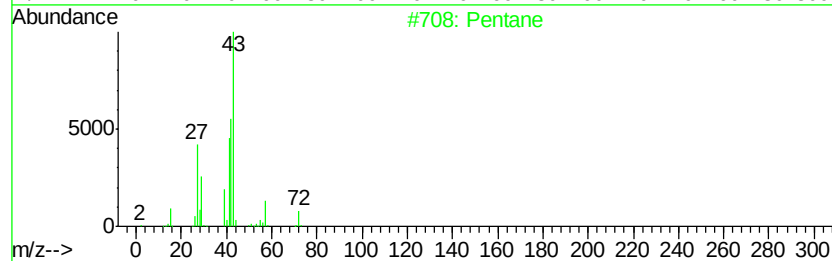
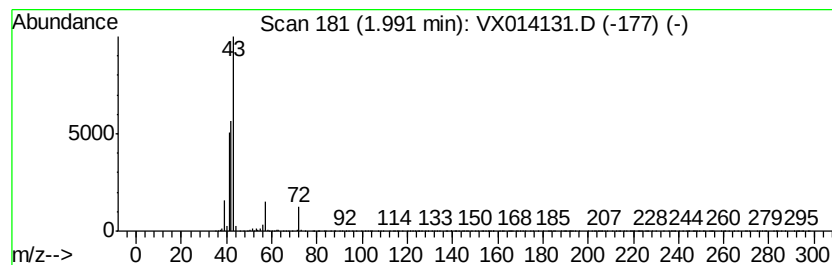
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	21.43 ug/l	653077	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	86
2	Oxirane, ethyl-		72	C4H8O	000106-88-7	9
3	Diaziridine,3,3-dimethyl-		72	C3H8N2	004901-76-2	9
4	Ethanone, 1-[6-(4-methyl-1,2,5-o...		234	C8H6N6O3	314728-61-5	9
5	5,9-Dodecadien-2-one, 6,10-dimet...		208	C14H24O	1000132-10-9	7



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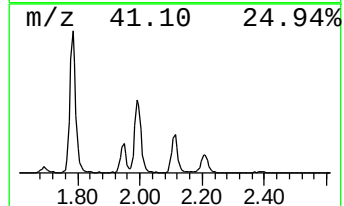
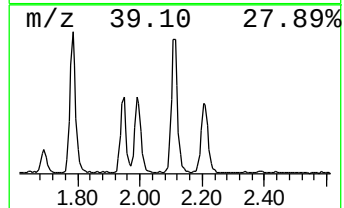
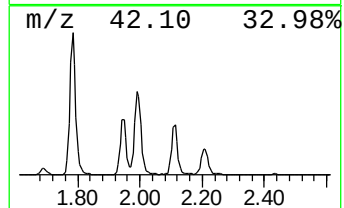
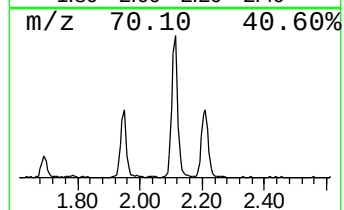
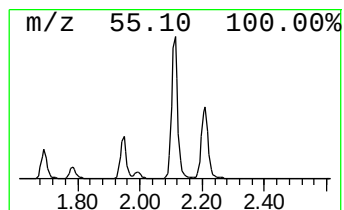
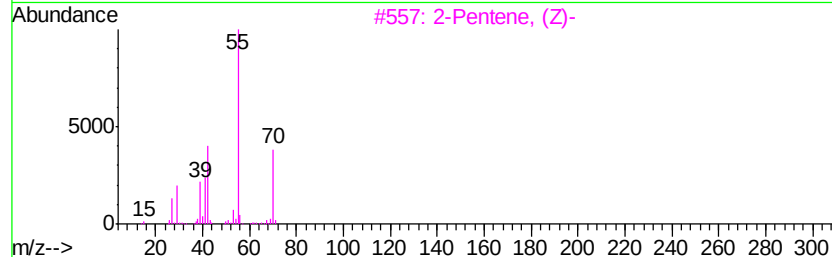
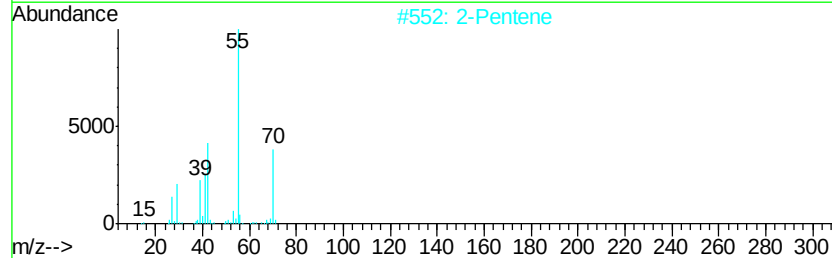
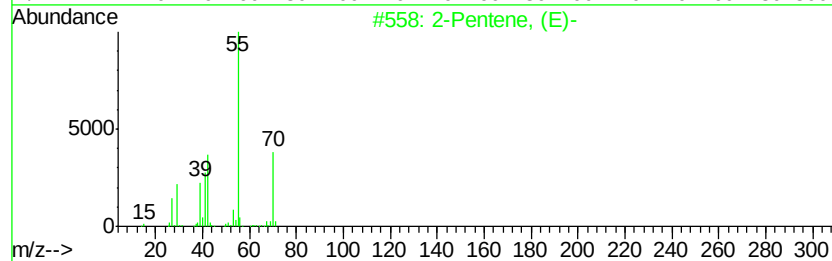
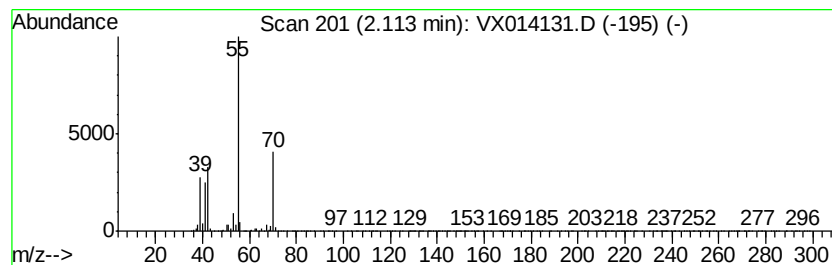
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Quant Title : SW846 8260

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

Peak Number 5 2-Pentene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	23.39 ug/l	712572	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentene, (E)-	70	C5H10	000646-04-8	90
2		2-Pentene	70	C5H10	000109-68-2	90
3		2-Pentene, (Z)-	70	C5H10	000627-20-3	90
4		2-Methyl-1-butene	70	C5H10	000563-46-2	90
5		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90



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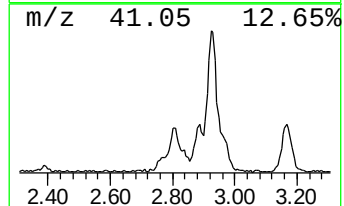
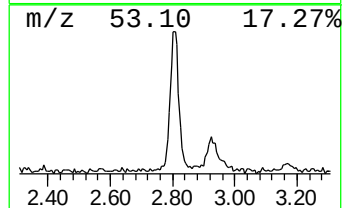
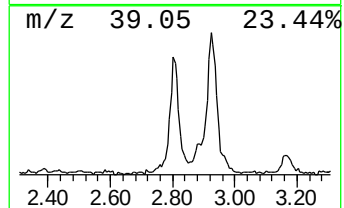
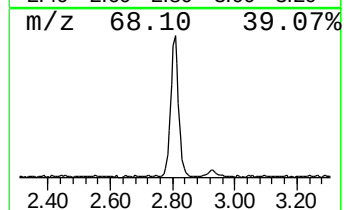
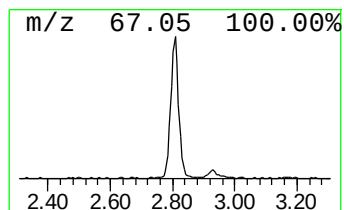
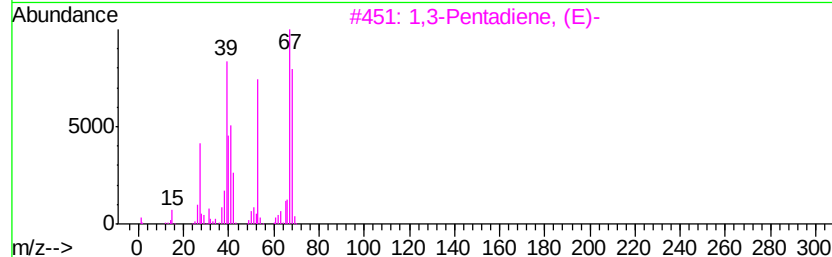
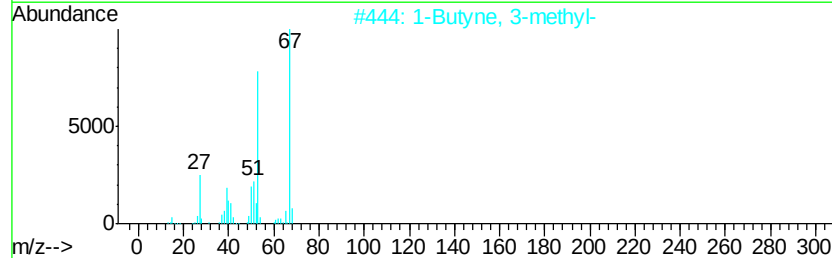
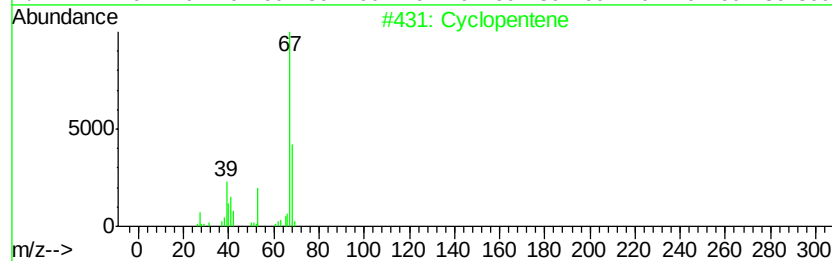
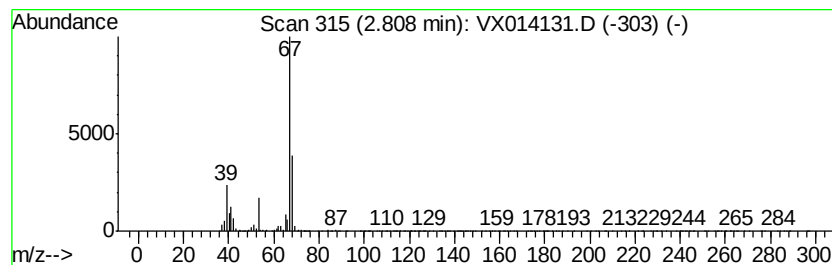
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	14.31 ug/l	435969	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentene	68	C5H8	000142-29-0	91
2		1-Butyne, 3-methyl-	68	C5H8	000598-23-2	53
3		1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	53
4		1,4-Pentadiene	68	C5H8	000591-93-5	52
5		1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014131.D
Acq On : 19 Dec 2019 19:20
Operator : JC/SP
Sample : K6347-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

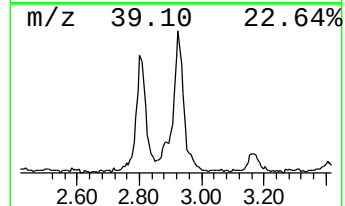
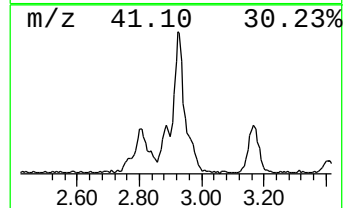
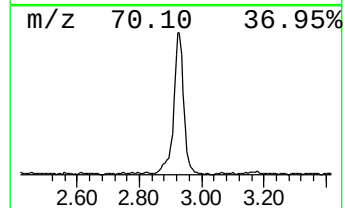
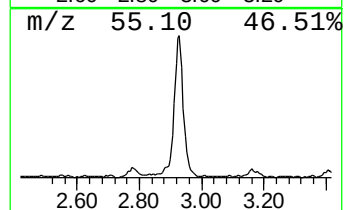
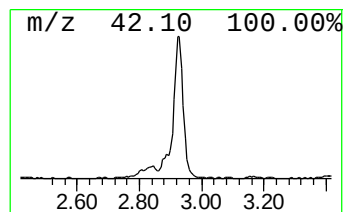
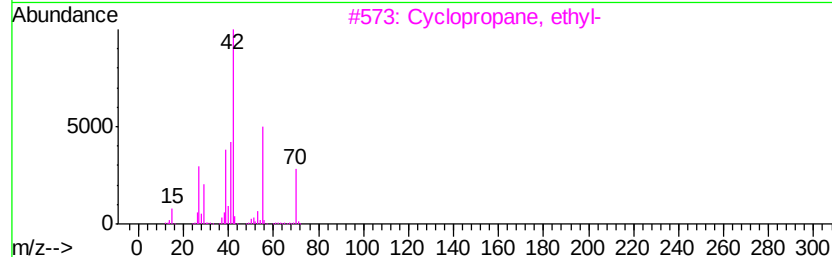
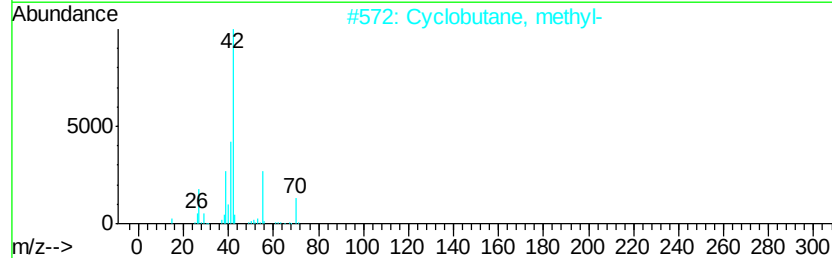
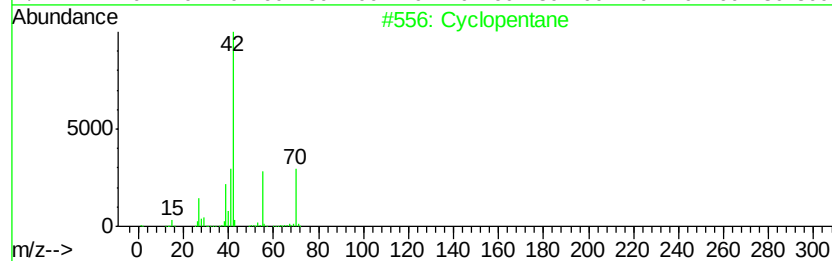
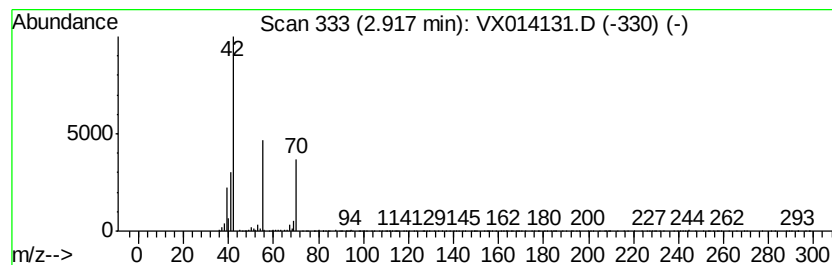
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.92	17.44 ug/l	531318	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane	70	C5H10	000287-92-3	80
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
4		1-Pentene	70	C5H10	000109-67-1	59
5		2H-Pyran-2,6(3H)-dione, dihydro-	114	C5H6O3	000108-55-4	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014131.D
Acq On : 19 Dec 2019 19:20
Operator : JC/SP
Sample : K6347-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

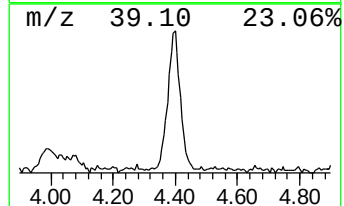
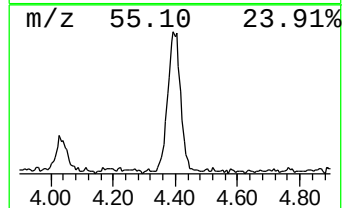
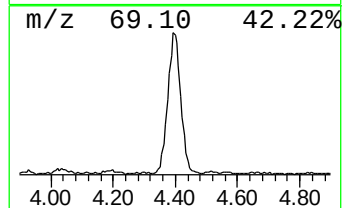
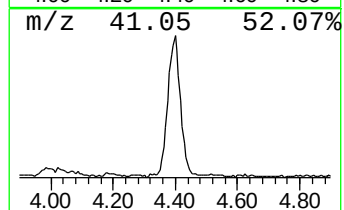
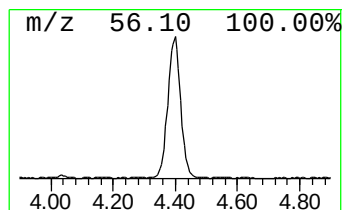
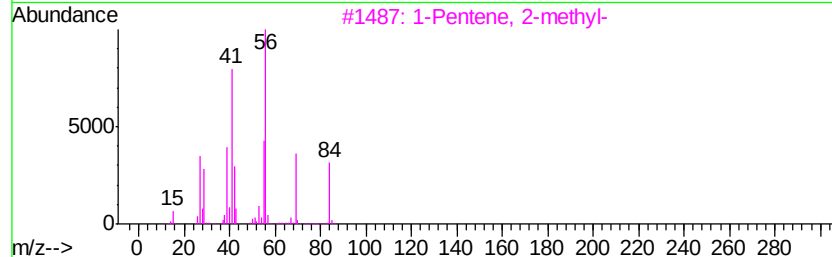
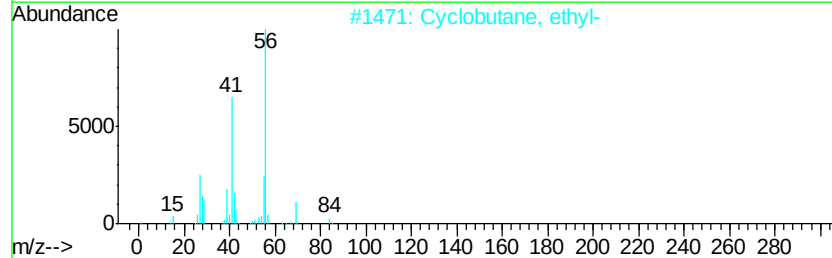
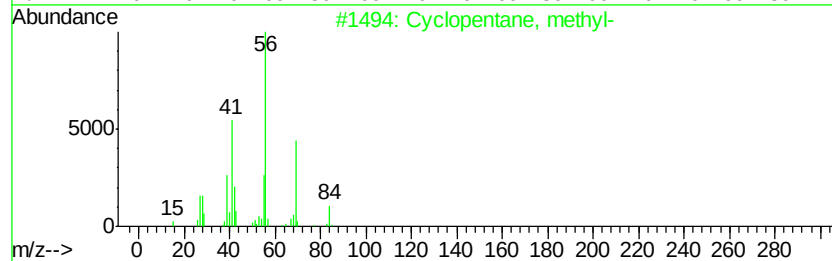
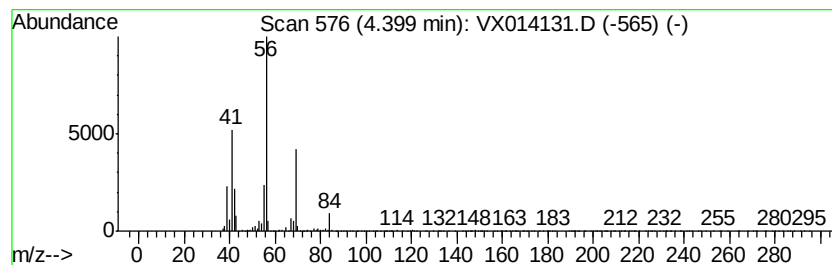
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	18.46 ug/l	562439	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014131.D
Acq On : 19 Dec 2019 19:20
Operator : JC/SP
Sample : K6347-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

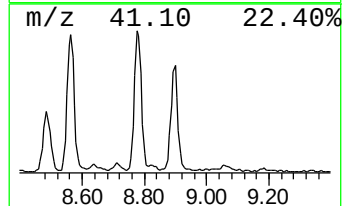
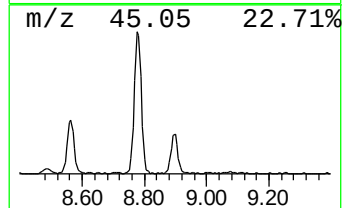
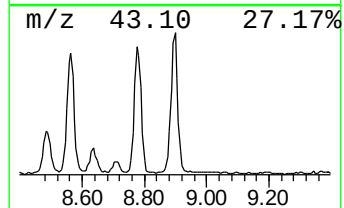
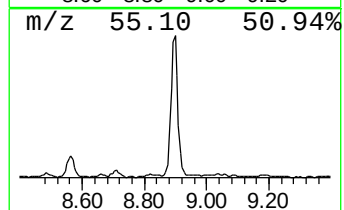
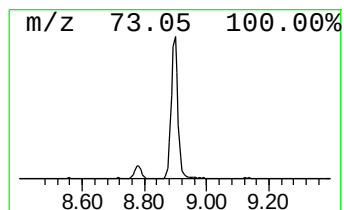
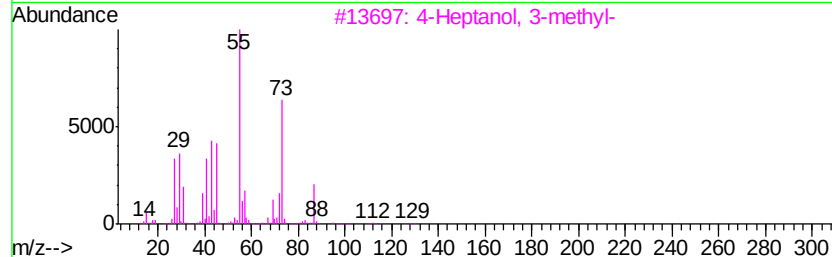
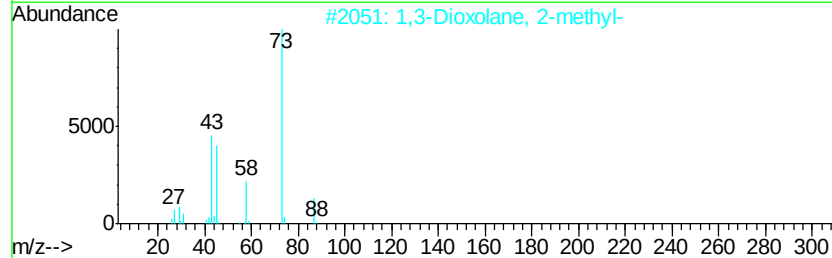
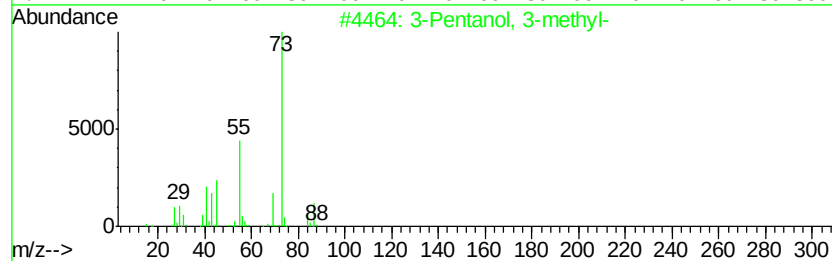
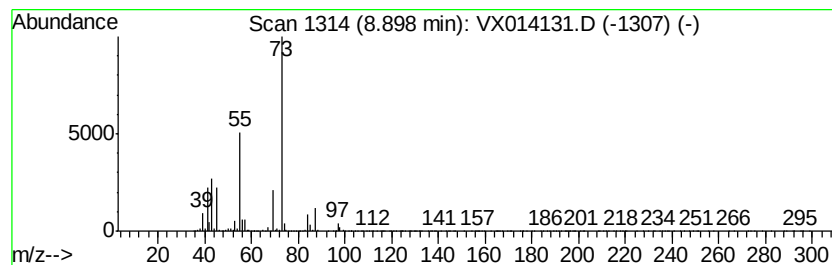
Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 9 3-Pentanol, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	14.55 ug/l	664782	Chlorobenzene-d5	10.11
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Pentanol, 3-methyl-	102 C6H14O	000077-74-7	86
2	1,3-Dioxolane, 2-methyl-	88 C4H8O2	000497-26-7	38
3	4-Heptanol, 3-methyl-	130 C8H18O	001838-73-9	38
4	3-Pentanol, 2,4-dimethyl-	116 C7H16O	000600-36-2	38
5	Propane, 2-methoxy-2-methyl-	88 C5H12O	001634-04-4	12



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014131.D
Acq On : 19 Dec 2019 19:20
Operator : JC/SP
Sample : K6347-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

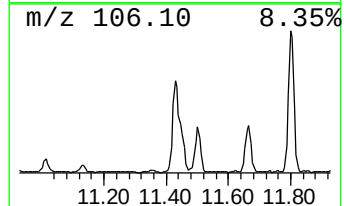
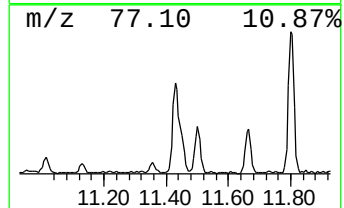
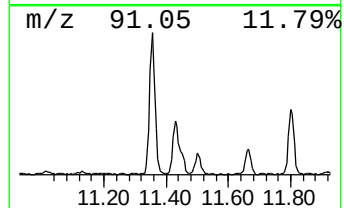
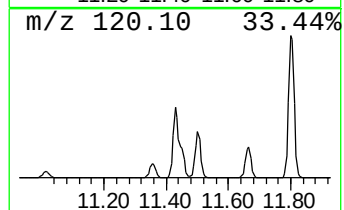
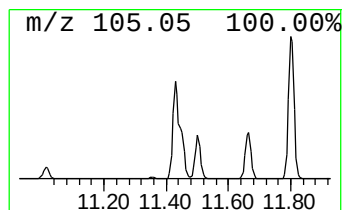
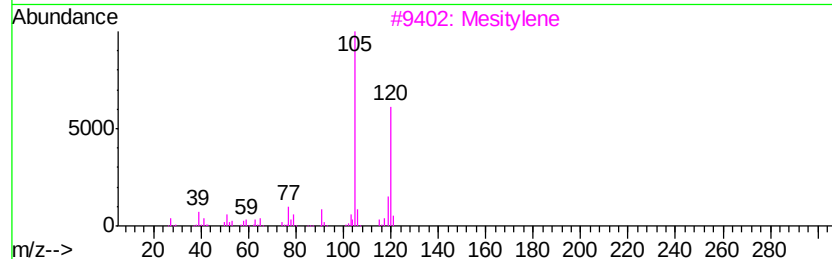
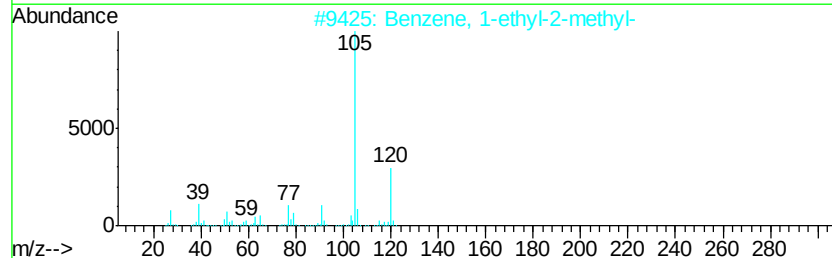
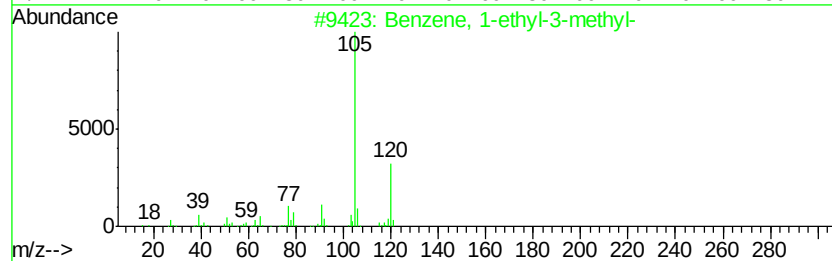
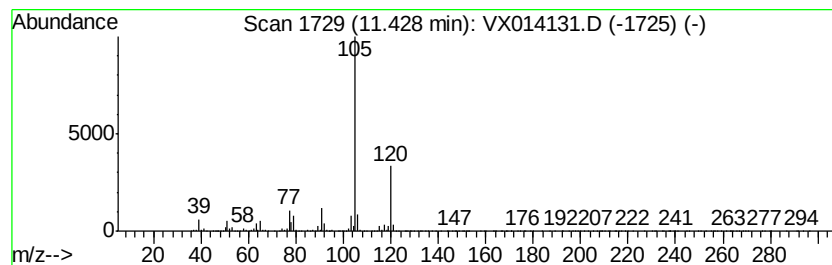
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	17.96 ug/l	770100	1,4-Dichlorobenzene-d4	12.07

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		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121919\
Data File : VX014131.D
Acq On : 19 Dec 2019 19:20
Operator : JC/SP
Sample : K6347-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.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	1.40	41.0	ug/l	1249780	1	5.65	1523560	50.0
Butane, 2-methyl-	1.78	38.5	ug/l	1173780	1	5.65	1523560	50.0
Pentane	1.99	21.4	ug/l	653077	1	5.65	1523560	50.0
2-Pentene, (E)-	2.11	23.4	ug/l	712572	1	5.65	1523560	50.0
Cyclopentene	2.81	14.3	ug/l	435969	1	5.65	1523560	50.0
Cyclopentane	2.92	17.4	ug/l	531318	1	5.65	1523560	50.0
Cyclopentane, met...	4.40	18.5	ug/l	562439	1	5.65	1523560	50.0
3-Pentanol, 3-met...	8.90	14.6	ug/l	664782	3	10.11	2284610	50.0
Benzene, 1-ethyl-...	11.43	18.0	ug/l	770100	4	12.07	2143540	50.0