

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
 Data File : VX000623.D
 Acq On : 01 Apr 2018 04:54
 Operator : JC/MD
 Sample : J2132-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 44 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	76	80	93	rBV	494336	570957	2.20%	0.356%
2	1.300	114	117	130	rVB	918361	938992	3.63%	0.585%
3	1.404	130	134	140	rBV	3829509	3950823	15.26%	2.462%
4	1.794	192	198	216	rBV	20075801	25895602	100.00%	16.139%
5	2.001	228	232	246	rVB2	2421574	3965808	15.31%	2.472%
6	2.123	246	252	258	rBV	570914	822957	3.18%	0.513%
7	2.221	263	268	271	rVV	234617	335332	1.29%	0.209%
8	2.270	271	276	287	rVB	1140150	1751546	6.76%	1.092%
9	2.398	287	297	303	rBV	417185	820241	3.17%	0.511%
10	2.788	350	361	363	rBV4	133319	309851	1.20%	0.193%
11	2.849	364	371	374	rVV	986574	2248486	8.68%	1.401%
12	2.892	374	378	382	rVV	2118055	4382664	16.92%	2.731%
13	2.934	382	385	405	rVB2	1450264	3298691	12.74%	2.056%
14	3.178	414	425	446	rVB	1786441	4031876	15.57%	2.513%
15	3.398	452	461	472	rBV2	159523	401104	1.55%	0.250%
16	3.526	473	482	494	rVB	194057	437198	1.69%	0.272%
17	3.818	523	530	539	rVB	257964	619832	2.39%	0.386%
18	3.928	539	548	554	rBV2	181881	467889	1.81%	0.292%
19	4.202	584	593	602	rVB	203553	515415	1.99%	0.321%
20	4.410	616	627	639	rVB	1285099	3701739	14.29%	2.307%
21	5.312	750	775	790	rVB3	165316	652686	2.52%	0.407%
22	5.513	793	808	812	rVV3	97440	297174	1.15%	0.185%
23	5.586	812	820	829	rVV3	480096	1597845	6.17%	0.996%
24	5.678	829	835	839	rVV2	150781	449469	1.74%	0.280%
25	5.732	840	844	864	rVB4	180149	561193	2.17%	0.350%
26	5.940	864	878	892	rBV4	189936	612874	2.37%	0.382%
27	6.153	907	913	922	rVV	110595	305935	1.18%	0.191%
28	6.263	923	931	941	rVV5	194896	875603	3.38%	0.546%
29	6.360	942	947	957	rVV4	241354	805741	3.11%	0.502%
30	6.464	957	964	976	rVB2	174313	487898	1.88%	0.304%
31	6.872	1022	1031	1038	rBV2	232791	695712	2.69%	0.434%
32	6.952	1040	1044	1057	rVB3	159332	392321	1.52%	0.245%
33	7.470	1117	1129	1141	rBV3	542849	1408736	5.44%	0.878%
34	7.964	1199	1210	1217	rBV3	89488	294524	1.14%	0.184%

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35	8.586	1306	1312	1320	rVB3	163850	370247	1.43%	0.231%
36	8.726	1329	1335	1340	rVB	482147	777806	3.00%	0.485%
37	8.793	1340	1346	1352	rBV	1222034	1815333	7.01%	1.131%
38	10.122	1553	1564	1569	rBV	528248	765305	2.96%	0.477%
39	10.262	1581	1587	1598	rBV	10274391	12841194	49.59%	8.003%
40	10.372	1598	1605	1611	rVB	9833953	13054459	50.41%	8.136%
41	10.707	1655	1660	1669	rVB	1078390	1366630	5.28%	0.852%
42	11.024	1706	1712	1719	rBV	964128	1204263	4.65%	0.751%
43	11.146	1724	1732	1737	rBV	542241	697700	2.69%	0.435%
44	11.366	1760	1768	1774	rBV	1849877	2266140	8.75%	1.412%
45	11.445	1774	1781	1782	rVV	2235490	2835257	10.95%	1.767%
46	11.463	1782	1784	1788	rVV	2240785	2383437	9.20%	1.485%
47	11.512	1788	1792	1798	rVB	2465100	3043779	11.75%	1.897%
48	11.677	1813	1819	1829	rBV	1932156	2345548	9.06%	1.462%
49	11.817	1837	1842	1847	rVB	3874170	4583265	17.70%	2.856%
50	12.085	1881	1886	1892	rVB2	869578	1116745	4.31%	0.696%
51	12.152	1892	1897	1901	rBV	705535	856931	3.31%	0.534%
52	12.311	1917	1923	1930	rBV	8063926	10150192	39.20%	6.326%
53	12.378	1930	1934	1942	rVB3	867856	1359357	5.25%	0.847%
54	12.475	1944	1950	1954	rBV2	392481	549120	2.12%	0.342%
55	12.524	1954	1958	1964	rVB	298317	356185	1.38%	0.222%
56	12.597	1964	1970	1972	rBV	897481	1157945	4.47%	0.722%
57	12.615	1972	1973	1978	rVB	372260	342906	1.32%	0.214%
58	12.676	1978	1983	1986	rBV	1603673	1873616	7.24%	1.168%
59	12.713	1986	1989	1993	rVV	549809	650900	2.51%	0.406%
60	12.762	1993	1997	2005	rVB	2513187	3252072	12.56%	2.027%
61	12.987	2026	2034	2037	rBV	873755	1081435	4.18%	0.674%
62	13.024	2037	2040	2046	rVB	955623	1185148	4.58%	0.739%
63	13.231	2070	2074	2080	rVB	1590569	1945967	7.51%	1.213%
64	13.359	2090	2095	2100	rVB2	3869035	4890955	18.89%	3.048%
65	13.408	2100	2103	2106	rBV3	215219	268639	1.04%	0.167%
66	13.487	2112	2116	2123	rVB	502866	639902	2.47%	0.399%
67	13.609	2132	2136	2139	rVV	395336	498932	1.93%	0.311%
68	13.652	2139	2143	2148	rVB2	275977	502153	1.94%	0.313%
69	13.731	2153	2156	2162	rVB2	405298	593110	2.29%	0.370%
70	13.841	2167	2174	2184	rVV	4155563	5387823	20.81%	3.358%
71	13.938	2184	2190	2194	rVB	370178	508787	1.96%	0.317%

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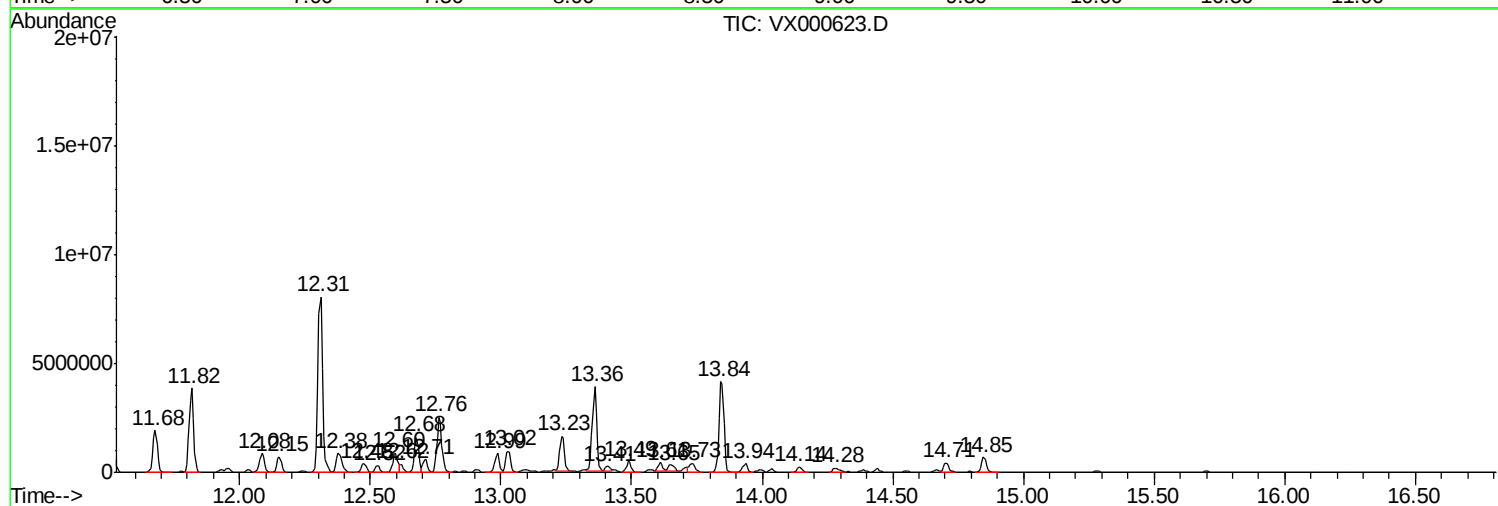
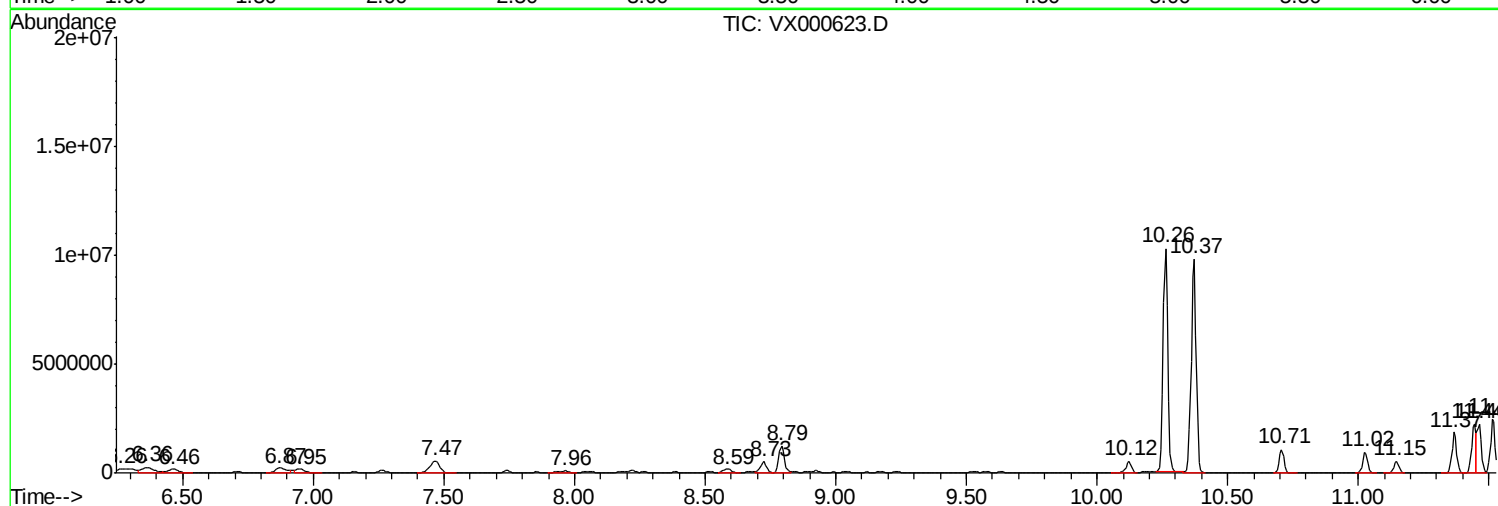
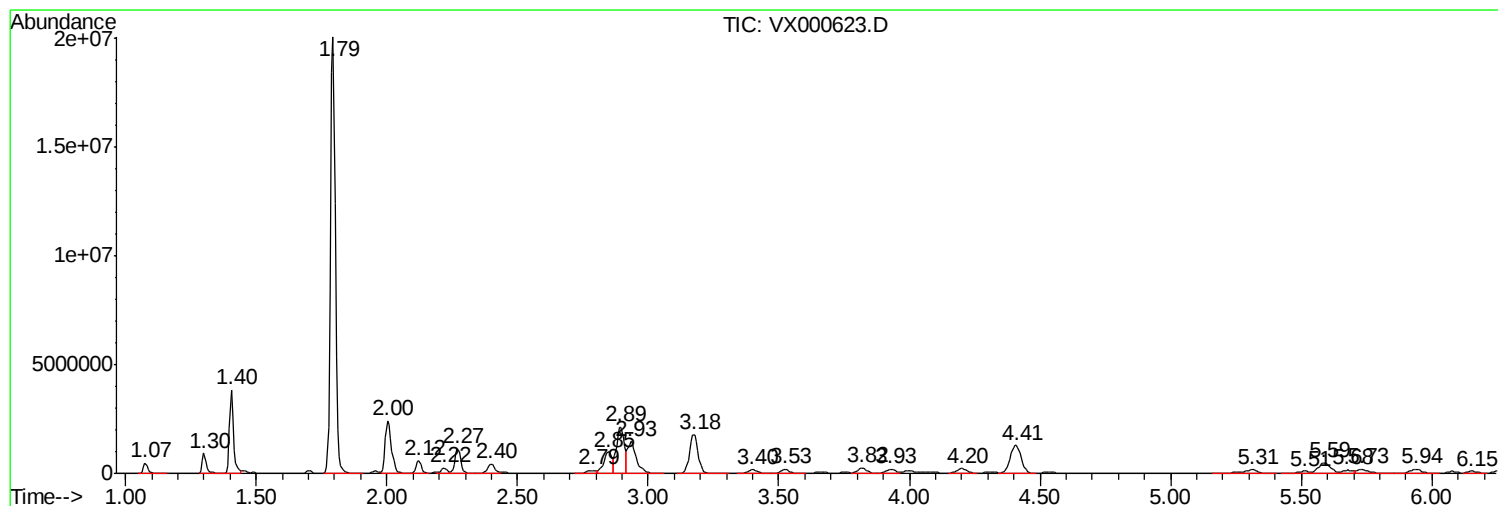
72	14.139	2218	2223	2229	rBV	254827	322854	1.25%	0.201%
73	14.280	2242	2246	2252	rBV2	187555	311003	1.20%	0.194%
74	14.706	2312	2316	2321	rVB	398785	504574	1.95%	0.314%
75	14.847	2334	2339	2348	rBV2	677240	895601	3.46%	0.558%

Sum of corrected areas: 160457929

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Quant Title : SW846 8260

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



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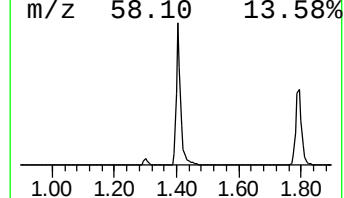
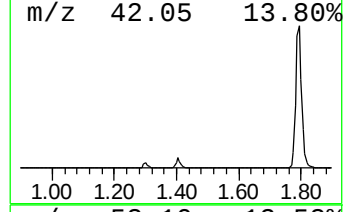
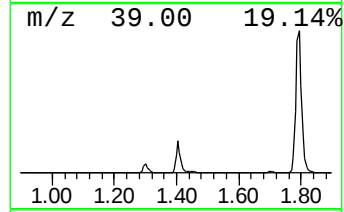
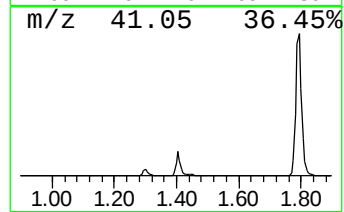
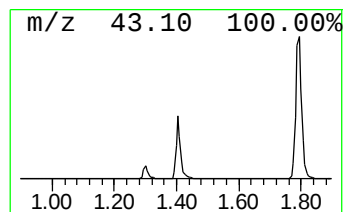
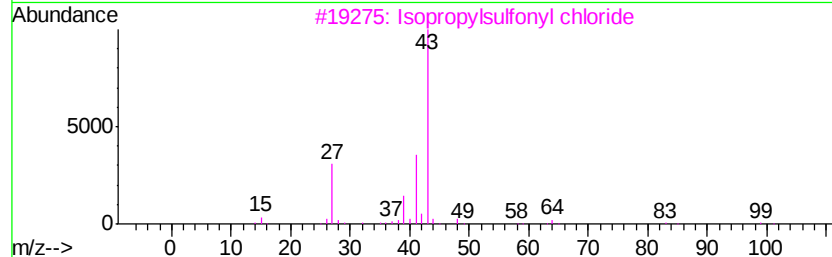
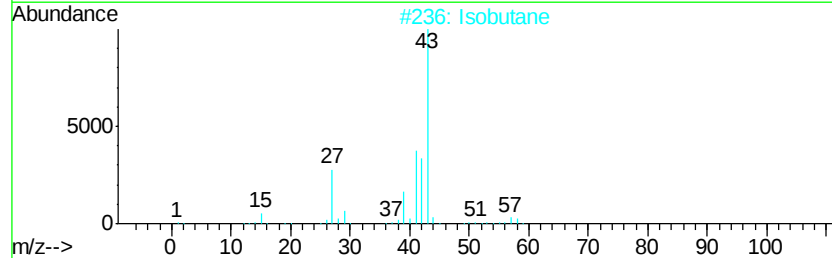
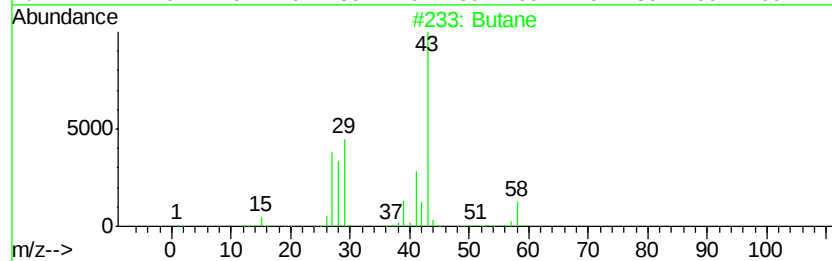
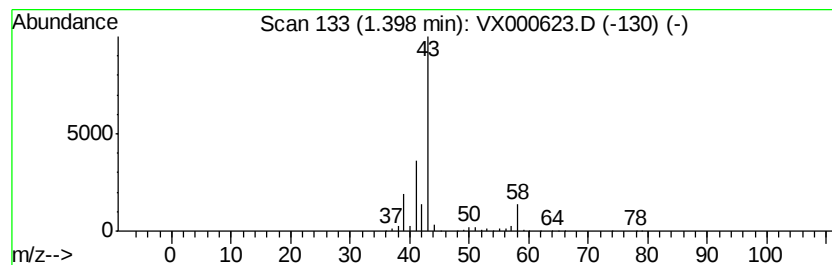
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	439.50 ug/l	3950820	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane	58	C4H10	000106-97-8	80
2		Isobutane	58	C4H10	000075-28-5	9
3		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5		Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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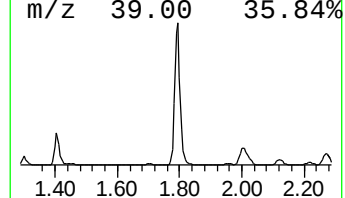
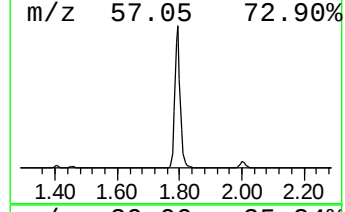
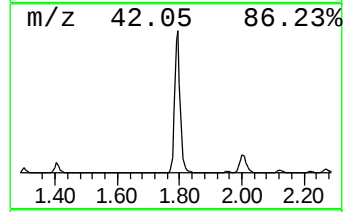
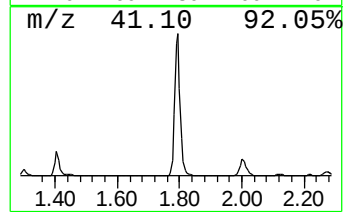
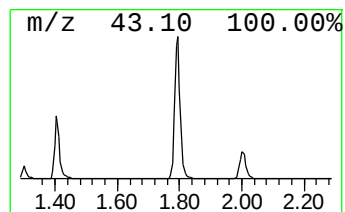
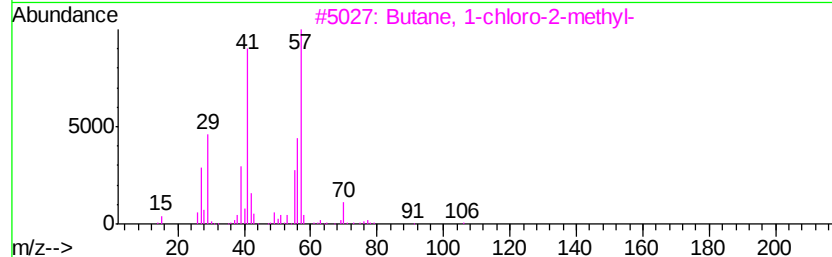
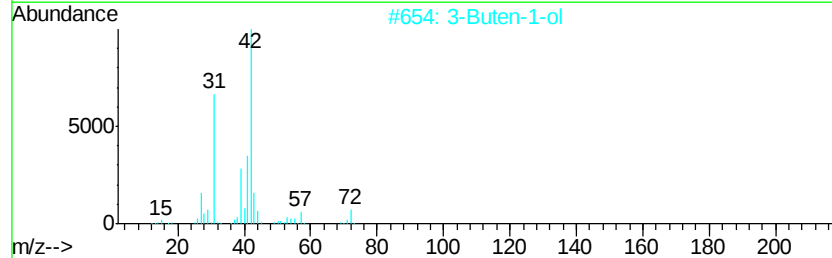
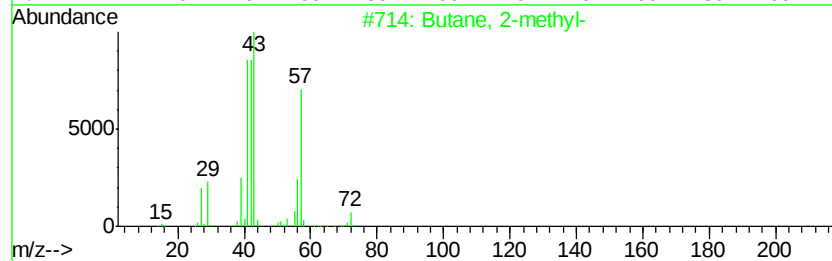
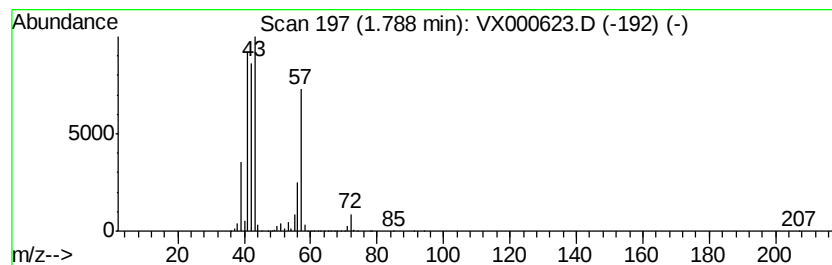
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	2880.69 ug/l	25895600	Pentafluorobenzene	5.67

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	43
3		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4		Pentane	72	C5H12	000109-66-0	28
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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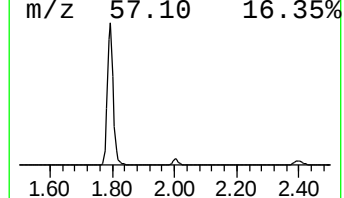
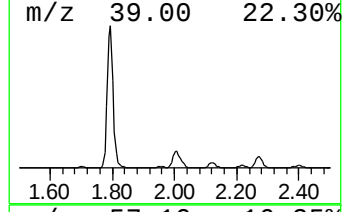
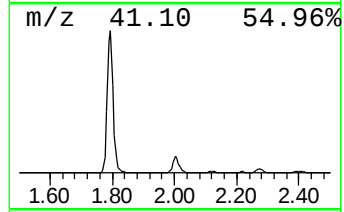
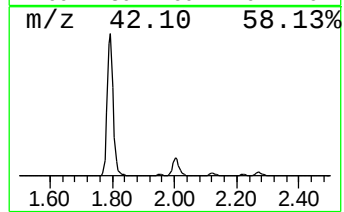
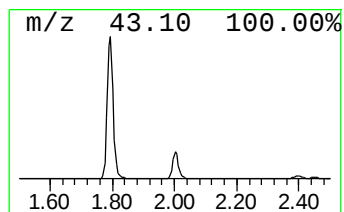
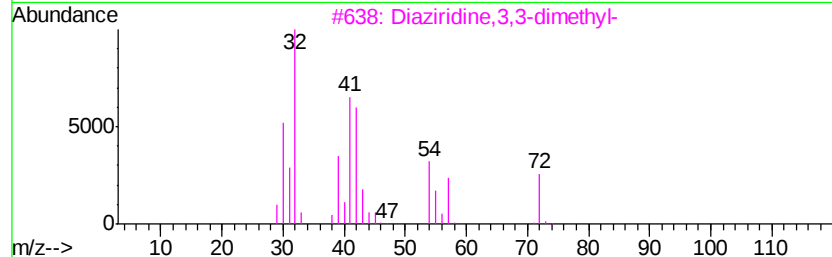
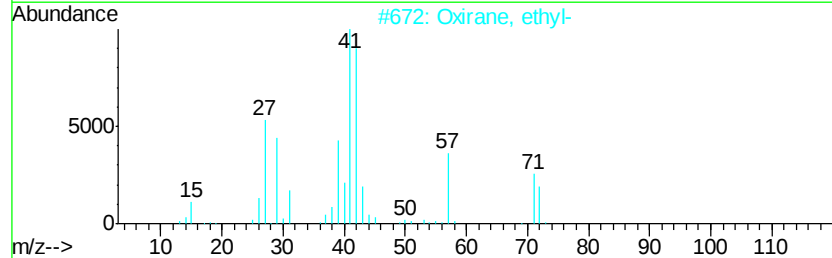
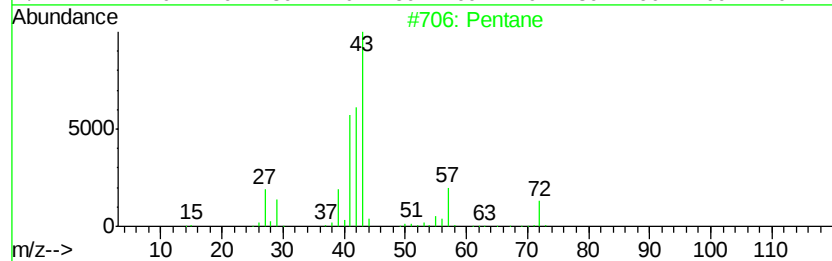
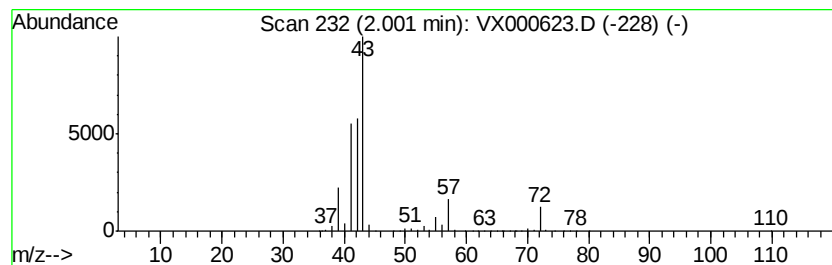
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	441.17 ug/l	3965810	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	90
2		Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	36
5		Cyclobutylamine	71	C4H9N	002516-34-9	9



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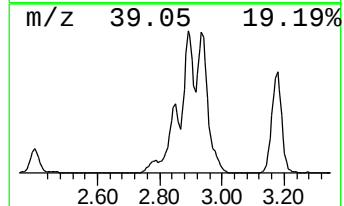
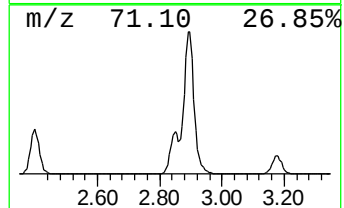
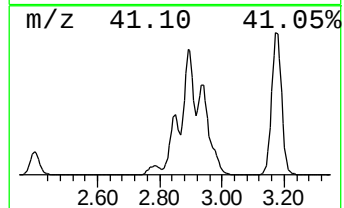
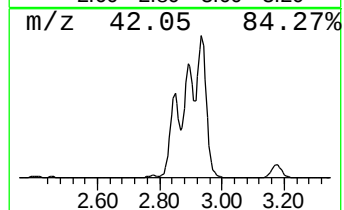
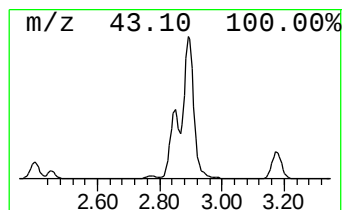
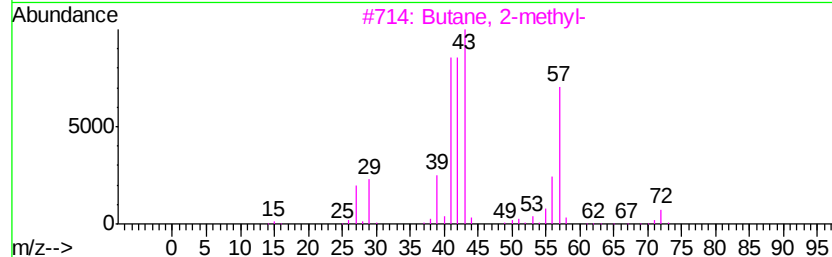
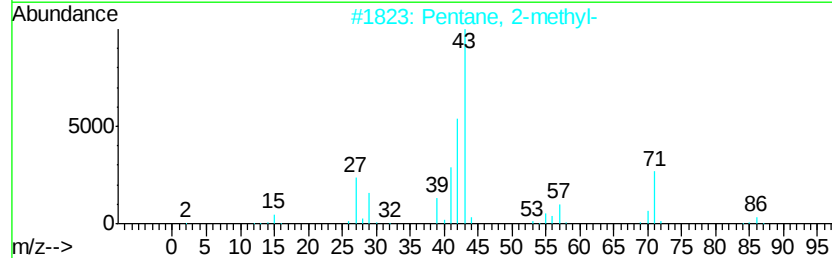
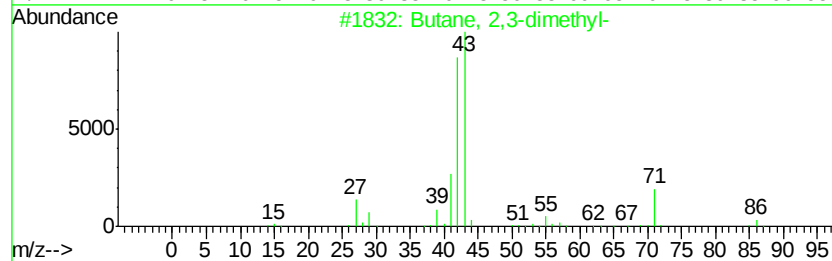
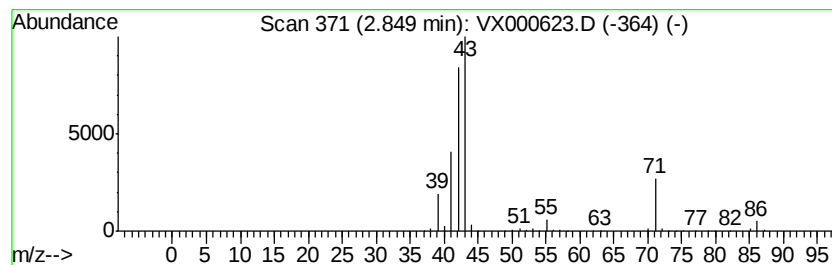
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	250.13 ug/l	2248490	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Butane, 2-methyl-	72	C5H12	000078-78-4	9
4		Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	9
5		Tetrahydrofuran	72	C4H8O	000109-99-9	9



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 44 Sample Multiplier: 1

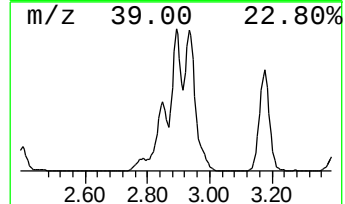
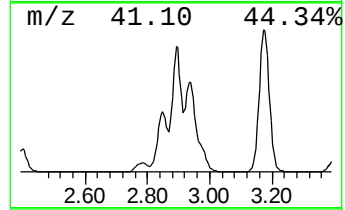
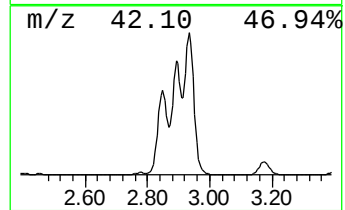
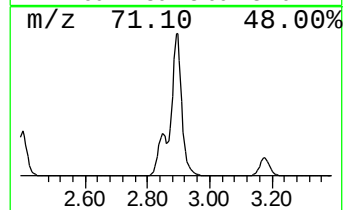
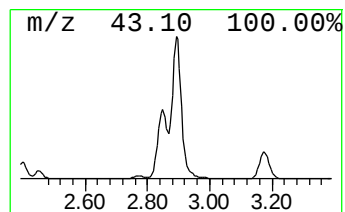
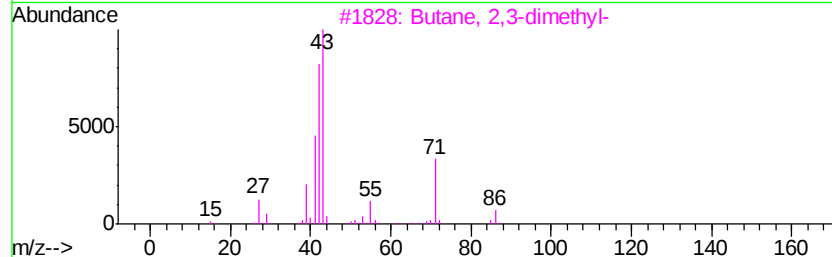
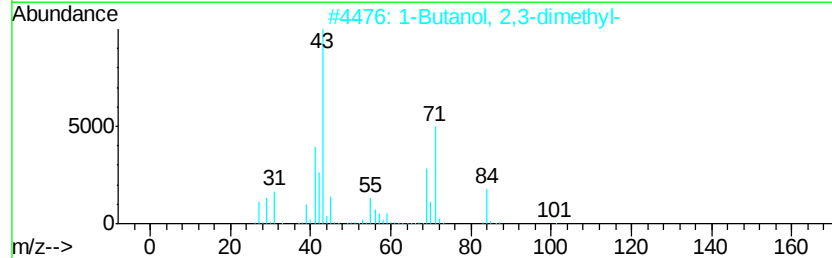
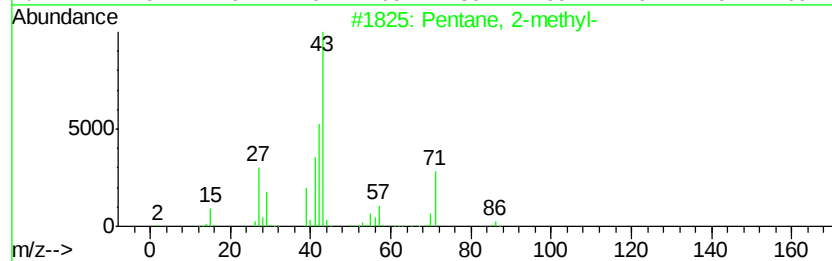
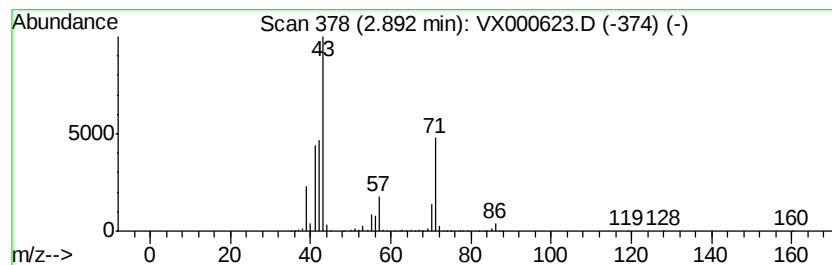
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	487.54 ug/l	4382660	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
4		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 44 Sample Multiplier: 1

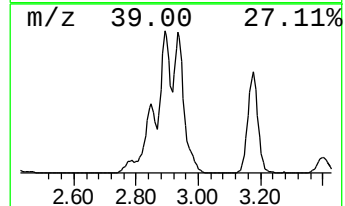
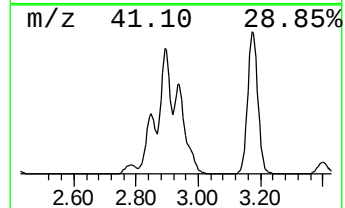
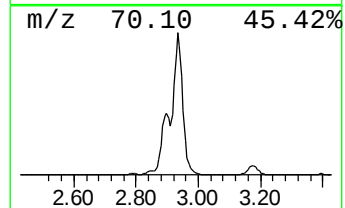
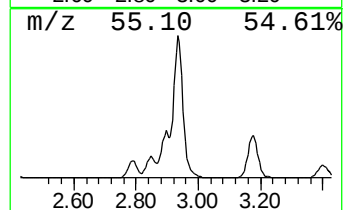
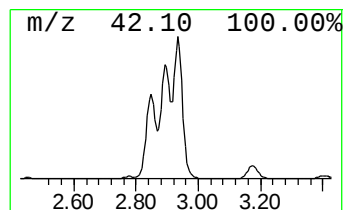
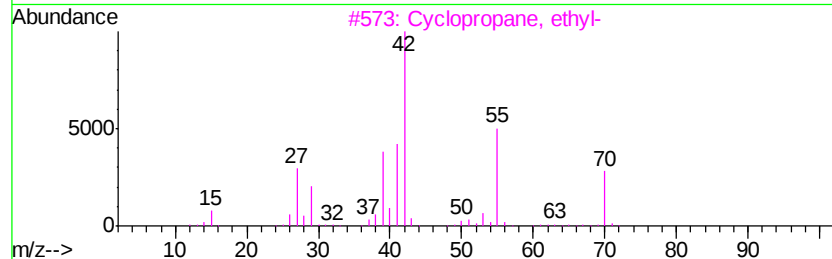
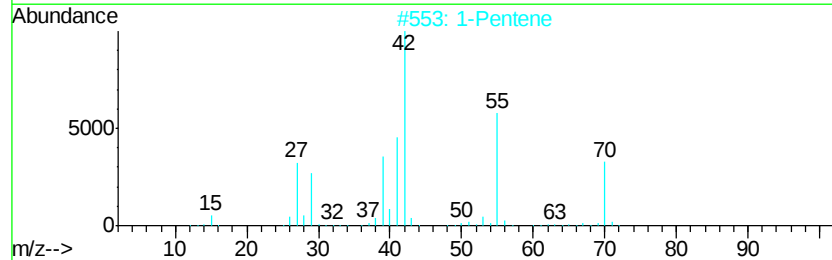
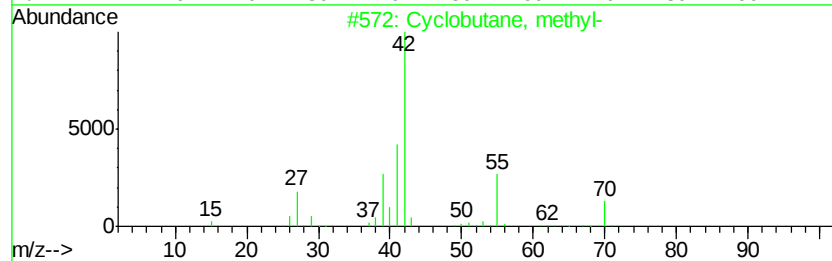
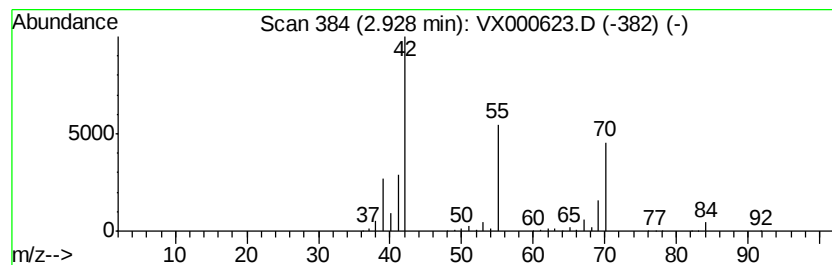
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclobutane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	366.95 ug/l	3298690	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2		1-Pentene	70	C5H10	000109-67-1	78
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
4		2-Pentene, (E)-	70	C5H10	000646-04-8	38
5		2-Pentene, (Z)-	70	C5H10	000627-20-3	37



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 44 Sample Multiplier: 1

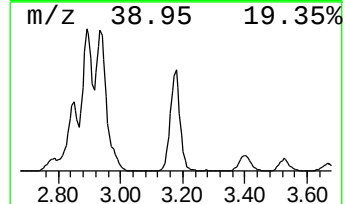
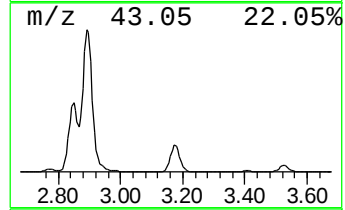
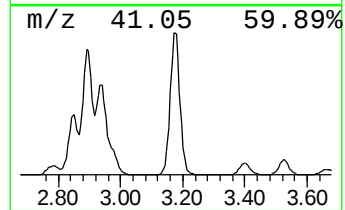
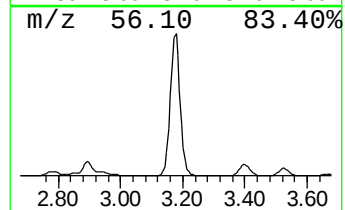
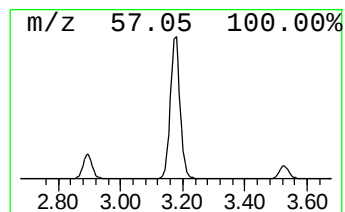
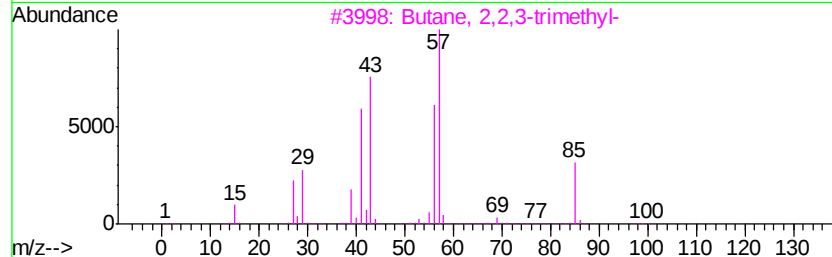
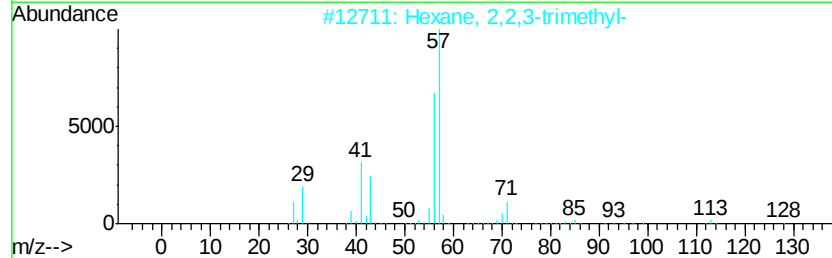
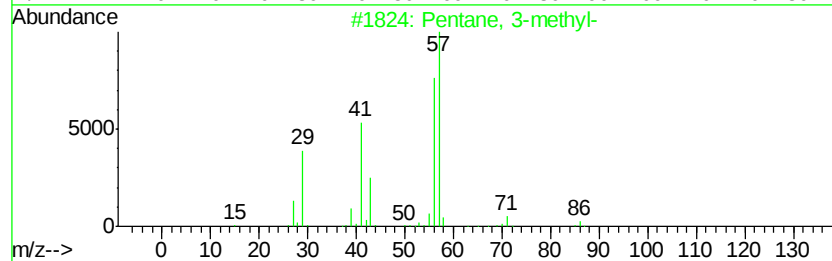
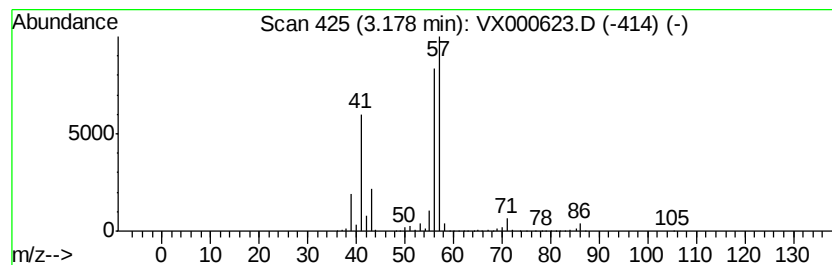
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 7 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	448.52 ug/l	4031880	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
4		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5		1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	40



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 44 Sample Multiplier: 1

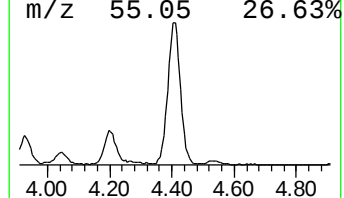
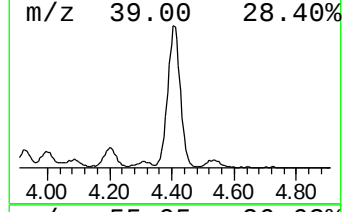
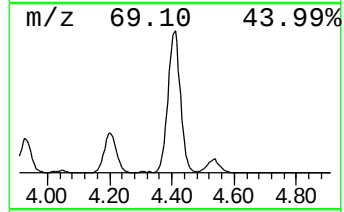
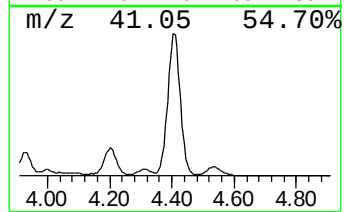
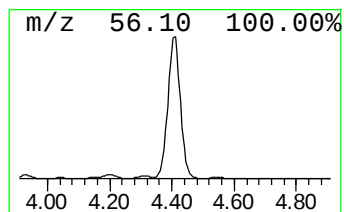
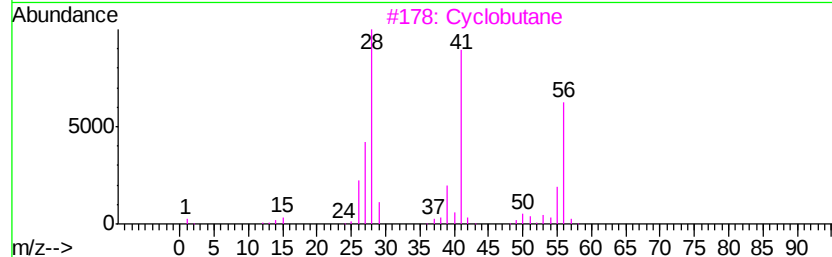
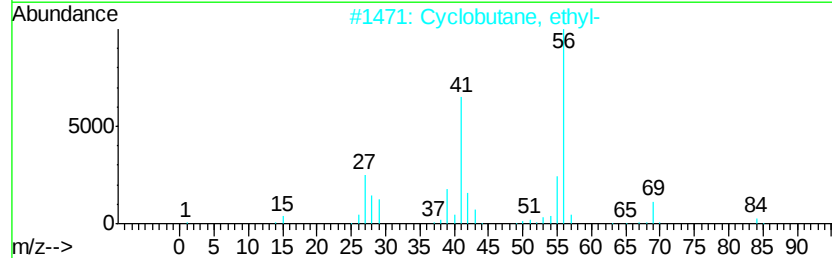
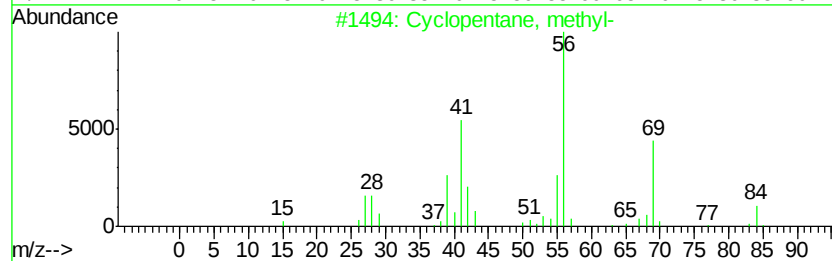
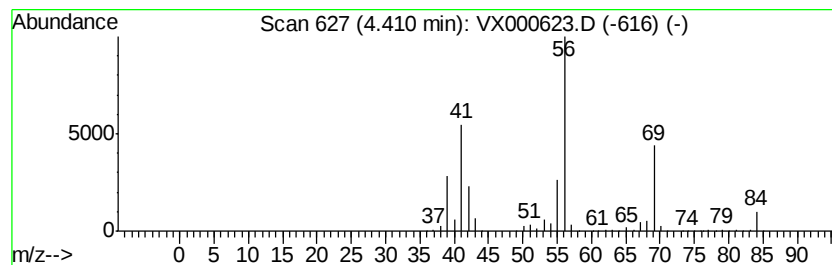
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	411.79 ug/l	3701740	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3		Cyclobutane	56	C4H8	000287-23-0	53
4		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53
5		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 44 Sample Multiplier: 1

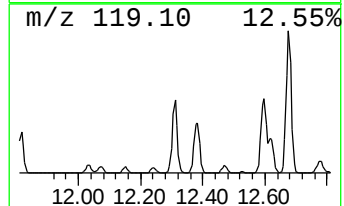
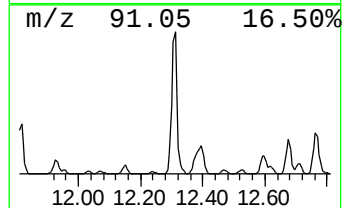
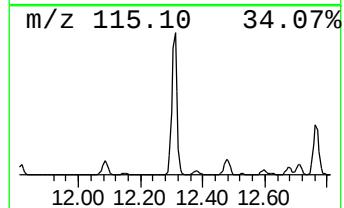
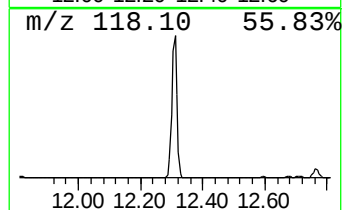
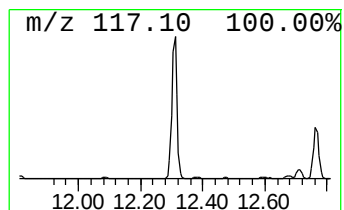
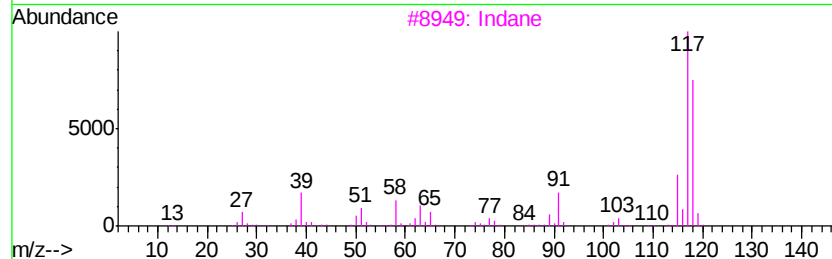
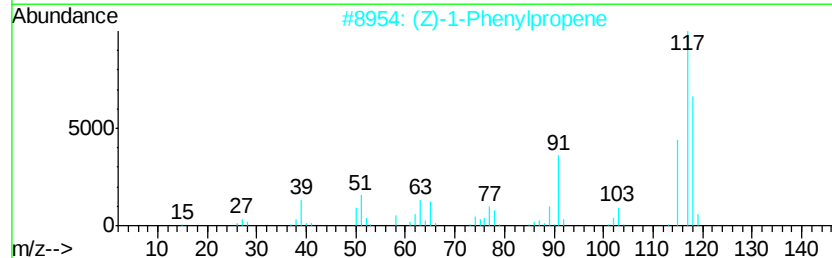
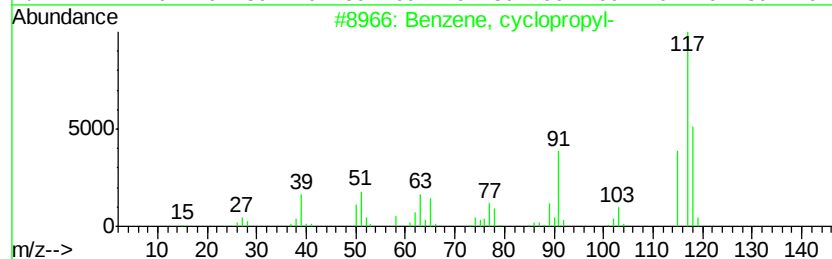
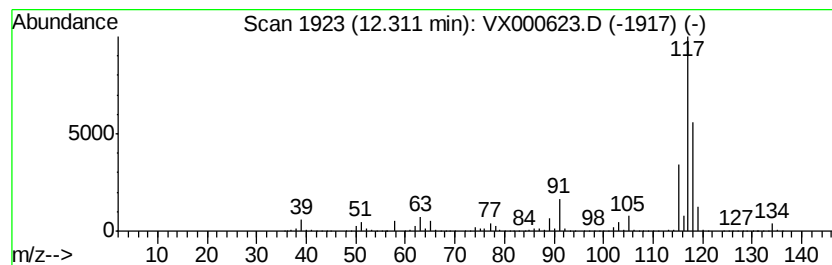
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, cyclopropyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	454.45 ug/l	10150200	1,4-Dichlorobenzene-d4	12.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, cvclopropyl-	118	C9H10	000873-49-4	81
2		(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81
3		Indane	118	C9H10	000496-11-7	81
4		Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5		Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 44 Sample Multiplier: 1

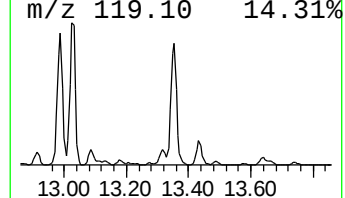
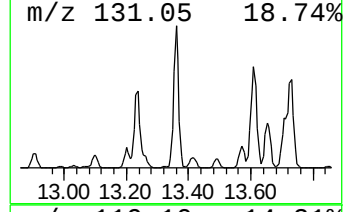
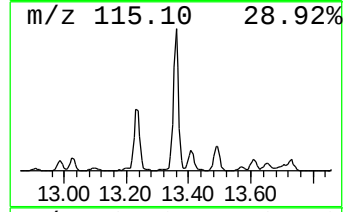
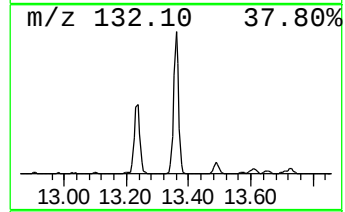
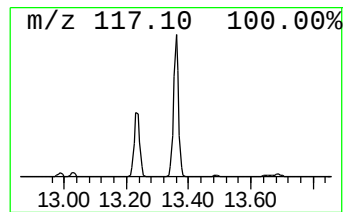
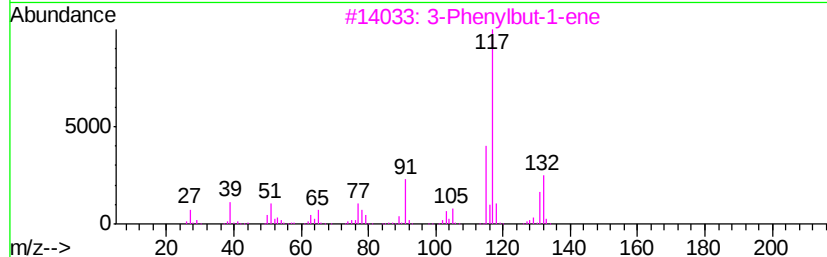
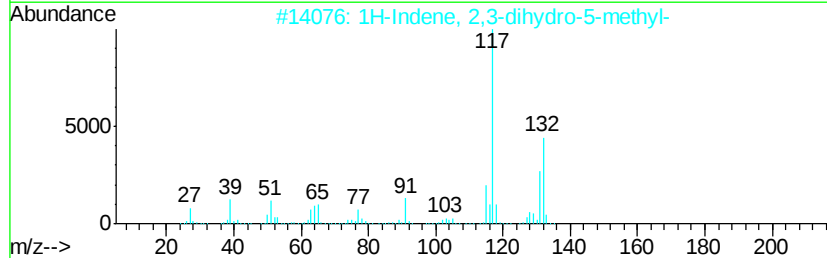
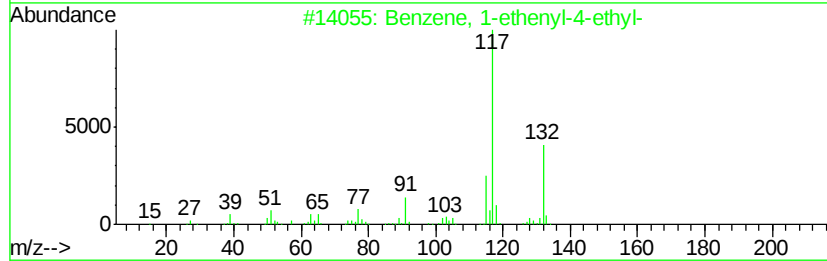
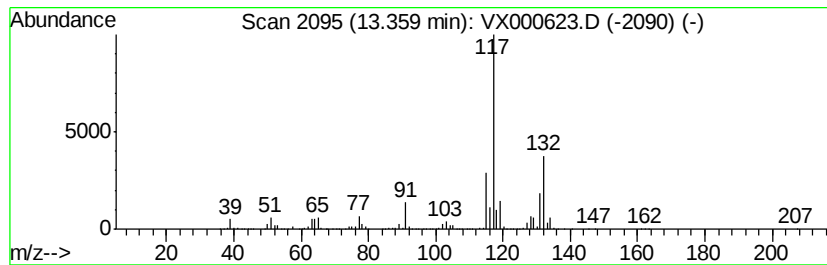
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	218.98 ug/l	4890960	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000623.D
Acq On : 01 Apr 2018 04:54
Operator : JC/MD
Sample : J2132-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 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
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Butane, 2-methyl-	1.79	2880.7	ug/l	25895600	1	5.67	449469	50.0
Pentane	2.00	441.2	ug/l	3965810	1	5.67	449469	50.0
Butane, 2,3-dimet...	2.85	250.1	ug/l	2248490	1	5.67	449469	50.0
Pentane, 2-methyl-	2.89	487.5	ug/l	4382660	1	5.67	449469	50.0
Cyclobutane, methyl-	2.93	366.9	ug/l	3298690	1	5.67	449469	50.0
Pentane, 3-methyl-	3.18	448.5	ug/l	4031880	1	5.67	449469	50.0
Cyclopentane, met...	4.41	411.8	ug/l	3701740	1	5.67	449469	50.0
Benzene, cyclopro...	12.31	454.4	ug/l	10150200	4	12.09	1116750	50.0
Benzene, 1-etheny...	13.36	219.0	ug/l	4890960	4	12.09	1116750	50.0