

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
 Data File : VX000621.D
 Acq On : 01 Apr 2018 04:03
 Operator : JC/MD
 Sample : J2132-07 50X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 42 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.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	1.075	75	80	89	rBV	315925	385623	58.40%	5.800%
2	1.794	193	198	205	rBV2	29090	43204	6.54%	0.650%
3	2.002	228	232	238	rVB	21521	31980	4.84%	0.481%
4	2.117	245	251	258	rVB3	6232	11733	1.78%	0.176%
5	2.270	271	276	280	rBV3	8720	12643	1.91%	0.190%
6	2.849	366	371	374	rBV5	4159	8621	1.31%	0.130%
7	2.892	374	378	382	rVV3	13658	25229	3.82%	0.379%
8	2.934	382	385	390	rVB3	8071	13333	2.02%	0.201%
9	3.172	417	424	433	rVB2	11875	27759	4.20%	0.418%
10	3.398	453	461	470	rBV5	4430	12759	1.93%	0.192%
11	3.526	475	482	491	rBV4	8361	19691	2.98%	0.296%
12	3.660	498	504	512	rVB7	3461	9829	1.49%	0.148%
13	3.751	512	519	525	rVV5	2558	6689	1.01%	0.101%
14	3.818	525	530	539	rVB5	4334	10774	1.63%	0.162%
15	4.196	582	592	602	rBV4	4451	11067	1.68%	0.166%
16	4.404	614	626	639	rBV3	20477	59109	8.95%	0.889%
17	5.312	766	775	784	rVB5	4640	12768	1.93%	0.192%
18	5.513	795	808	817	rBV	70700	207354	31.40%	3.119%
19	5.678	825	835	846	rVB	112869	314259	47.59%	4.727%
20	6.086	890	902	911	rBV	77361	206930	31.34%	3.113%
21	6.873	1021	1031	1041	rBV	186202	436422	66.09%	6.564%
22	6.940	1041	1042	1049	rVB5	4902	8630	1.31%	0.130%
23	7.275	1087	1097	1102	rBV6	2868	6943	1.05%	0.104%
24	7.470	1118	1129	1136	rBV5	8346	20390	3.09%	0.307%
25	8.220	1245	1252	1257	rBV3	4329	7690	1.16%	0.116%
26	8.726	1327	1335	1342	rBV	392700	620671	93.99%	9.336%
27	8.787	1342	1345	1353	rVB2	10325	16416	2.49%	0.247%
28	10.122	1557	1564	1572	rBV	425985	575450	87.15%	8.656%
29	10.256	1581	1586	1592	rBV	146638	198360	30.04%	2.984%
30	10.366	1598	1604	1612	rVB	390929	508833	77.06%	7.654%
31	10.707	1654	1660	1666	rVB	110983	144352	21.86%	2.171%
32	11.024	1708	1712	1720	rVB	14747	18680	2.83%	0.281%
33	11.146	1725	1732	1741	rBV	383835	472913	71.62%	7.113%
34	11.366	1763	1768	1773	rBV	38424	46750	7.08%	0.703%

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35	11.439	1775	1780	1788	rVV	162427	285973	43.31%	4.301%
36	11.512	1788	1792	1798	rVB	82693	99097	15.01%	1.491%
37	11.677	1813	1819	1825	rBV	77045	97778	14.81%	1.471%
38	11.817	1836	1842	1847	rBV	316309	391740	59.32%	5.892%
39	12.085	1880	1886	1892	rBV	541384	660335	100.00%	9.932%
40	12.152	1892	1897	1901	rVB	84445	104298	15.79%	1.569%
41	12.305	1917	1922	1930	rBV2	89367	123295	18.67%	1.855%
42	12.378	1930	1934	1942	rVB3	21202	31375	4.75%	0.472%
43	12.524	1955	1958	1964	rBV2	4994	6619	1.00%	0.100%
44	12.591	1964	1969	1971	rVV2	13086	16413	2.49%	0.247%
45	12.615	1971	1973	1978	rVV2	12065	14129	2.14%	0.213%
46	12.676	1978	1983	1986	rVV	19365	23476	3.56%	0.353%
47	12.707	1986	1988	1992	rVB3	6276	7208	1.09%	0.108%
48	12.762	1992	1997	2005	rBV2	18149	25163	3.81%	0.378%
49	12.908	2018	2021	2028	rBV2	5813	7869	1.19%	0.118%
50	12.987	2028	2034	2037	rVV	10890	14224	2.15%	0.214%
51	13.024	2037	2040	2047	rVB2	16686	20941	3.17%	0.315%
52	13.231	2067	2074	2079	rBV2	16595	21047	3.19%	0.317%
53	13.359	2089	2095	2099	rBV2	31074	43047	6.52%	0.647%
54	13.487	2112	2116	2121	rVB5	7220	8959	1.36%	0.135%
55	13.841	2164	2174	2179	rBV	85218	102396	15.51%	1.540%
56	14.707	2312	2316	2323	rVB	15222	19685	2.98%	0.296%
57	14.847	2335	2339	2346	rBV3	6689	9389	1.42%	0.141%

Sum of corrected areas: 6648310

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ALS Vial : 42 Sample Multiplier: 1

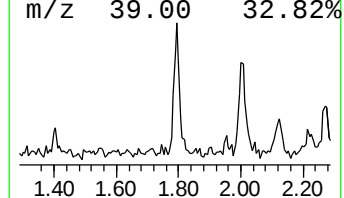
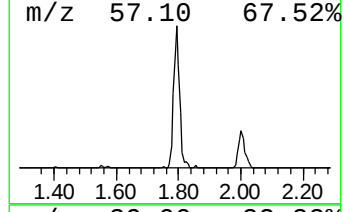
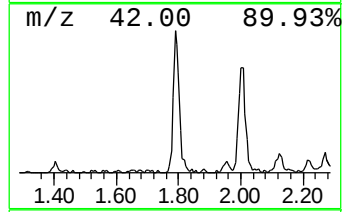
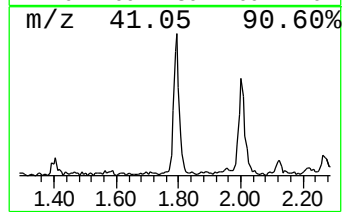
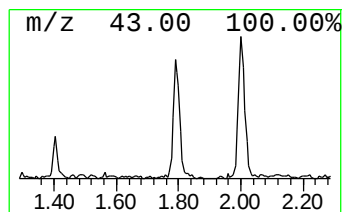
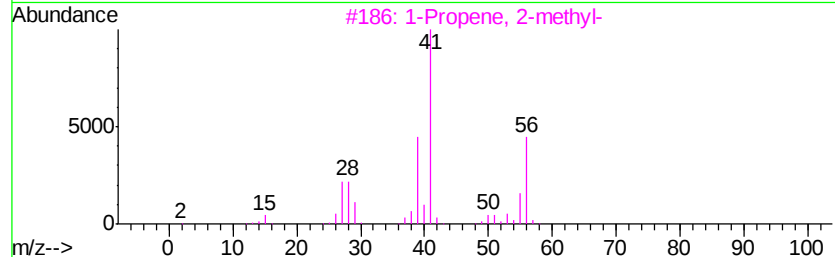
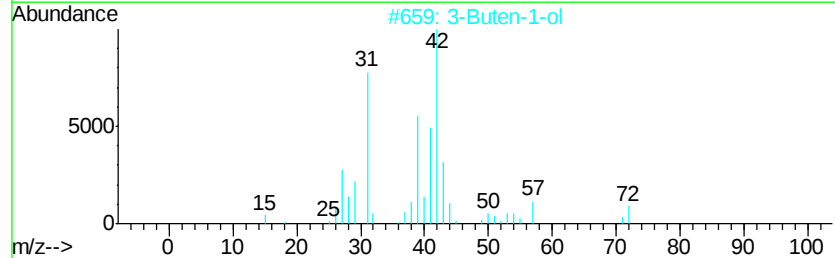
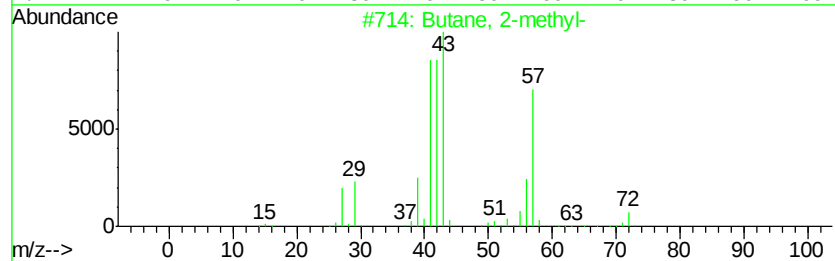
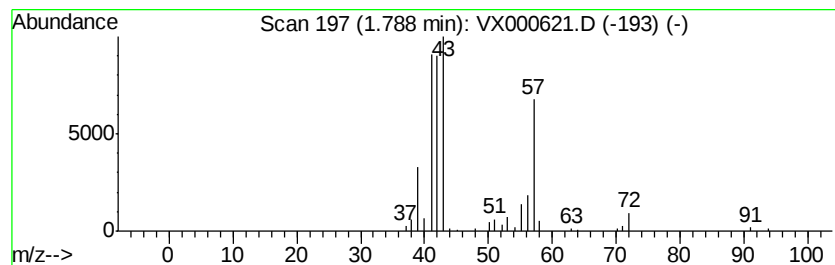
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	6.87 ug/l	43204	Pentafluorobenzene	5.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	72
2		3-Buten-1-ol	72	C4H8O	000627-27-0	33
3		1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
4		1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25
5		Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	23



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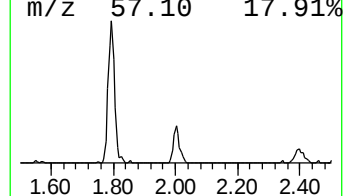
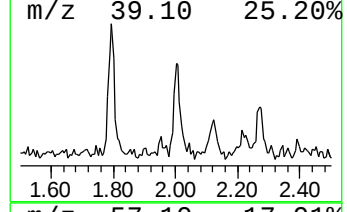
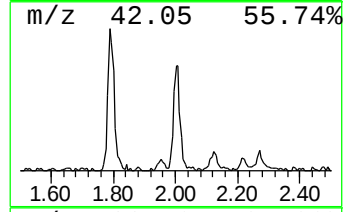
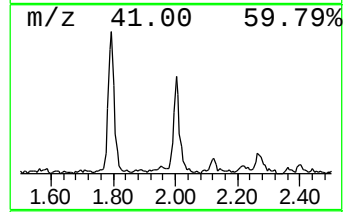
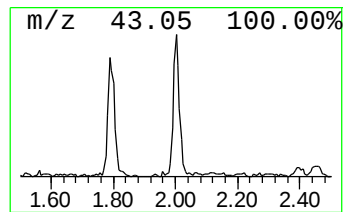
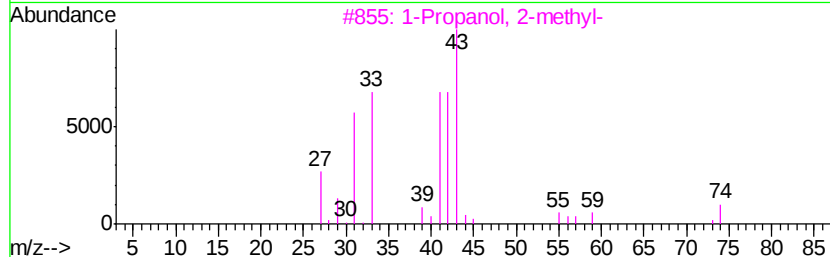
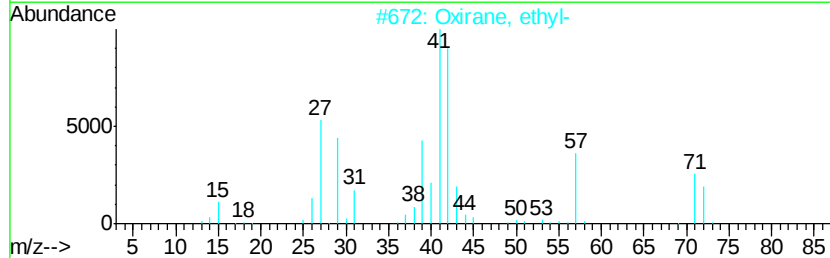
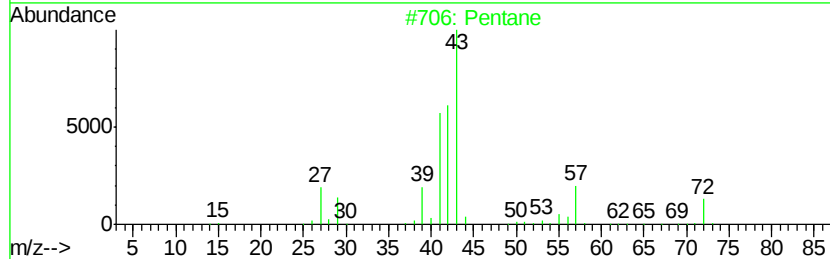
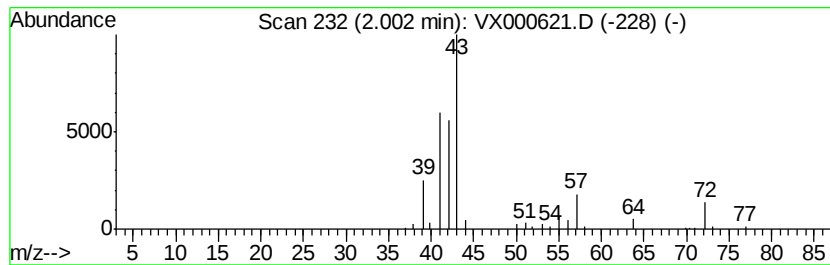
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	5.09 ug/l	31980	Pentafluorobenzene	5.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	91
2		Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	50
4		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	37
5		Butanal, 2-ethyl-	100	C6H12O	000097-96-1	12



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ALS Vial : 42 Sample Multiplier: 1

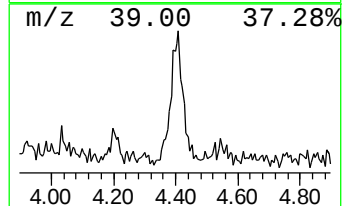
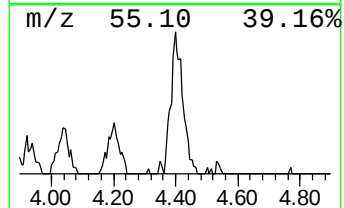
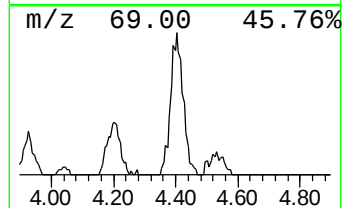
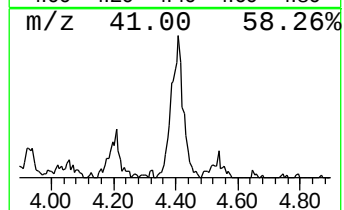
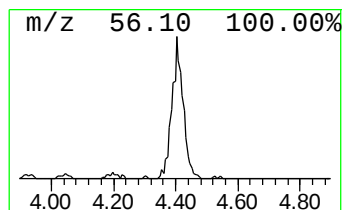
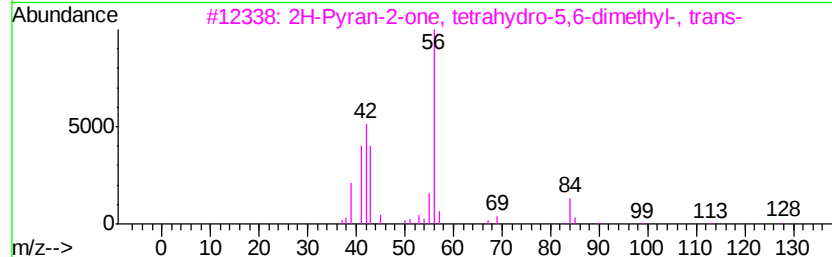
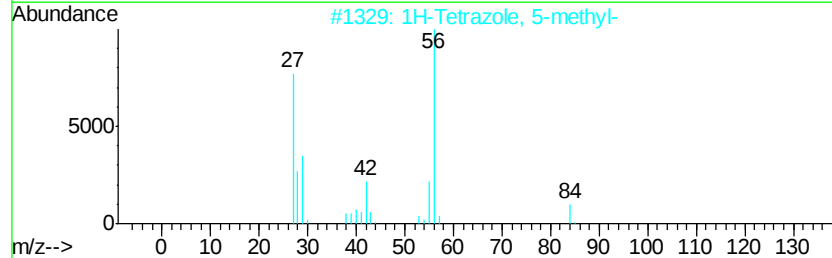
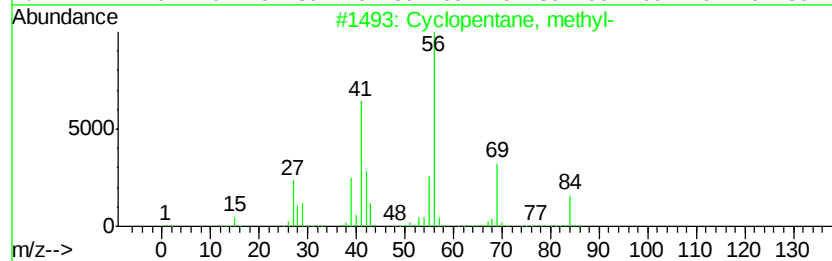
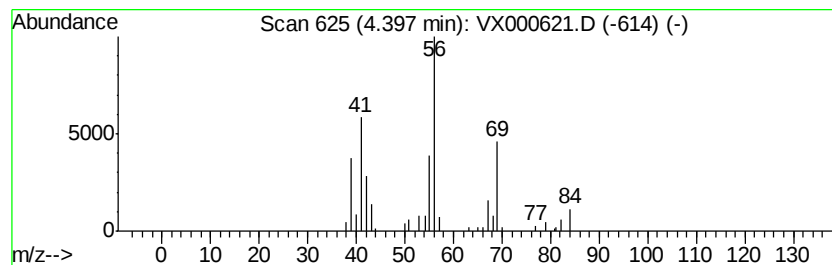
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	9.40 ug/l	59109	Pentafluorobenzene	5.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3		2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	50
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	40
5		4-Penten-2-ol, 3-methyl-	100	C6H12O	001569-59-1	25



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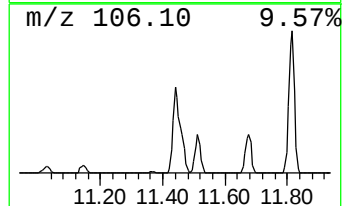
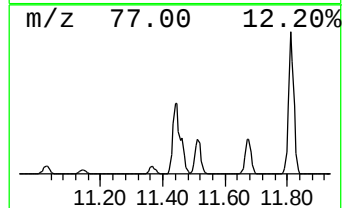
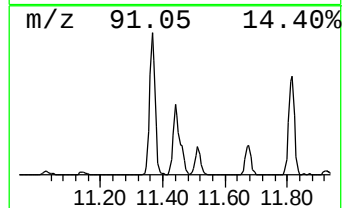
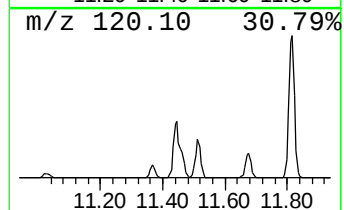
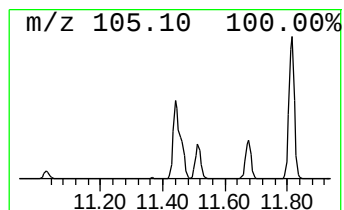
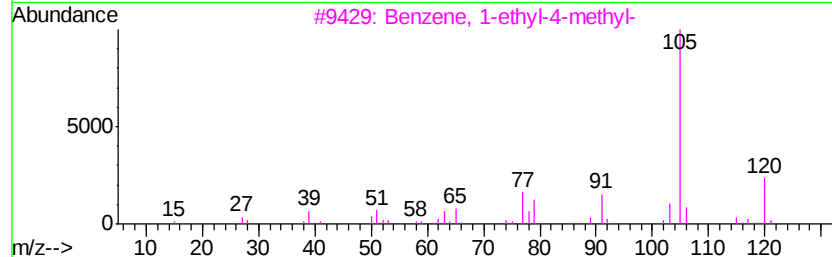
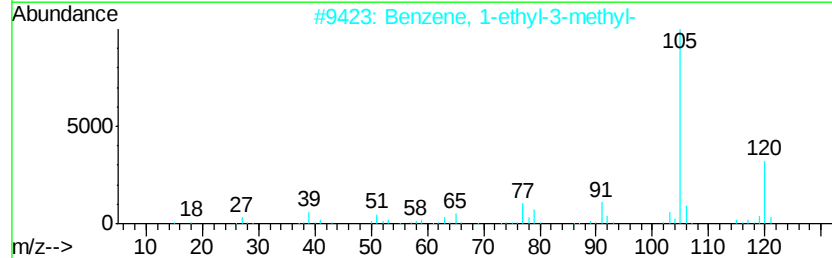
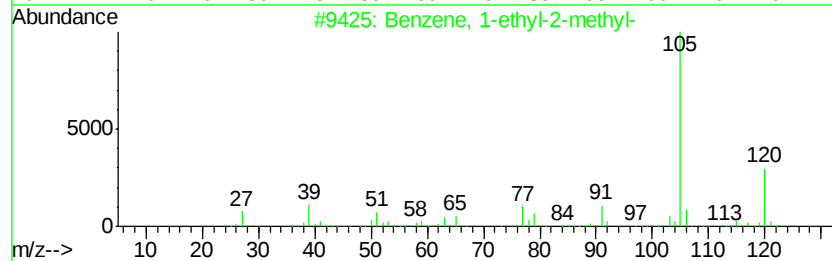
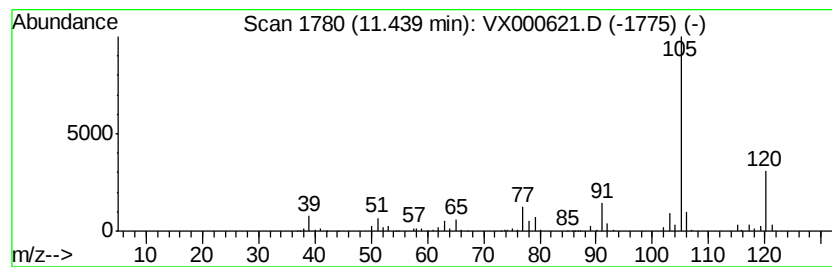
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	21.65 ug/l	285973	1,4-Dichlorobenzene-d4	12.09

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-3-methyl-	120	C9H12	000620-14-4	94
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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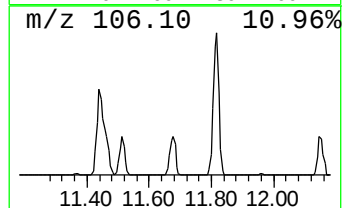
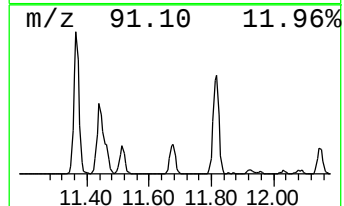
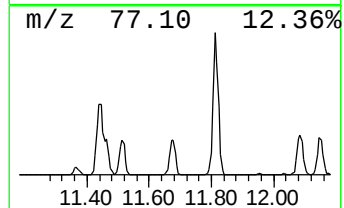
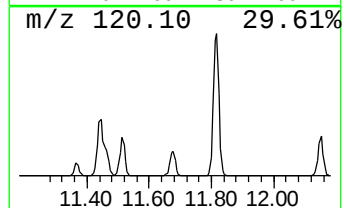
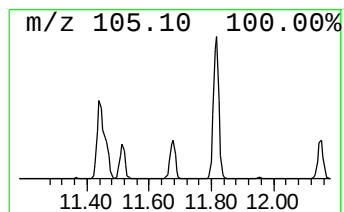
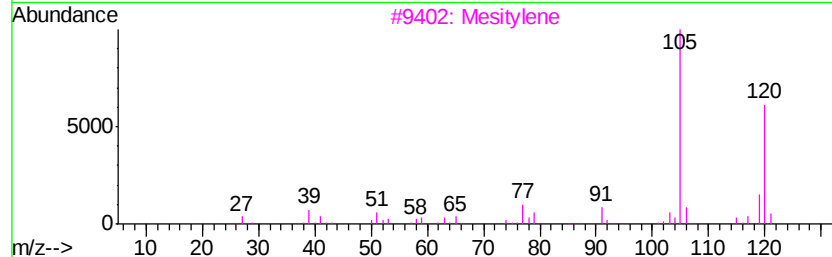
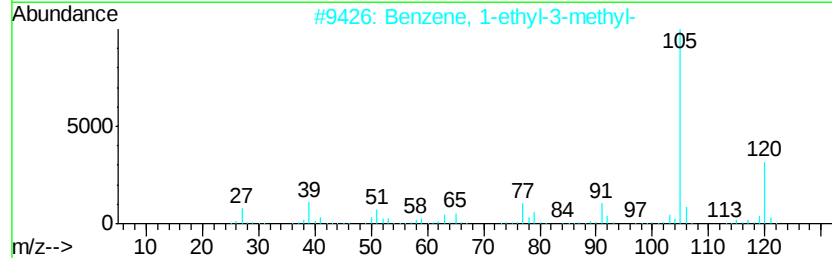
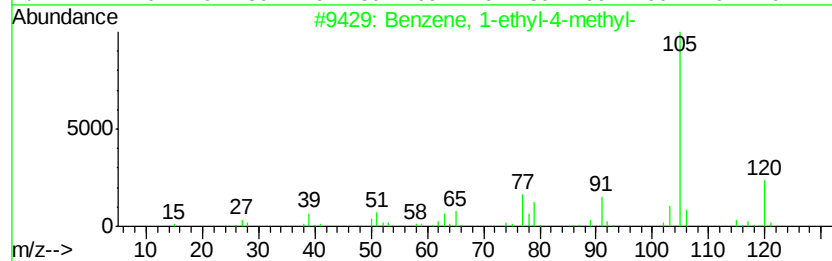
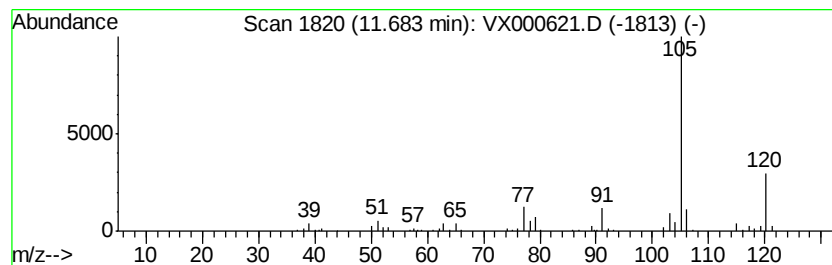
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	7.40 ug/l	97778	1,4-Dichlorobenzene-d4	12.09

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



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000621.D
Acq On : 01 Apr 2018 04:03
Operator : JC/MD
Sample : J2132-07 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 42 Sample Multiplier: 1

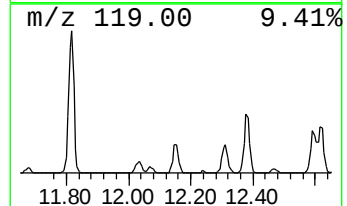
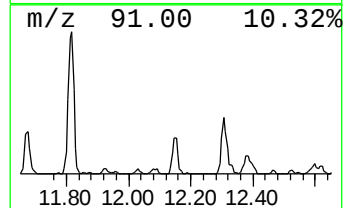
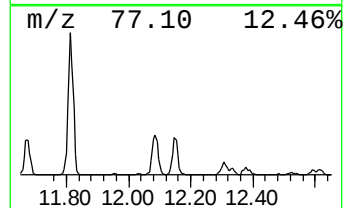
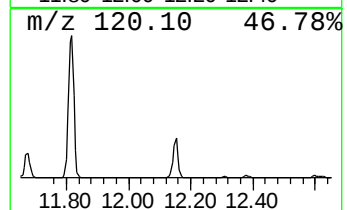
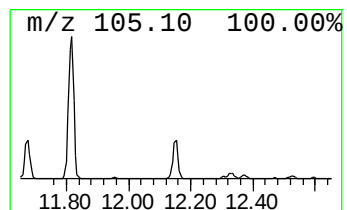
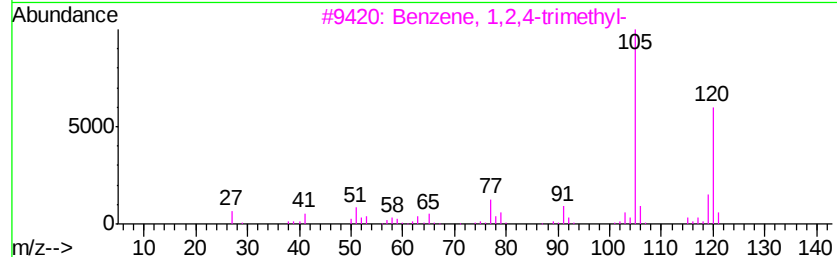
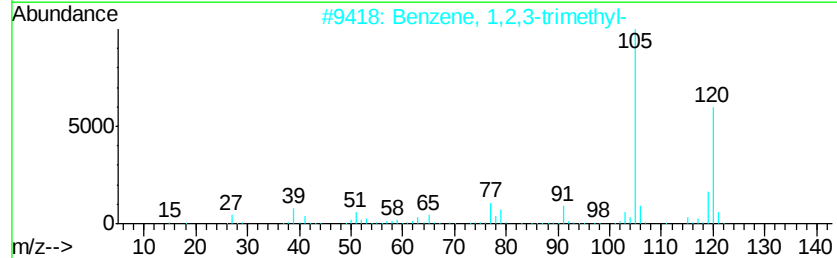
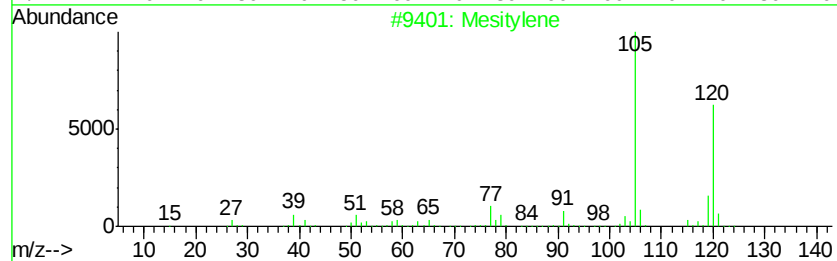
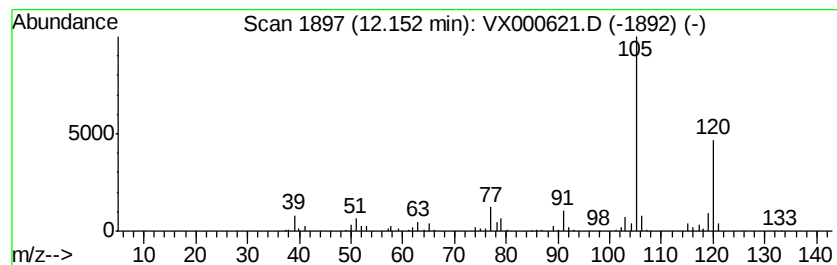
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Quant Title : SW846 8260

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

Peak Number 7 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	7.90 ug/l	104298	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	94
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	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-4-methyl-	120	C9H12	000622-96-8	90



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000621.D
Acq On : 01 Apr 2018 04:03
Operator : JC/MD
Sample : J2132-07 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 42 Sample Multiplier: 1

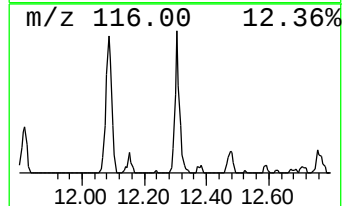
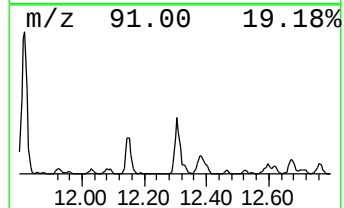
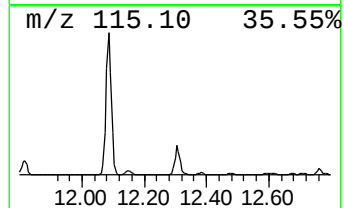
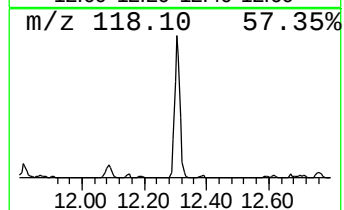
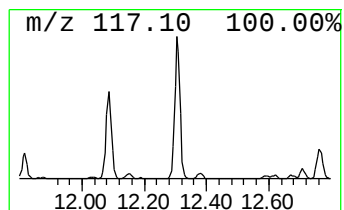
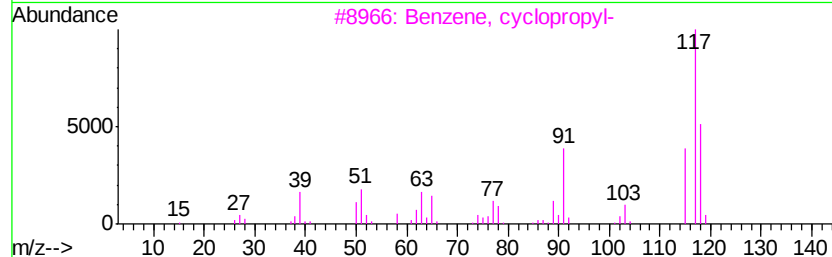
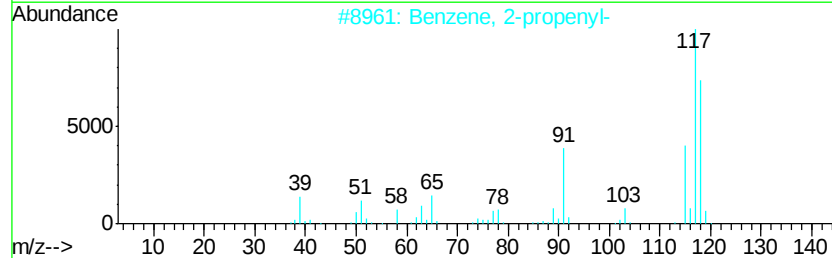
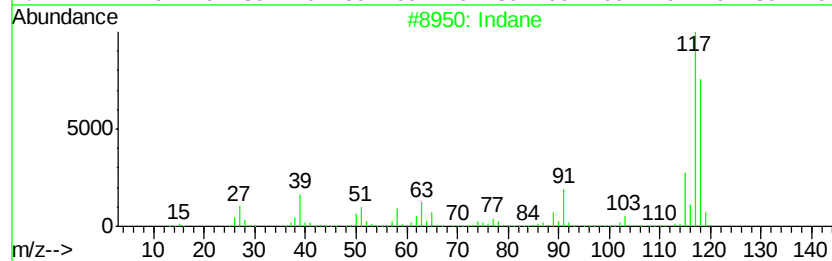
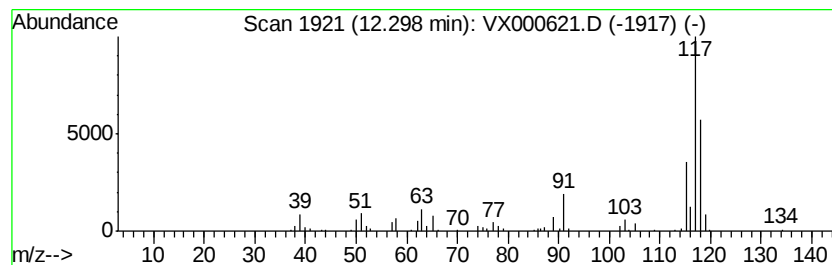
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	9.34 ug/l	123295	1,4-Dichlorobenzene-d4	12.09

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	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	64
5	trans-Cinnamyl bromide		196	C9H9Br	026146-77-0	64



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000621.D
Acq On : 01 Apr 2018 04:03
Operator : JC/MD
Sample : J2132-07 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.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-	1.79	6.9	ug/l	43204	1	5.68	314259	50.0
Pentane	2.00	5.1	ug/l	31980	1	5.68	314259	50.0
Cyclopentane, met...	4.40	9.4	ug/l	59109	1	5.68	314259	50.0
Benzene, 1-ethyl-...	11.44	21.6	ug/l	285973	4	12.09	660335	50.0
Benzene, 1-ethyl-...	11.68	7.4	ug/l	97778	4	12.09	660335	50.0
Mesitylene	12.15	7.9	ug/l	104298	4	12.09	660335	50.0
Indane	12.30	9.3	ug/l	123295	4	12.09	660335	50.0