

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX080918\
 Data File : VX003951.D
 Acq On : 09 Aug 2018 15:30
 Operator : JC/MD
 Sample : J4387-10
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0567

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\82X080618W.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	73	80	95	rBV	1240054	1702479	7.59%	1.262%
2	1.398	130	133	139	rBV	246324	248762	1.11%	0.184%
3	1.788	191	197	210	rVB	1722495	2382586	10.63%	1.766%
4	1.996	226	231	242	rVB	488441	705258	3.15%	0.523%
5	2.843	361	370	374	rBV	655910	1461285	6.52%	1.083%
6	2.886	374	377	382	rVB	334595	577728	2.58%	0.428%
7	3.166	414	423	441	rVB	621863	1418434	6.33%	1.051%
8	3.520	472	481	494	rVB	160704	367358	1.64%	0.272%
9	4.300	597	609	615	rBV	115022	341511	1.52%	0.253%
10	4.398	615	625	640	rVB	889484	2606813	11.63%	1.932%
11	5.507	795	807	811	rBV2	225409	643351	2.87%	0.477%
12	5.574	811	818	828	rVV3	833841	2931659	13.08%	2.173%
13	5.666	828	833	838	rVV	346007	966812	4.31%	0.717%
14	5.720	838	842	861	rVB	298328	833851	3.72%	0.618%
15	5.928	861	876	890	rBV4	347585	1190467	5.31%	0.883%
16	6.074	890	900	908	rBV	235271	597548	2.67%	0.443%
17	6.257	919	930	937	rBV2	253540	799088	3.56%	0.592%
18	6.348	938	945	954	rVV3	471269	1428252	6.37%	1.059%
19	6.452	954	962	978	rVB2	356970	988883	4.41%	0.733%
20	6.867	1019	1030	1039	rBV	498843	1182348	5.27%	0.876%
21	7.464	1113	1128	1140	rBV	2414928	5591933	24.94%	4.145%
22	7.732	1166	1172	1182	rVB	274810	532281	2.37%	0.395%
23	7.848	1182	1191	1199	rVB2	143487	306315	1.37%	0.227%
24	8.055	1213	1225	1234	rVB2	356890	893572	3.99%	0.662%
25	8.177	1237	1245	1253	rBV	482699	992702	4.43%	0.736%
26	8.385	1275	1279	1285	rVB2	170266	313910	1.40%	0.233%
27	8.500	1294	1298	1302	rBV	179908	297698	1.33%	0.221%
28	8.665	1318	1325	1329	rBV2	506481	980223	4.37%	0.727%
29	8.714	1329	1333	1342	rVB	1266615	2191138	9.77%	1.624%
30	8.842	1348	1354	1358	rBV	288188	487960	2.18%	0.362%
31	9.043	1381	1387	1393	rVB	552796	882138	3.93%	0.654%
32	9.165	1398	1407	1413	rBV	282049	462136	2.06%	0.343%
33	9.573	1468	1474	1478	rBV3	217008	362893	1.62%	0.269%
34	9.622	1478	1482	1487	rVB	476737	656311	2.93%	0.487%

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Integrator: RTE
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35	9.677	1487	1491	1496	rBV	328020	487751	2.18%	0.362%
36	10.116	1558	1563	1568	rBV	1091683	1409810	6.29%	1.045%
37	10.189	1568	1575	1579	rBV	273876	388127	1.73%	0.288%
38	10.256	1579	1586	1591	rVB	1479545	1984642	8.85%	1.471%
39	10.360	1594	1603	1610	rBV	16217530	22418626	100.00%	16.619%
40	10.646	1639	1650	1655	rBV3	128183	358977	1.60%	0.266%
41	10.701	1655	1659	1669	rVB	490012	681165	3.04%	0.505%
42	10.835	1670	1681	1689	rBV2	174666	332470	1.48%	0.246%
43	10.915	1689	1694	1702	rBV5	125712	229038	1.02%	0.170%
44	11.018	1706	1711	1717	rBV	1584558	2001166	8.93%	1.483%
45	11.140	1725	1731	1735	rBV	1093429	1351709	6.03%	1.002%
46	11.360	1762	1767	1774	rBV	1887318	2326523	10.38%	1.725%
47	11.439	1774	1780	1787	rVV	4983255	9436167	42.09%	6.995%
48	11.506	1787	1791	1800	rVB	4608626	5713102	25.48%	4.235%
49	11.671	1812	1818	1826	rBV	3677234	4422777	19.73%	3.279%
50	11.811	1836	1841	1846	rVB	9732860	11510538	51.34%	8.533%
51	11.921	1853	1859	1861	rBV	170045	239289	1.07%	0.177%
52	11.945	1861	1863	1869	rVB	322398	398381	1.78%	0.295%
53	12.030	1869	1877	1880	rBV	610026	776170	3.46%	0.575%
54	12.079	1880	1885	1890	rVB2	1476850	2055313	9.17%	1.524%
55	12.146	1890	1896	1901	rBV	3778812	4453923	19.87%	3.302%
56	12.305	1915	1922	1924	rBV	1103796	1577282	7.04%	1.169%
57	12.372	1929	1933	1942	rVB3	1250641	1817340	8.11%	1.347%
58	12.463	1943	1948	1953	rBV	203691	258902	1.15%	0.192%
59	12.518	1953	1957	1963	rVB	554945	689265	3.07%	0.511%
60	12.591	1963	1969	1970	rBV	580482	703021	3.14%	0.521%
61	12.610	1970	1972	1977	rVV	644600	765567	3.41%	0.568%
62	12.670	1977	1982	1985	rVV	825062	914209	4.08%	0.678%
63	12.701	1985	1987	1992	rVB	185142	225052	1.00%	0.167%
64	12.762	1992	1997	2004	rVB3	536169	1095649	4.89%	0.812%
65	12.902	2016	2020	2025	rVB2	509321	718373	3.20%	0.533%
66	12.981	2025	2033	2036	rBV	634974	861738	3.84%	0.639%
67	13.018	2036	2039	2046	rVB	1041002	1292431	5.76%	0.958%
68	13.085	2046	2050	2055	rBV2	176303	330330	1.47%	0.245%
69	13.225	2070	2073	2077	rVB2	219299	254707	1.14%	0.189%
70	13.347	2089	2093	2099	rVB2	1770002	2370828	10.58%	1.758%
71	13.481	2109	2115	2124	rVB	738796	945129	4.22%	0.701%

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Integration Parameters: RTEINT.P

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72	13.640	2137	2141	2146	rBV4	273950	468094	2.09%	0.347%
73	13.725	2153	2155	2160	rVB2	262942	364421	1.63%	0.270%
74	13.835	2165	2173	2181	rVB	1777236	2527015	11.27%	1.873%
75	13.987	2191	2198	2202	rBV2	250925	394194	1.76%	0.292%
76	14.292	2241	2248	2255	rVB2	288389	570828	2.55%	0.423%
77	14.542	2284	2289	2298	rBV2	314003	444987	1.98%	0.330%
78	14.701	2308	2315	2319	rBV	1305320	1683292	7.51%	1.248%
79	14.841	2333	2338	2347	rBV	1093817	1384218	6.17%	1.026%
80	15.554	2449	2455	2460	rBV	201733	315468	1.41%	0.234%
81	15.694	2470	2478	2481	rBV	235633	396764	1.77%	0.294%
82	15.731	2481	2484	2492	rVB	156041	226069	1.01%	0.168%

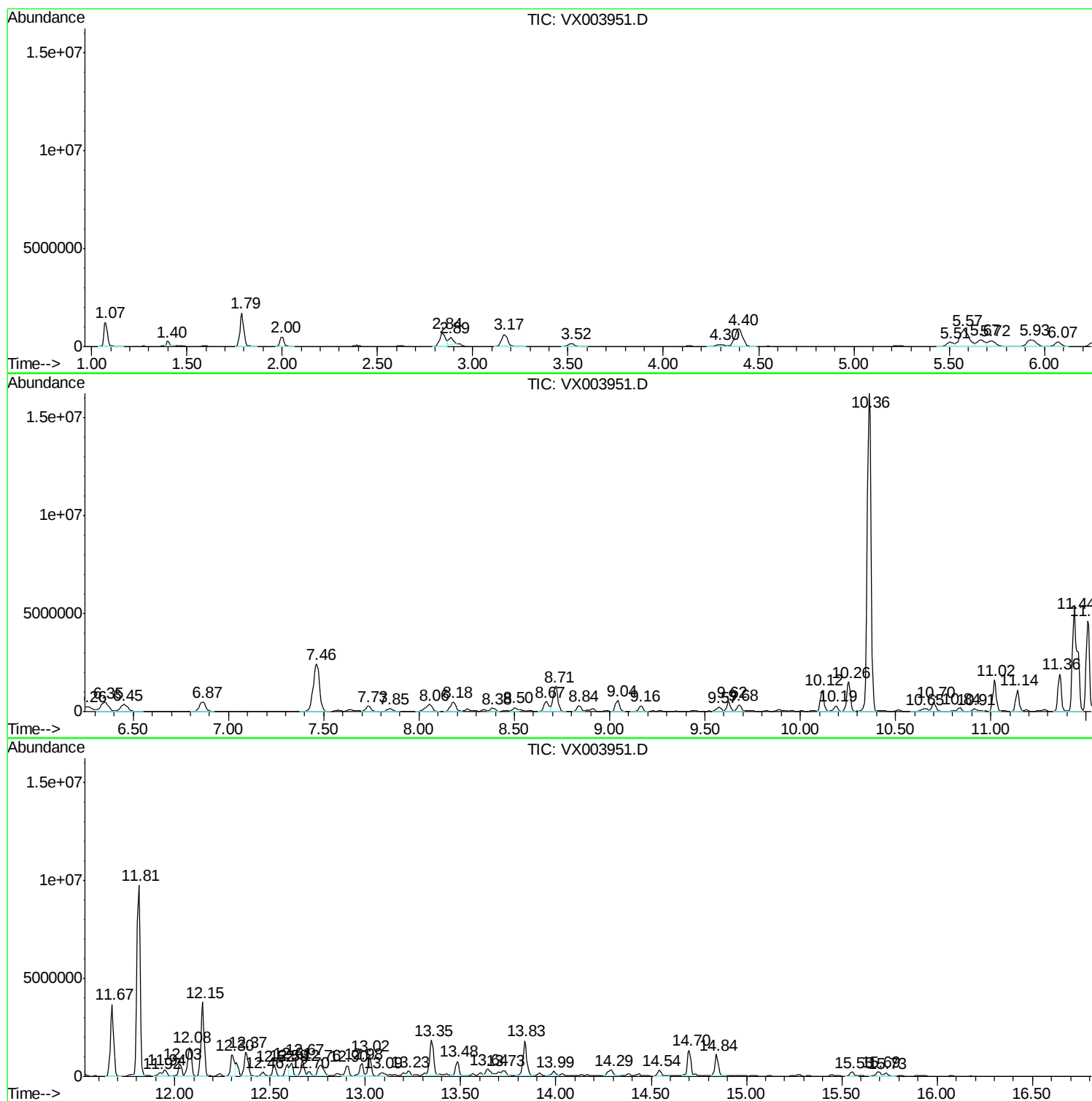
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X080618W.M
Quant Title : SW846 8260

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



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Instrument :
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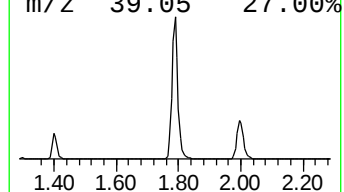
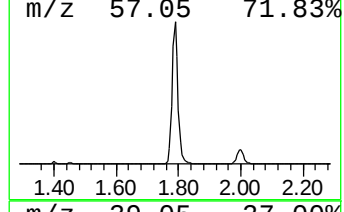
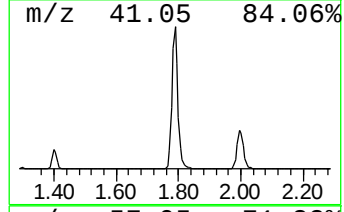
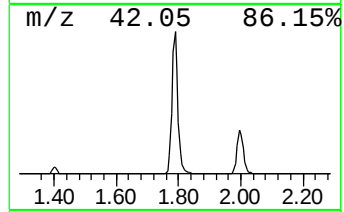
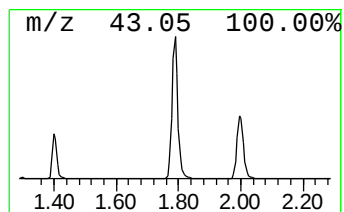
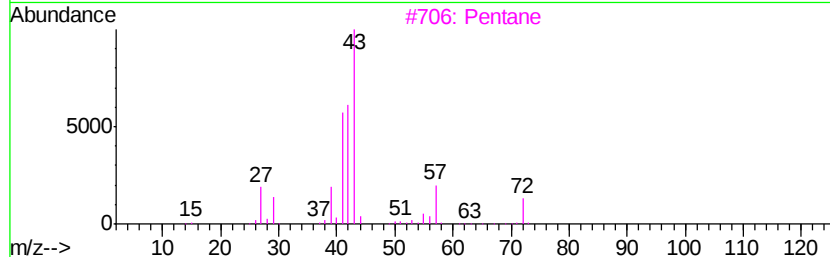
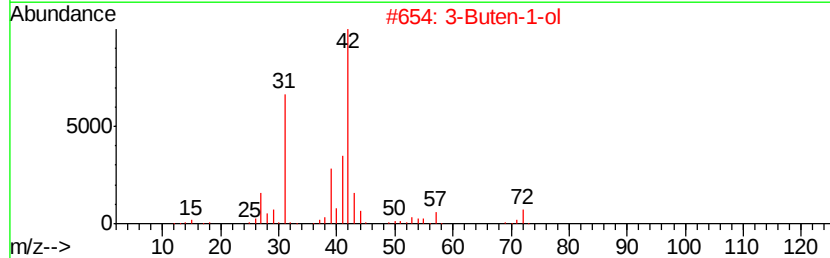
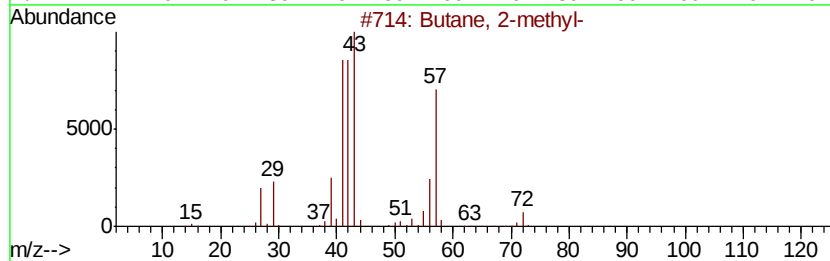
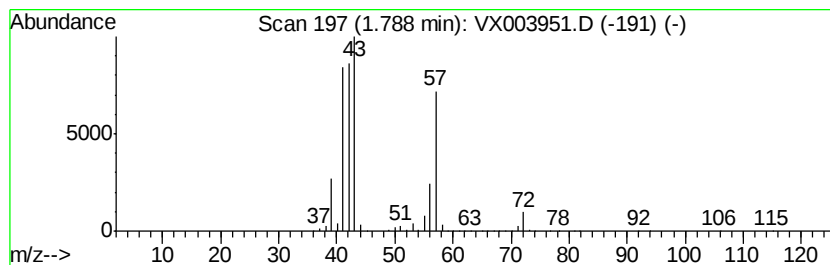
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X080618W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	123.22 ug/l	2382590	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	47
3		Pentane	72	C5H12	000109-66-0	43
4		1-Butene	56	C4H8	000106-98-9	10
5		Cyclobutane	56	C4H8	000287-23-0	9



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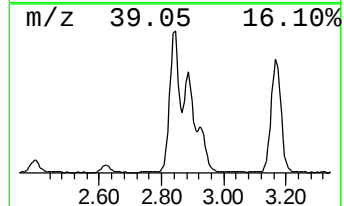
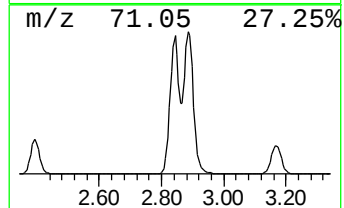
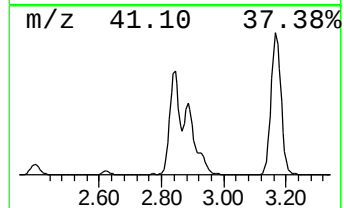
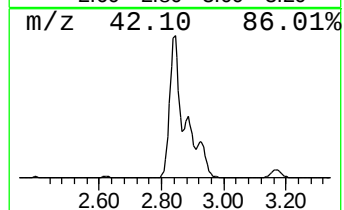
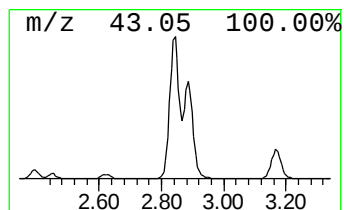
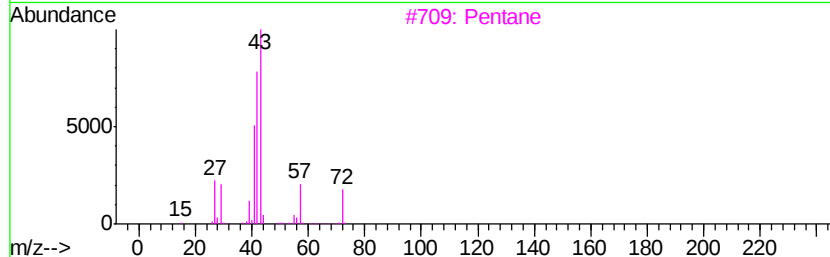
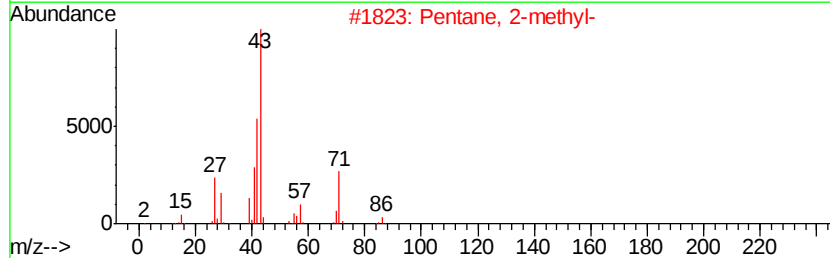
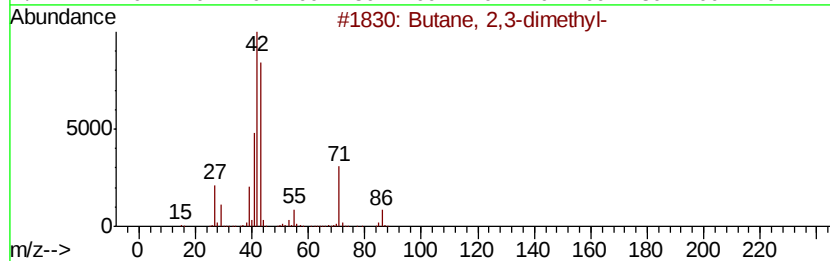
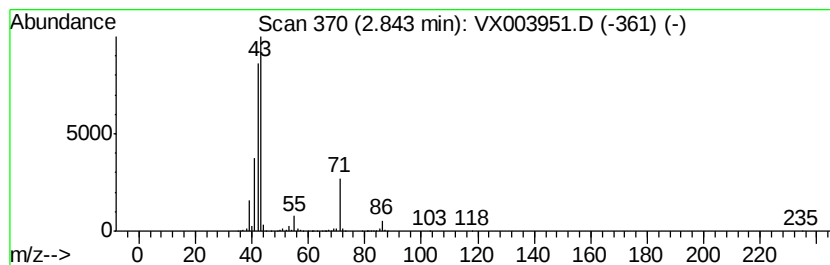
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	75.57 ug/l	1461290	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Pentane	72	C5H12	000109-66-0	36
4		C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	12
5		Pyrrolidine	71	C4H9N	000123-75-1	10



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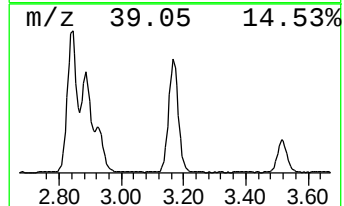
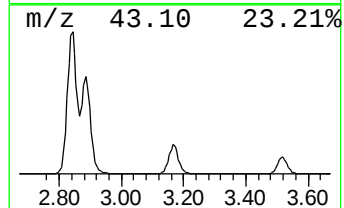
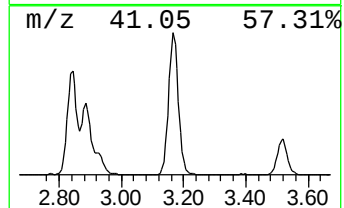
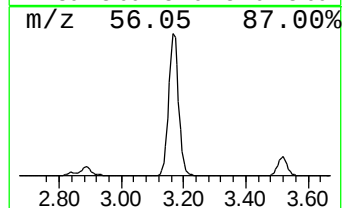
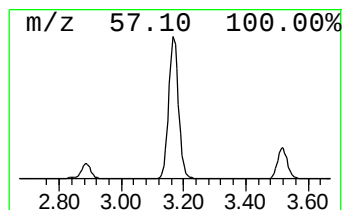
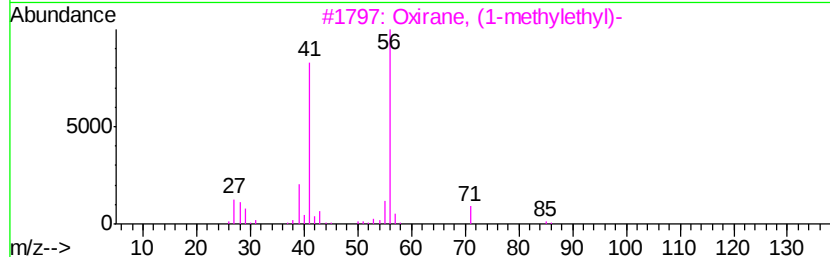
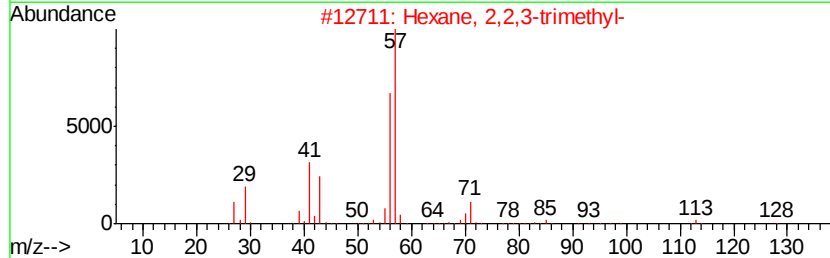
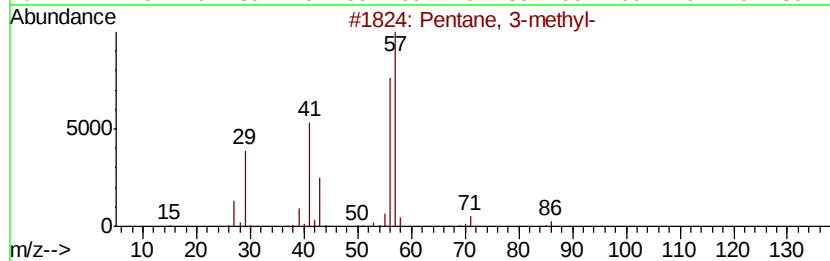
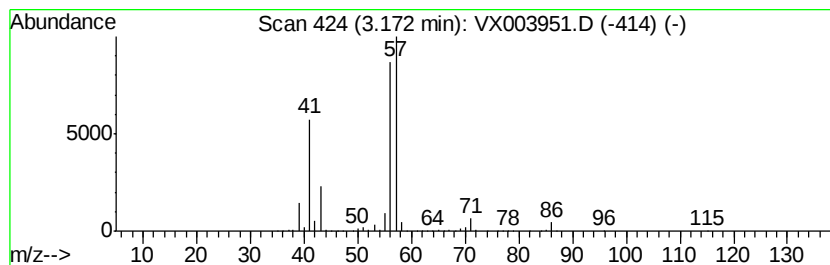
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	73.36 ug/l	1418430	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
4		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
5		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50



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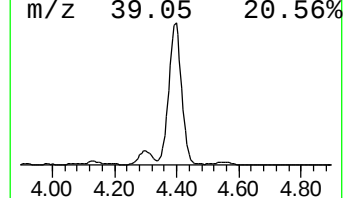
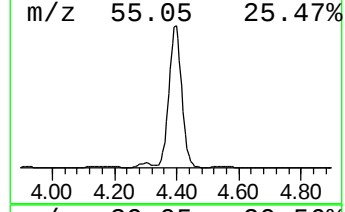
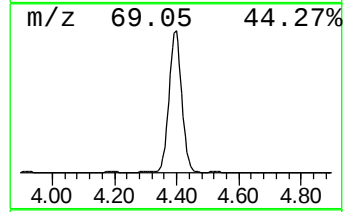
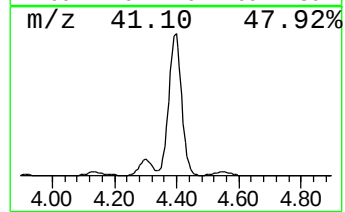
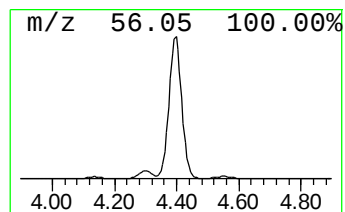
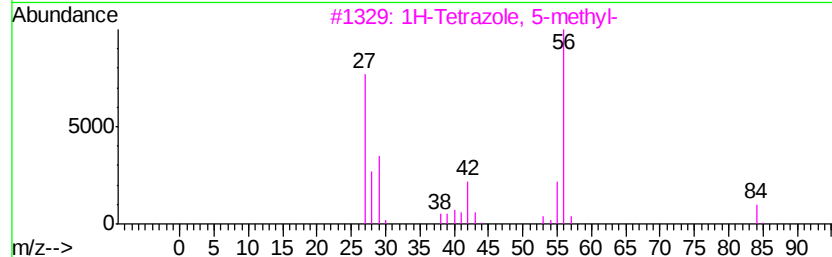
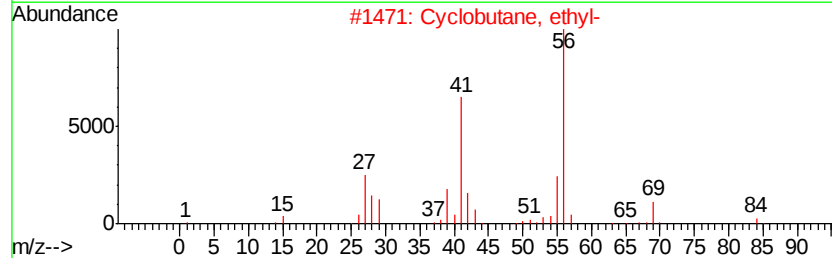
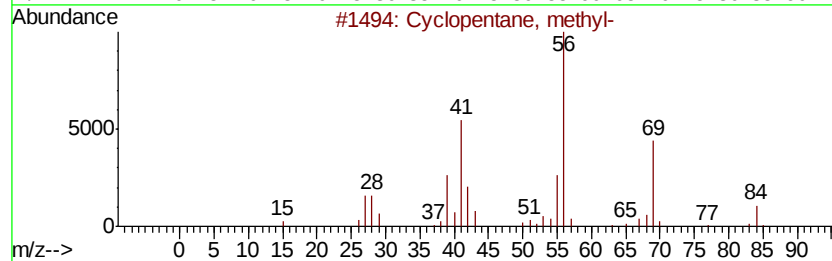
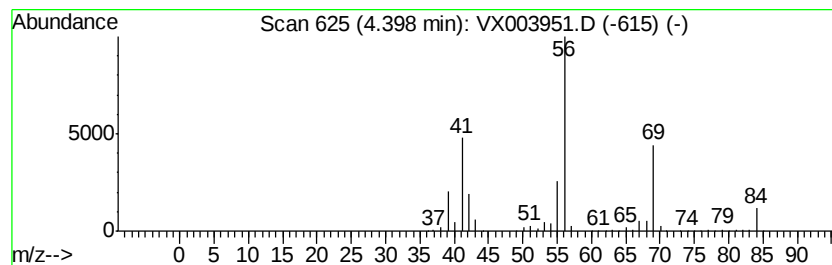
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	134.82 ug/l	2606810	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46
5		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX080918\
Data File : VX003951.D
Acq On : 09 Aug 2018 15:30
Operator : JC/MD
Sample : J4387-10
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleID :
FL-0567

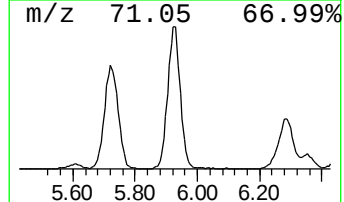
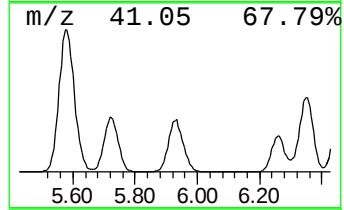
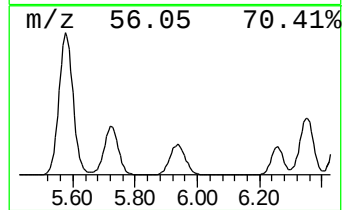
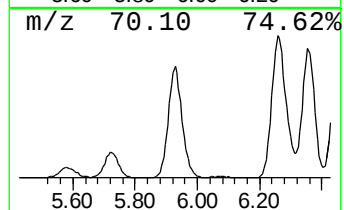
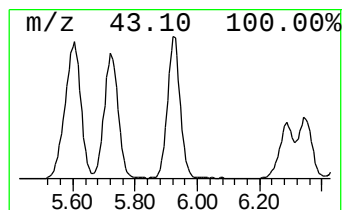
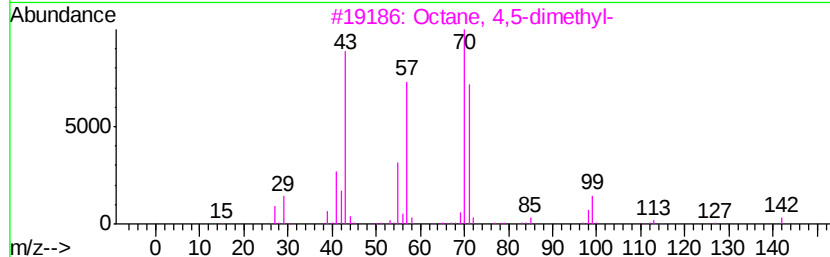
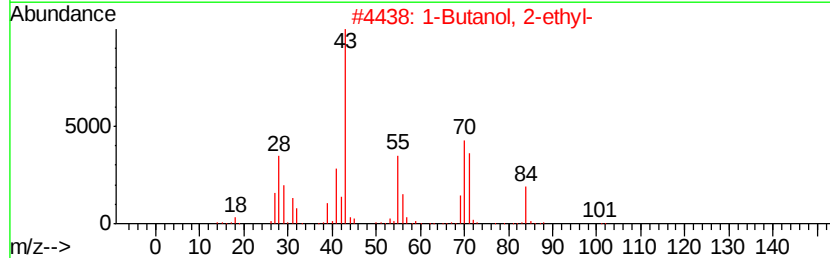
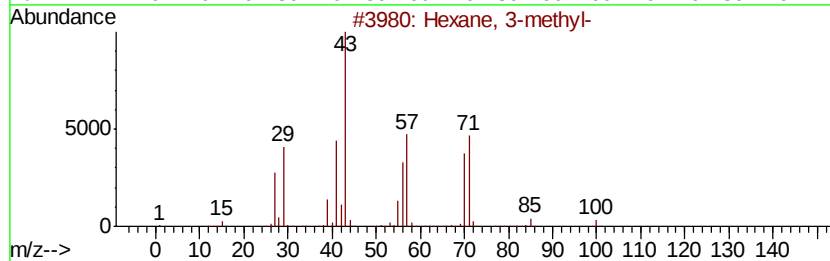
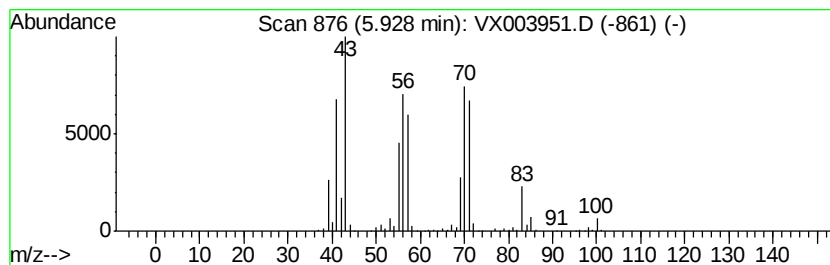
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Quant Title : SW846 8260

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

Peak Number 6 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	61.57 ug/l	1190470	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
2		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	59
3		Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	53
4		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	50
5		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX080918\
Data File : VX003951.D
Acq On : 09 Aug 2018 15:30
Operator : JC/MD
Sample : J4387-10
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0567

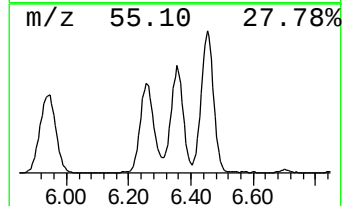
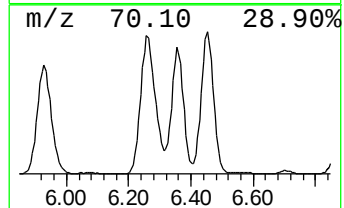
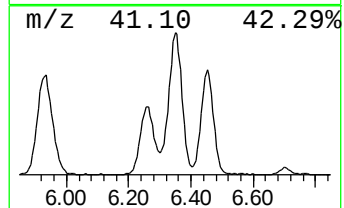
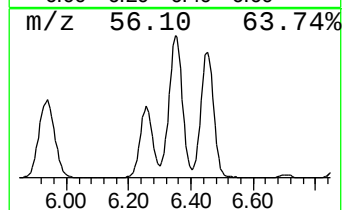
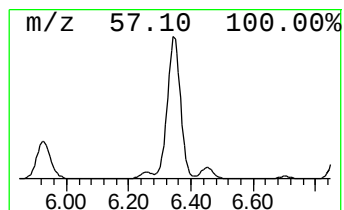
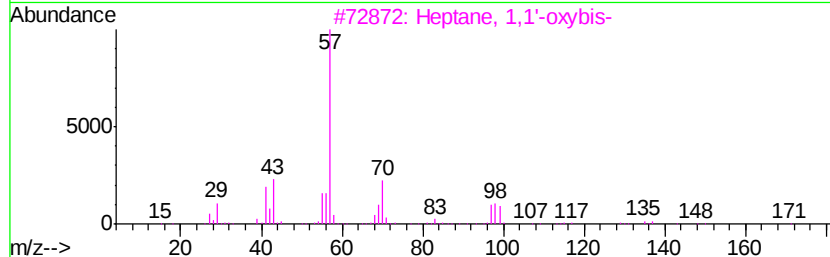
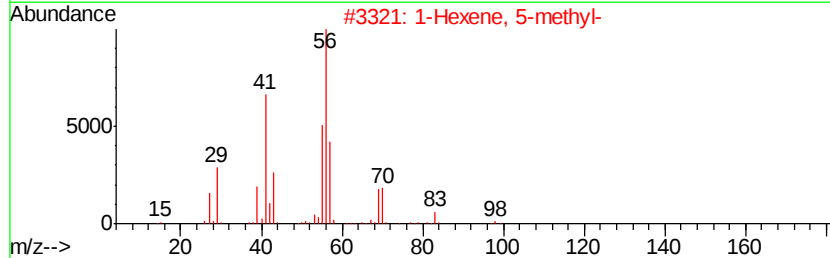
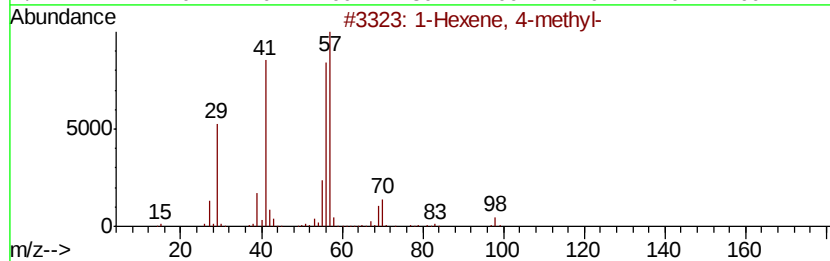
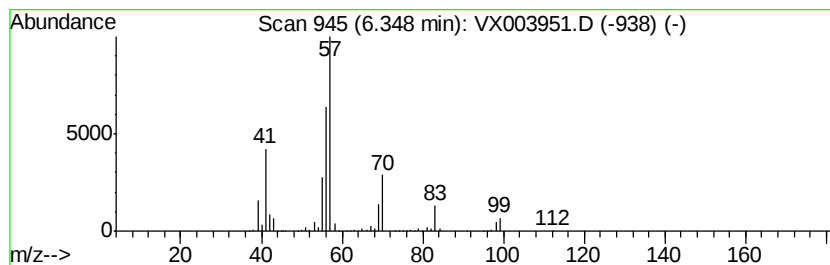
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexene, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	60.40 ug/l	1428250	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	59
2		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	53
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	49
5		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX080918\
Data File : VX003951.D
Acq On : 09 Aug 2018 15:30
Operator : JC/MD
Sample : J4387-10
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

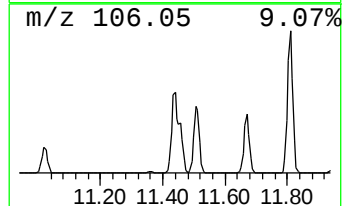
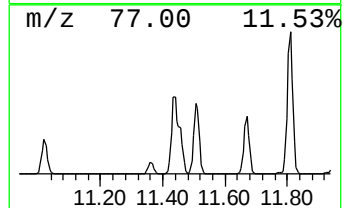
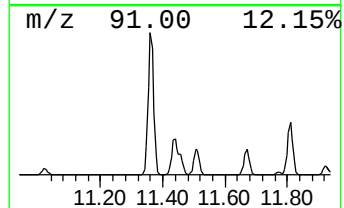
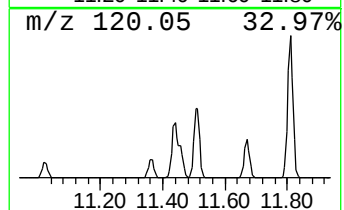
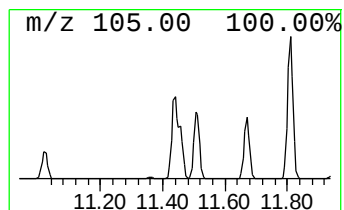
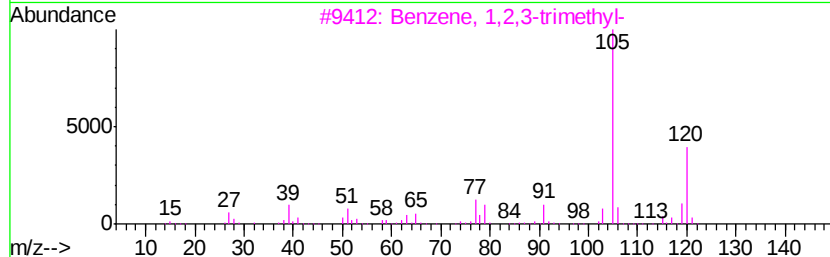
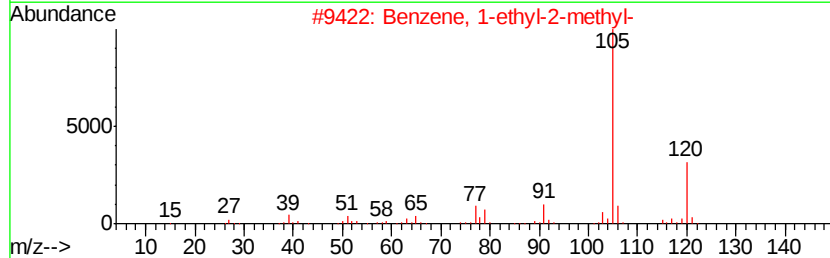
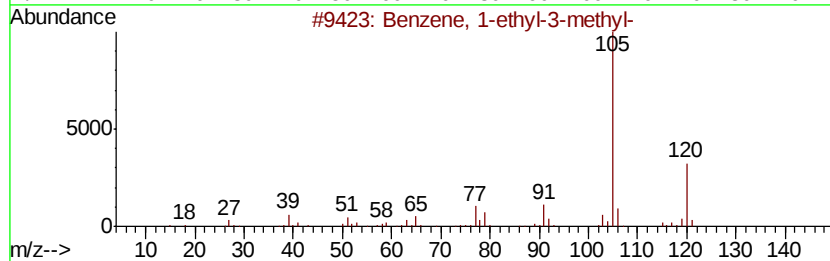
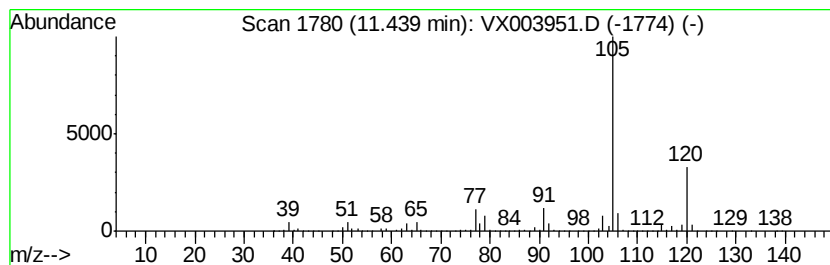
Instrument :
MSVOA_X
ClientSampleId :
FL-0567

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X080618W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	229.56 ug/l	9436170	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		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, 1,2,3-trimethyl-	120 C9H12	000526-73-8 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:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX080918\
Data File : VX003951.D
Acq On : 09 Aug 2018 15:30
Operator : JC/MD
Sample : J4387-10
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0567

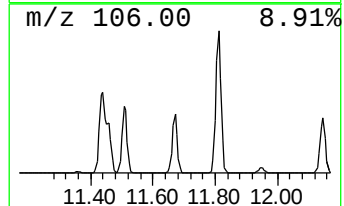
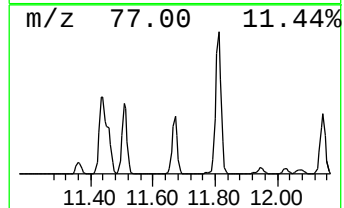
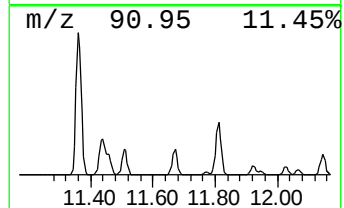
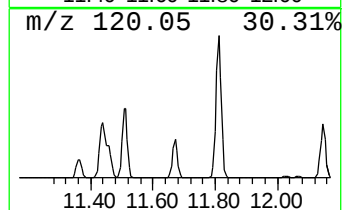
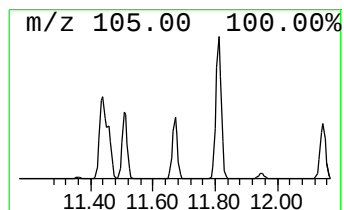
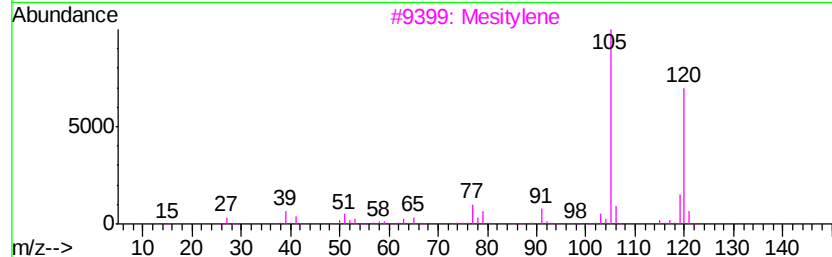
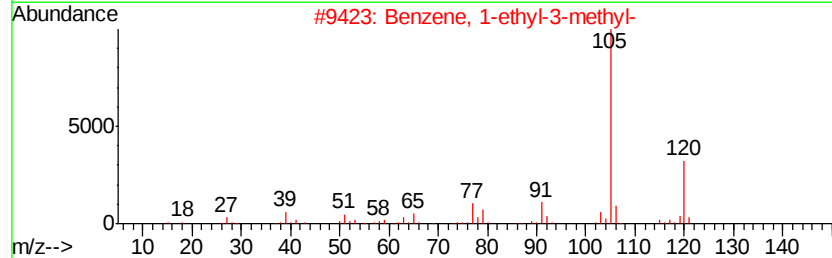
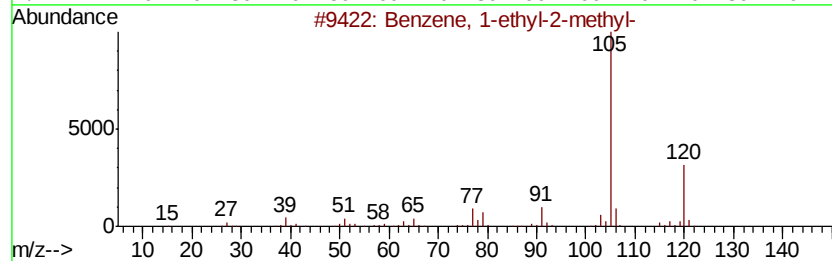
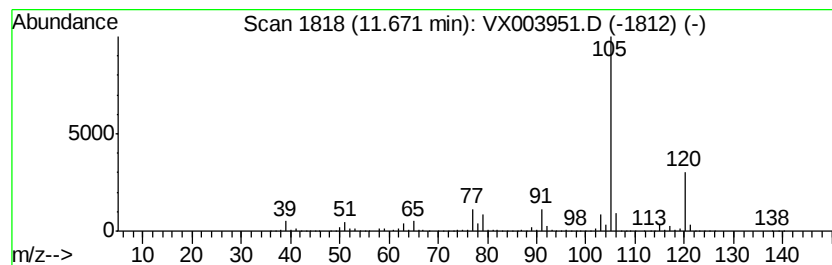
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X080618W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	107.59 ug/l	4422780	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
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\VX080918\
Data File : VX003951.D
Acq On : 09 Aug 2018 15:30
Operator : JC/MD
Sample : J4387-10
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0567

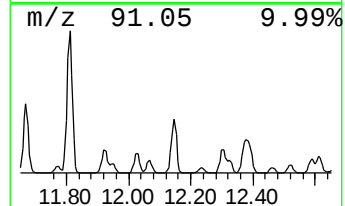
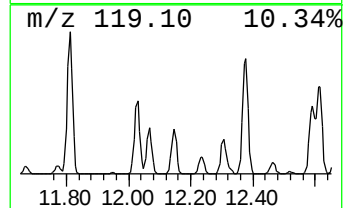
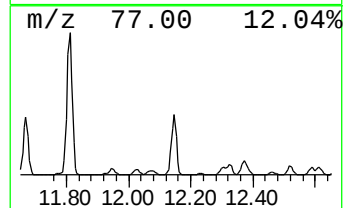
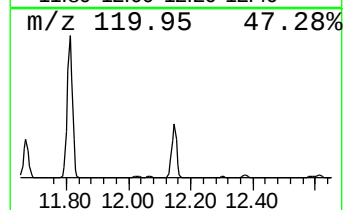
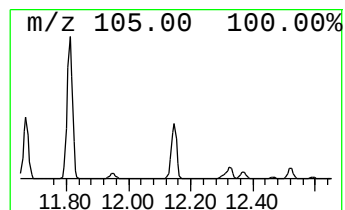
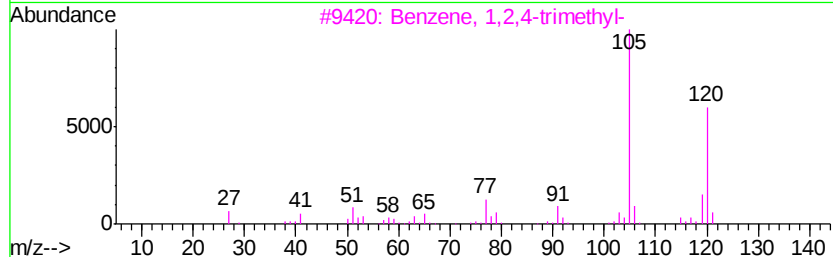
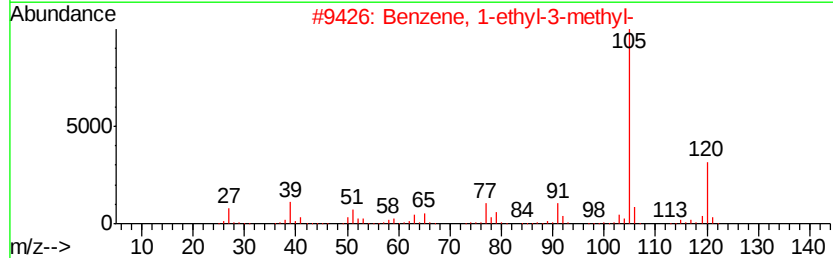
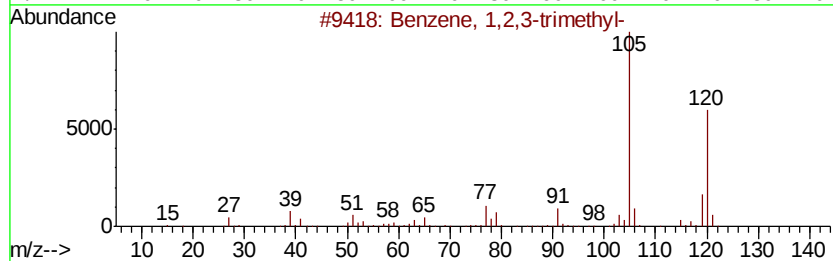
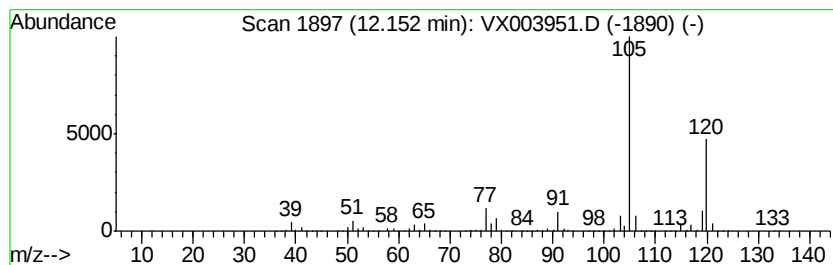
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X080618W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	108.35 ug/l	4453920	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX080918\
Data File : VX003951.D
Acq On : 09 Aug 2018 15:30
Operator : JC/MD
Sample : J4387-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0567

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X080618W.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	123.2	ug/l	2382590	1	5.67	966812	50.0
Butane, 2,3-dimet...	2.84	75.6	ug/l	1461290	1	5.67	966812	50.0
Pentane, 3-methyl-	3.17	73.4	ug/l	1418430	1	5.67	966812	50.0
Cyclopentane, met...	4.40	134.8	ug/l	2606810	1	5.67	966812	50.0
Hexane, 3-methyl-	5.93	61.6	ug/l	1190470	1	5.67	966812	50.0
1-Hexene, 4-methyl-	6.35	60.4	ug/l	1428250	2	6.87	1182350	50.0
Benzene, 1-ethyl-...	11.44	229.6	ug/l	9436170	4	12.08	2055310	50.0
Benzene, 1-ethyl-...	11.67	107.6	ug/l	4422780	4	12.08	2055310	50.0
Benzene, 1,2,3-tr...	12.15	108.3	ug/l	4453920	4	12.08	2055310	50.0