

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082218\
 Data File : VX004210.D
 Acq On : 22 Aug 2018 20:23
 Operator : JC/MD
 Sample : J4579-05
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0548

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\82X082218W.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	113	rBV	1337084	1848891	9.63%	1.348%
2	1.398	130	133	139	rBV	278442	281323	1.47%	0.205%
3	1.788	191	197	214	rVB	1064557	1502436	7.83%	1.095%
4	1.996	226	231	247	rVB	914538	1304723	6.80%	0.951%
5	2.392	289	296	302	rBV	116125	225465	1.17%	0.164%
6	2.843	362	370	372	rBV	177755	367766	1.92%	0.268%
7	2.886	372	377	381	rVV	745618	1572465	8.19%	1.146%
8	2.922	381	383	404	rVB	373792	685133	3.57%	0.499%
9	3.166	413	423	438	rVB	644384	1461345	7.61%	1.065%
10	3.514	470	480	495	rBV	677409	1529687	7.97%	1.115%
11	4.391	614	624	638	rVB	1555596	4541092	23.65%	3.311%
12	5.501	790	806	810	rBV	216913	595753	3.10%	0.434%
13	5.574	810	818	828	rVV2	1151221	3764756	19.61%	2.745%
14	5.660	828	832	839	rVB	202032	480975	2.51%	0.351%
15	5.928	862	876	890	rBV4	425759	1398946	7.29%	1.020%
16	6.068	890	899	913	rVB	225985	587115	3.06%	0.428%
17	6.257	914	930	939	rBV2	231644	744098	3.88%	0.542%
18	6.355	939	946	954	rVV	234848	635741	3.31%	0.463%
19	6.452	954	962	975	rVB	342588	939356	4.89%	0.685%
20	6.702	993	1003	1020	rBV2	214970	522961	2.72%	0.381%
21	6.861	1020	1029	1038	rBV	491035	1145378	5.97%	0.835%
22	7.464	1114	1128	1139	rBV	2483535	5715583	29.77%	4.167%
23	7.732	1165	1172	1182	rVB	242151	465762	2.43%	0.340%
24	7.848	1182	1191	1199	rVB2	102378	217620	1.13%	0.159%
25	8.025	1206	1220	1236	rVB2	81909	206681	1.08%	0.151%
26	8.342	1267	1272	1275	rBV	121920	195328	1.02%	0.142%
27	8.385	1275	1279	1285	rVB2	112295	203492	1.06%	0.148%
28	8.501	1293	1298	1302	rBV	160619	264864	1.38%	0.193%
29	8.665	1318	1325	1328	rBV2	394918	685700	3.57%	0.500%
30	8.714	1328	1333	1344	rVB	1257135	2131989	11.11%	1.554%
31	8.836	1347	1353	1358	rBV	157781	270892	1.41%	0.197%
32	9.037	1381	1386	1393	rVB	292730	481035	2.51%	0.351%
33	9.165	1398	1407	1413	rBV	192688	319845	1.67%	0.233%
34	9.573	1467	1474	1478	rBV3	145593	260152	1.36%	0.190%

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35	9.622	1478	1482	1487	rVB	397073	536942	2.80%	0.391%
36	9.677	1487	1491	1495	rBV	139741	206509	1.08%	0.151%
37	10.116	1558	1563	1569	rVB	965128	1282983	6.68%	0.935%
38	10.189	1569	1575	1579	rVB	134099	195750	1.02%	0.143%
39	10.256	1579	1586	1592	rBV	6417790	8548735	44.53%	6.232%
40	10.360	1594	1603	1609	rBV	14440964	19197928	100.00%	13.996%
41	10.701	1653	1659	1672	rVB	7607513	9720318	50.63%	7.086%
42	11.018	1706	1711	1716	rBV	1041979	1279581	6.67%	0.933%
43	11.140	1725	1731	1735	rBV	1044366	1323794	6.90%	0.965%
44	11.360	1758	1767	1774	rBV	1530596	1825186	9.51%	1.331%
45	11.433	1774	1779	1787	rVV	4600449	8279578	43.13%	6.036%
46	11.506	1787	1791	1800	rVB	3478227	4115846	21.44%	3.001%
47	11.671	1812	1818	1826	rBV	2279858	2831086	14.75%	2.064%
48	11.811	1836	1841	1846	rVB	8540427	10236591	53.32%	7.463%
49	11.945	1861	1863	1869	rVB	224676	257463	1.34%	0.188%
50	12.024	1869	1876	1880	rBV	426879	538663	2.81%	0.393%
51	12.079	1880	1885	1890	rVB2	1417493	1922781	10.02%	1.402%
52	12.146	1890	1896	1901	rBV	3307331	4053421	21.11%	2.955%
53	12.299	1915	1921	1924	rBV	1169753	1643843	8.56%	1.198%
54	12.372	1929	1933	1941	rVB4	1013972	1589127	8.28%	1.159%
55	12.518	1952	1957	1963	rVB	354231	422224	2.20%	0.308%
56	12.585	1963	1968	1970	rBV	496812	612923	3.19%	0.447%
57	12.610	1970	1972	1977	rVV	595332	675188	3.52%	0.492%
58	12.670	1977	1982	1985	rVV	740053	894269	4.66%	0.652%
59	12.701	1985	1987	1992	rVB	188415	212753	1.11%	0.155%
60	12.762	1992	1997	2004	rBV4	451109	867277	4.52%	0.632%
61	12.902	2016	2020	2025	rVB2	405618	540128	2.81%	0.394%
62	12.975	2025	2032	2036	rBV	494779	676500	3.52%	0.493%
63	13.018	2036	2039	2046	rVB	816036	948093	4.94%	0.691%
64	13.085	2046	2050	2055	rBV3	104205	208367	1.09%	0.152%
65	13.225	2069	2073	2077	rVB2	321791	399482	2.08%	0.291%
66	13.347	2089	2093	2098	rVB2	1333354	1778118	9.26%	1.296%
67	13.481	2110	2115	2124	rVB	987878	1206989	6.29%	0.880%
68	13.640	2137	2141	2146	rBV3	166179	287074	1.50%	0.209%
69	13.725	2152	2155	2160	rVB3	148978	236010	1.23%	0.172%
70	13.835	2165	2173	2180	rVB	2632574	3308078	17.23%	2.412%
71	13.914	2181	2186	2190	rVB	148355	200306	1.04%	0.146%

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Integration Parameters: RTEINT.P

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72	13.987	2190	2198	2202	rBV2	194714	300012	1.56%	0.219%
73	14.292	2240	2248	2255	rVB	312946	537449	2.80%	0.392%
74	14.542	2284	2289	2298	rBV2	253701	353612	1.84%	0.258%
75	14.701	2307	2315	2319	rBV	2041222	2633692	13.72%	1.920%
76	14.841	2333	2338	2347	rBV	1370242	1688437	8.79%	1.231%
77	15.274	2400	2409	2414	rBV2	128622	212821	1.11%	0.155%
78	15.554	2448	2455	2461	rBV	167196	273359	1.42%	0.199%
79	15.688	2469	2477	2480	rBV	201336	325453	1.70%	0.237%
80	15.725	2480	2483	2491	rVB	145071	229009	1.19%	0.167%

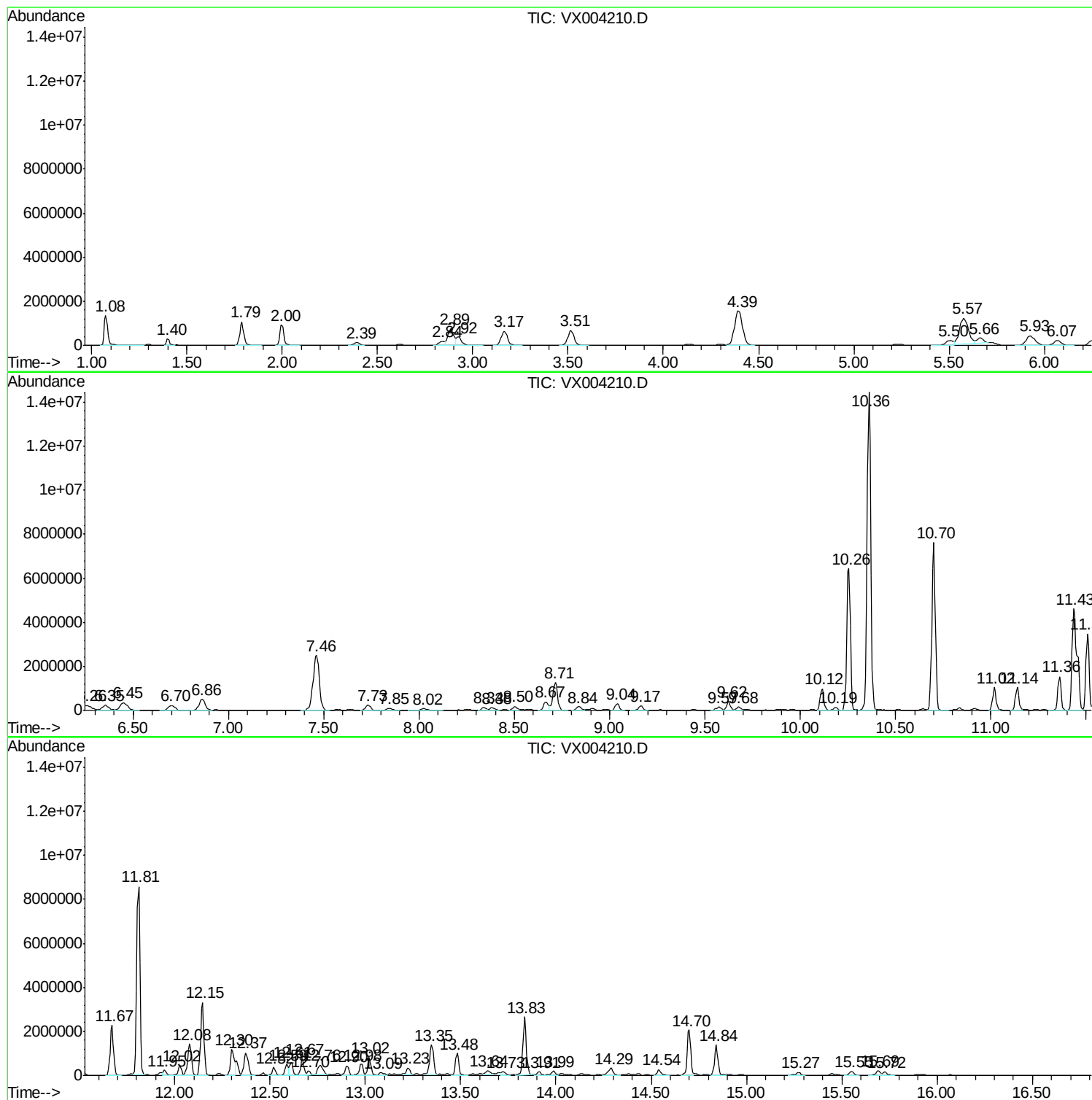
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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



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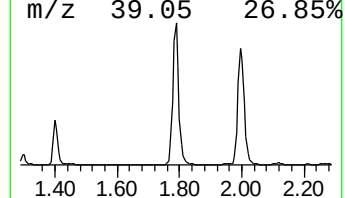
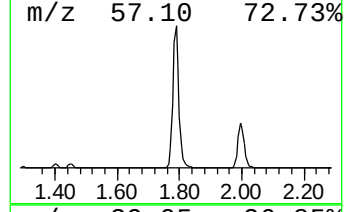
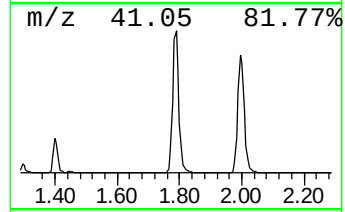
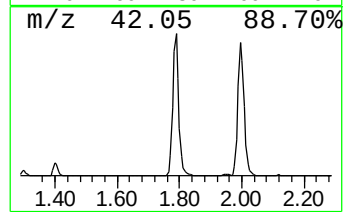
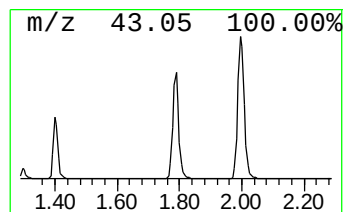
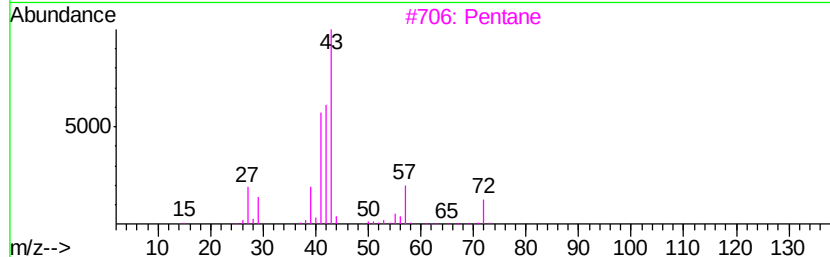
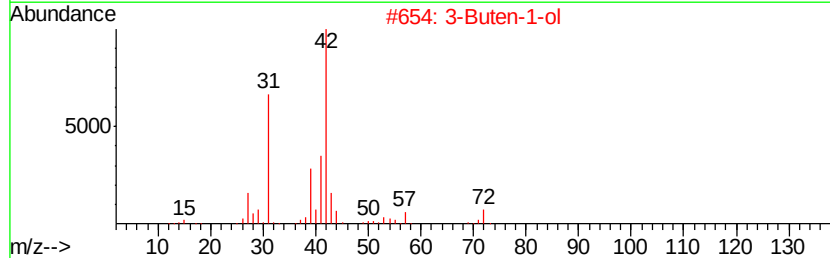
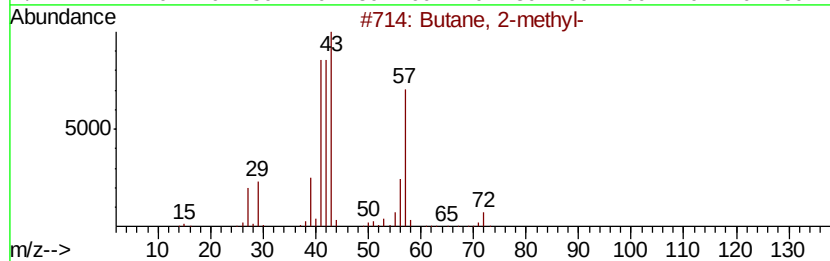
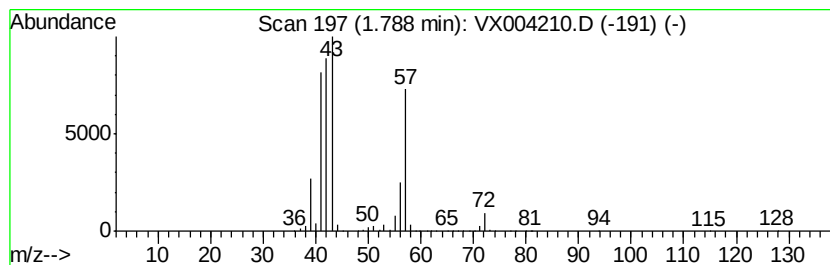
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	156.19 ug/l	1502440	Pentafluorobenzene	5.66

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		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampled :
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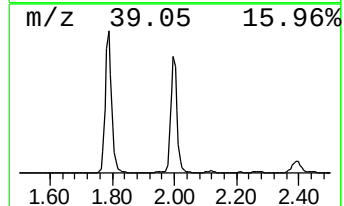
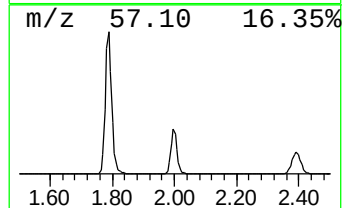
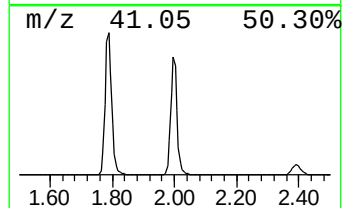
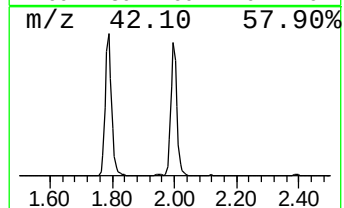
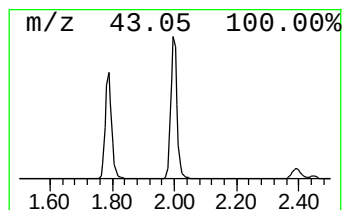
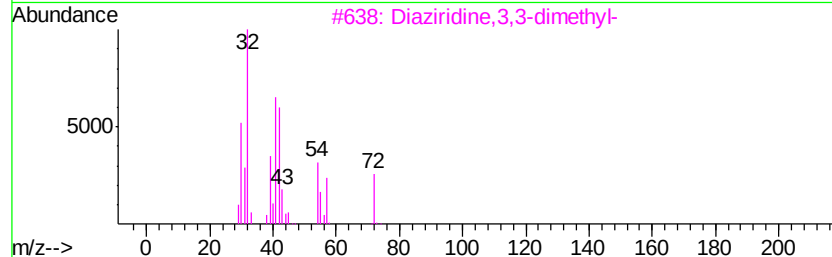
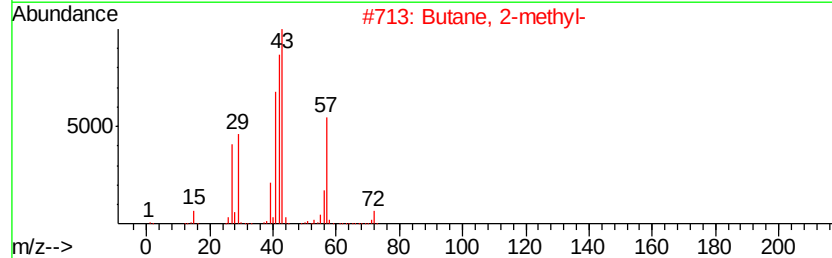
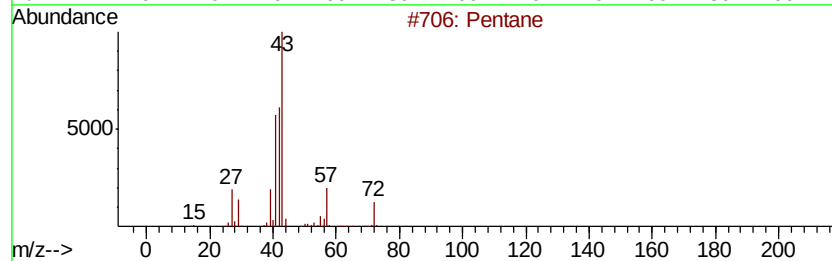
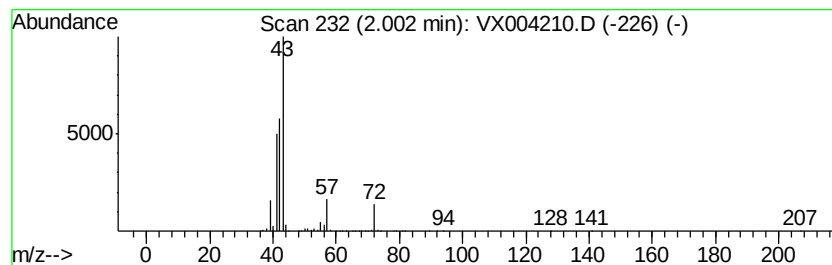
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	135.63 ug/l	1304720	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	38
3		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	25
4		Oxirane, ethyl-	72	C4H8O	000106-88-7	9
5		Propanal, 2-methyl-	72	C4H8O	000078-84-2	9



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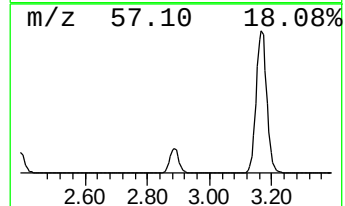
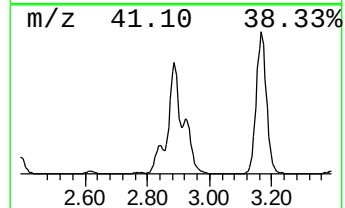
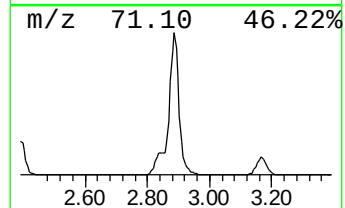
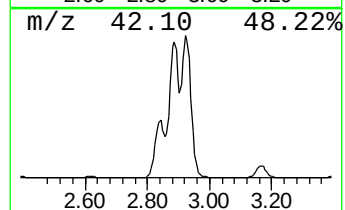
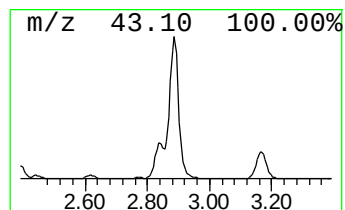
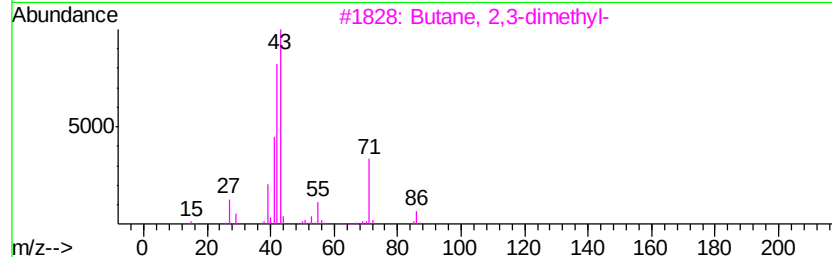
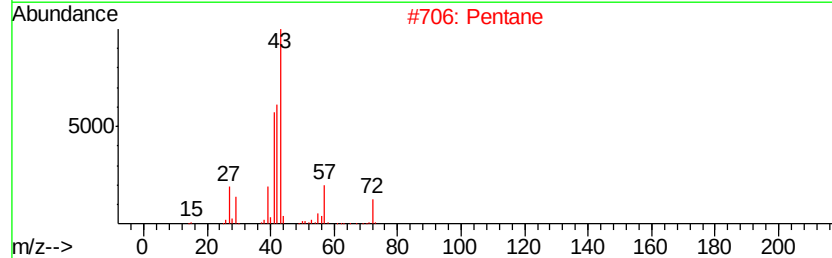
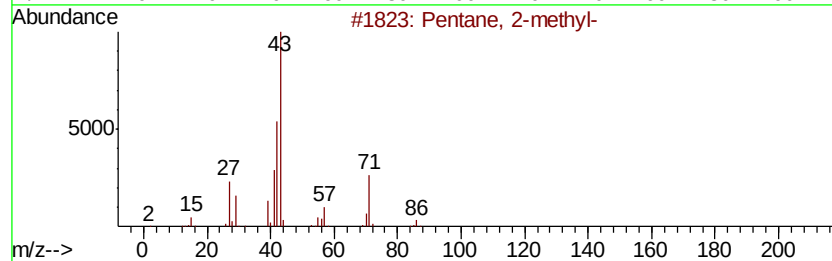
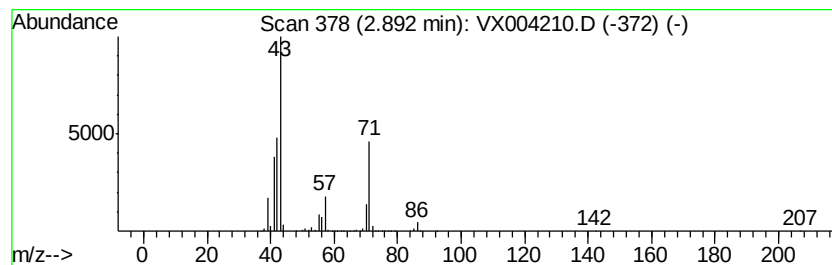
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	163.47 ug/l	1572470	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2		Pentane	72	C5H12	000109-66-0	46
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
4		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40
5		Ether, hexyl pentyl	172	C11H24O	032357-83-8	33



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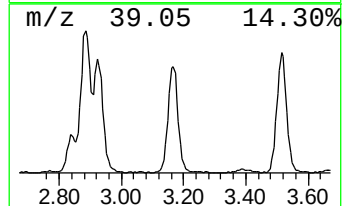
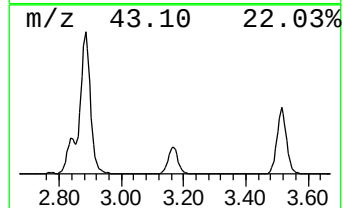
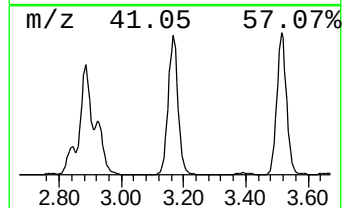
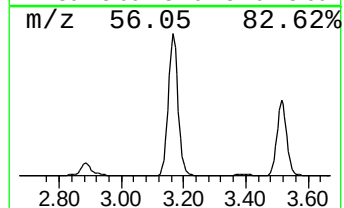
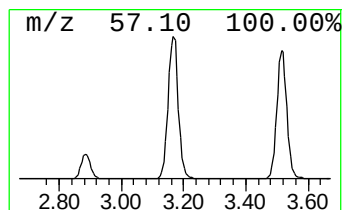
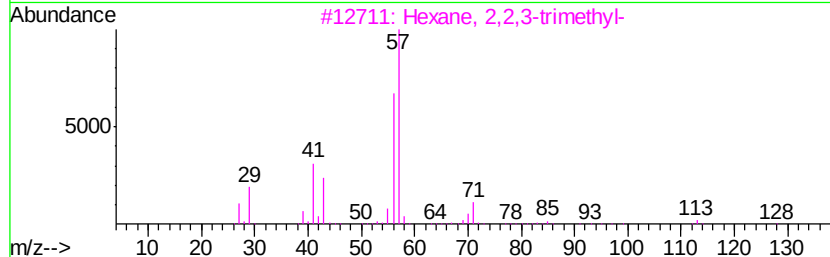
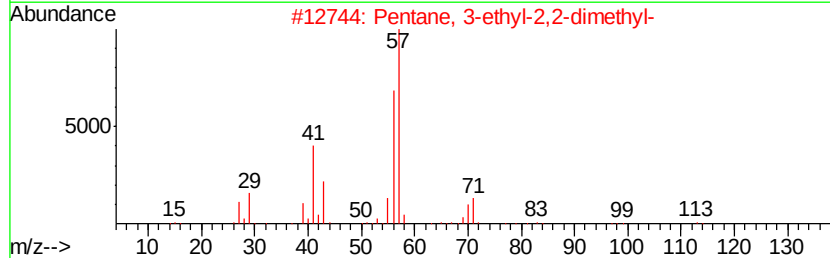
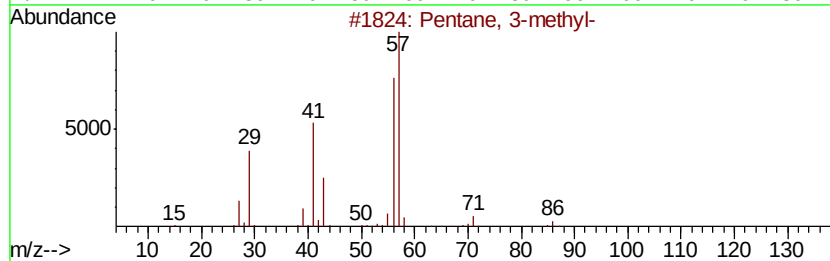
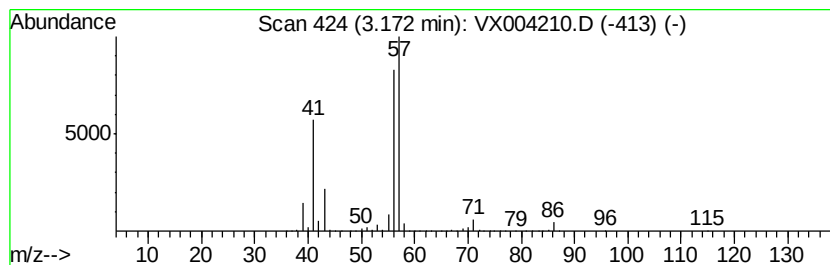
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	151.92 ug/l	1461350	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91	
2	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64	
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64	
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59	
5	n-Hexane	86	C6H14	000110-54-3	43	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004210.D
Acq On : 22 Aug 2018 20:23
Operator : JC/MD
Sample : J4579-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0548

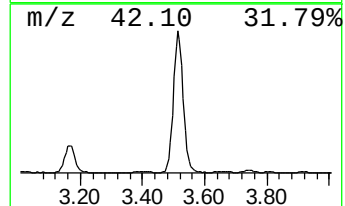
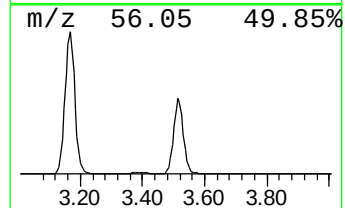
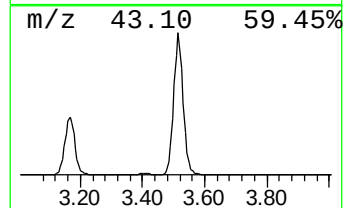
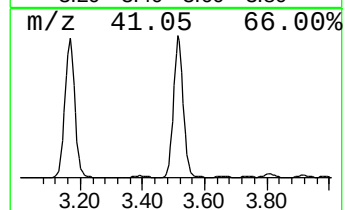
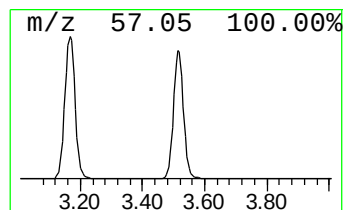
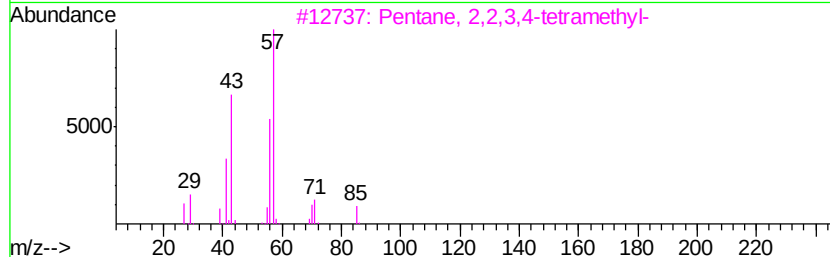
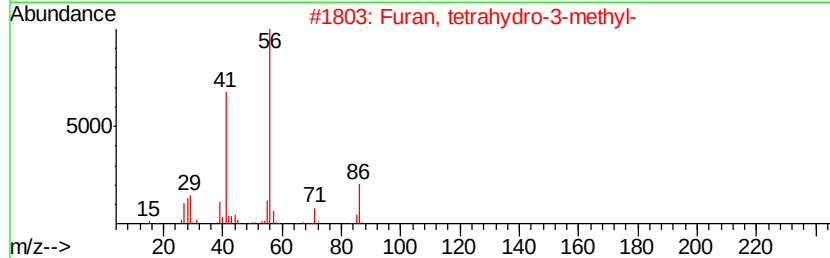
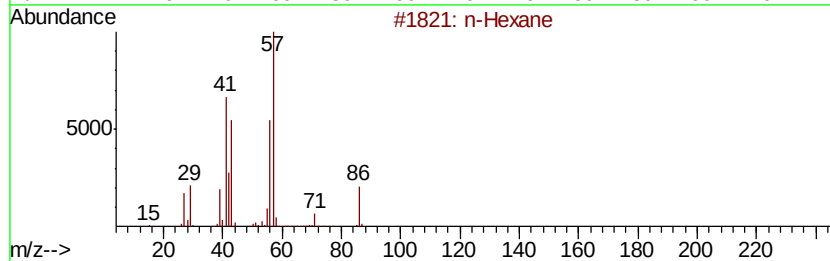
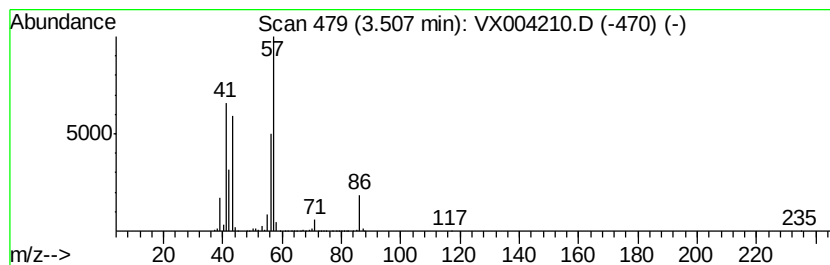
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Quant Title : SW846 8260

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

Peak Number 6 n-Hexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.51	159.02 ug/l	1529690	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	94
2		Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	50
3		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
5		Butanal, 2-methyl-	86	C5H10O	000096-17-3	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004210.D
Acq On : 22 Aug 2018 20:23
Operator : JC/MD
Sample : J4579-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0548

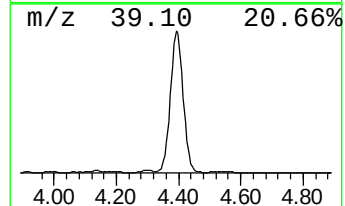
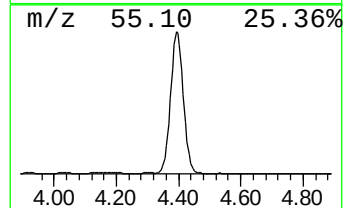
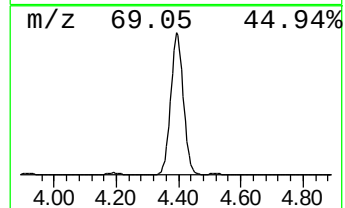
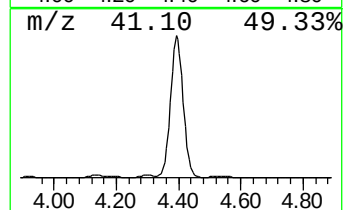
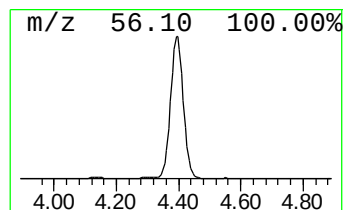
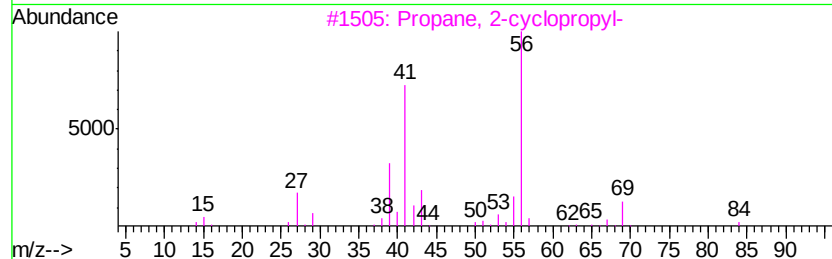
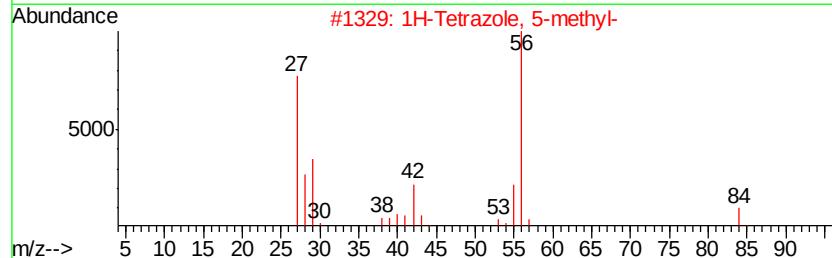
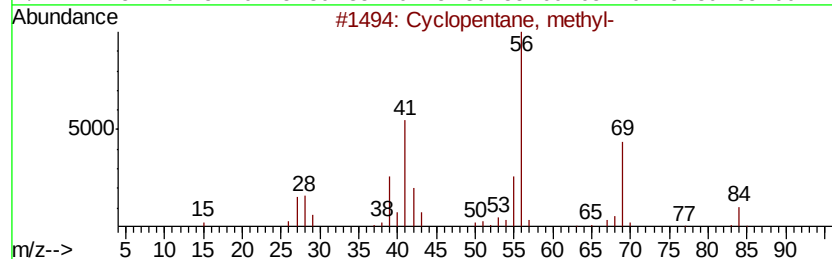
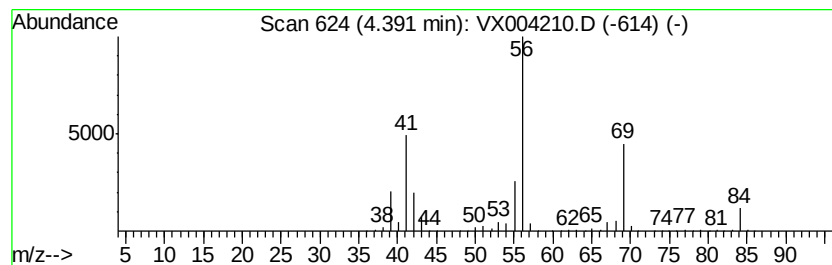
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	472.07 ug/l	4541090	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004210.D
Acq On : 22 Aug 2018 20:23
Operator : JC/MD
Sample : J4579-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

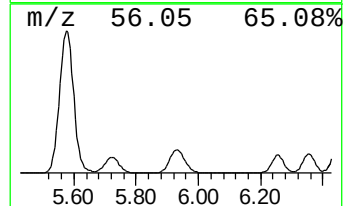
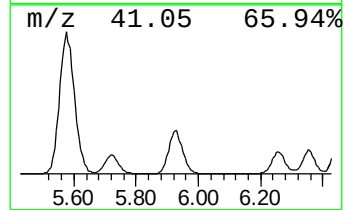
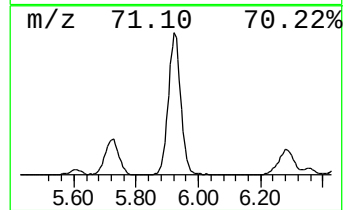
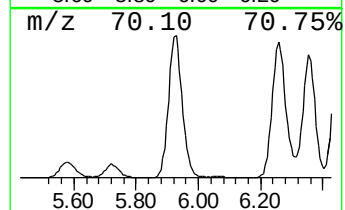
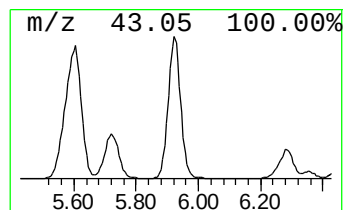
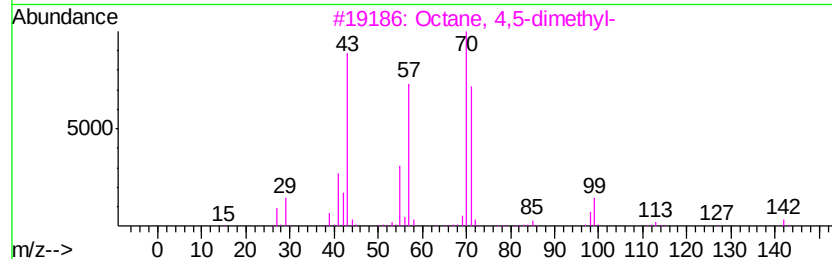
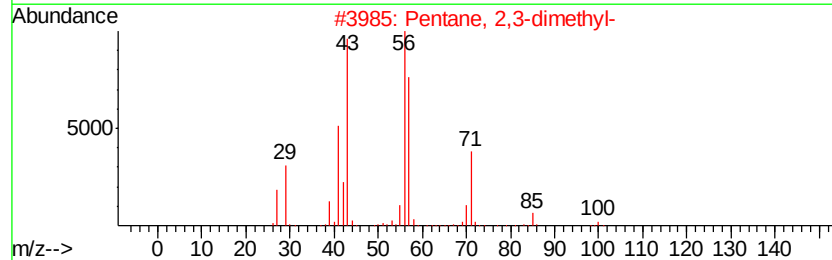
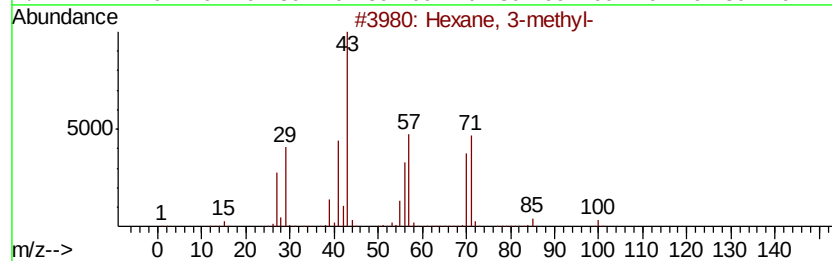
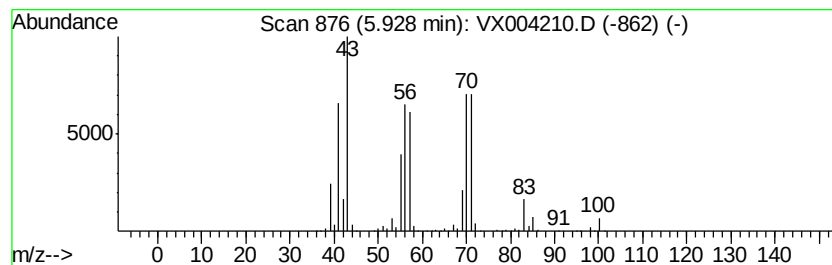
Instrument :
MSVOA_X
ClientSampleId :
FL-0548

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 8 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
5.93	145.43 ug/l	1398950	Pentafluorobenzene	5.66		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-		100	C7H16	000589-34-4	72
2	Pentane, 2,3-dimethyl-		100	C7H16	000565-59-3	53
3	Octane, 4,5-dimethyl-		142	C10H22	015869-96-2	53
4	3,3-Dimethyl-2-pentanol		116	C7H16O	019781-24-9	53
5	Heptane		100	C7H16	000142-82-5	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004210.D
Acq On : 22 Aug 2018 20:23
Operator : JC/MD
Sample : J4579-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

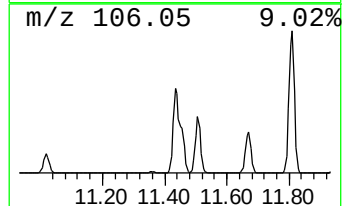
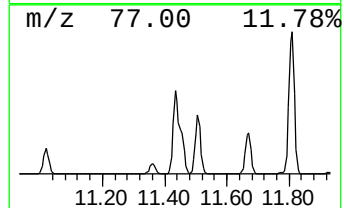
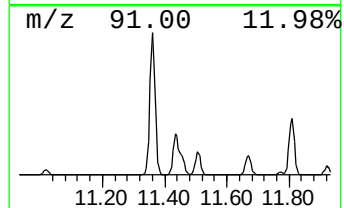
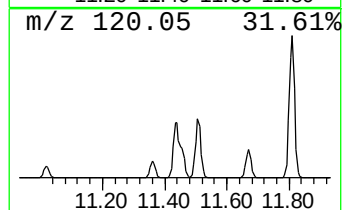
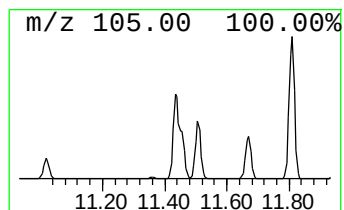
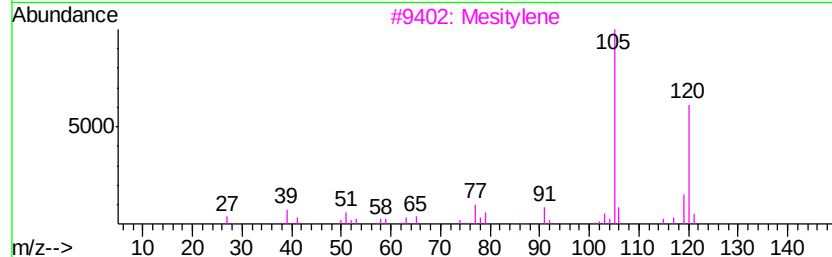
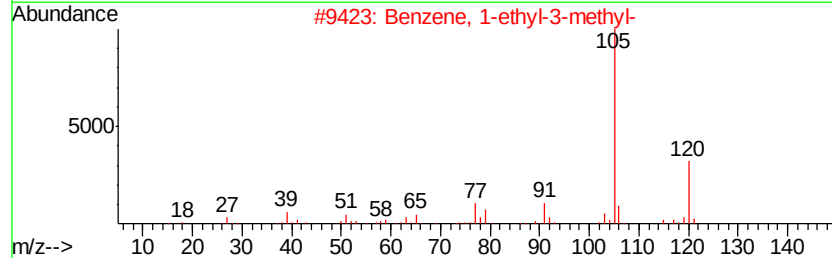
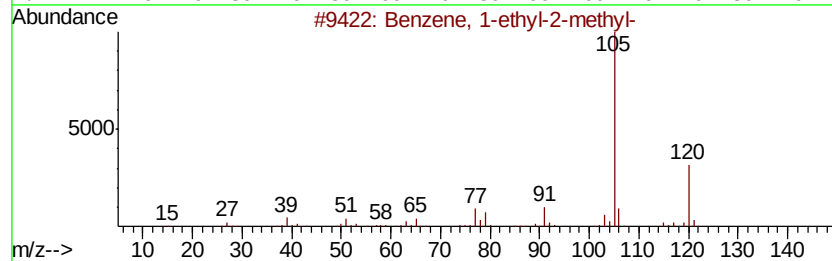
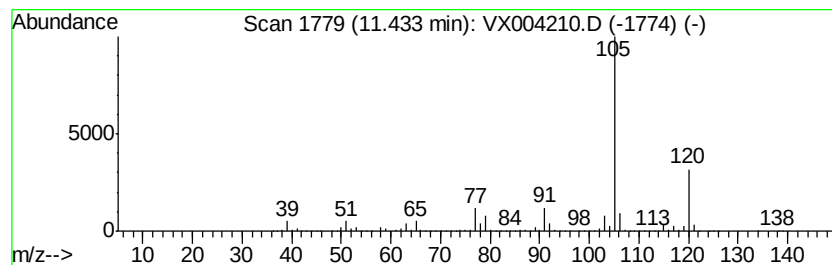
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	215.30 ug/l	8279580	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 95
2		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 95
3		Mesitylene	120 C9H12	000108-67-8 91
4		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 91
5		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004210.D
Acq On : 22 Aug 2018 20:23
Operator : JC/MD
Sample : J4579-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0548

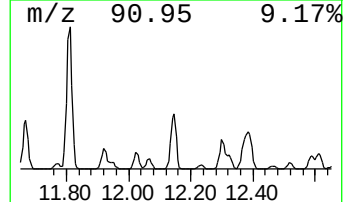
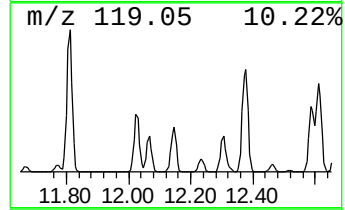
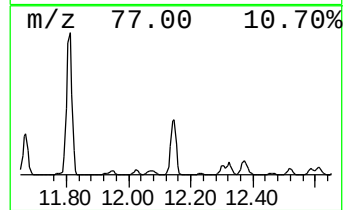
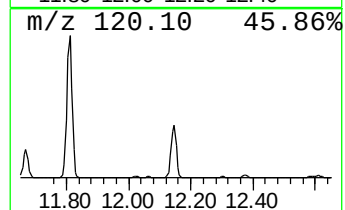
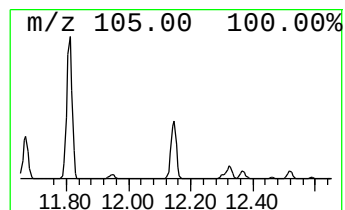
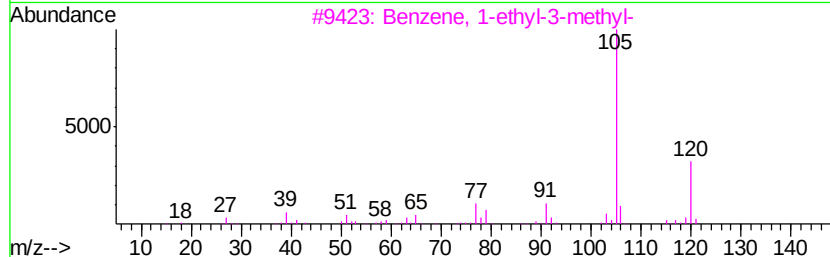
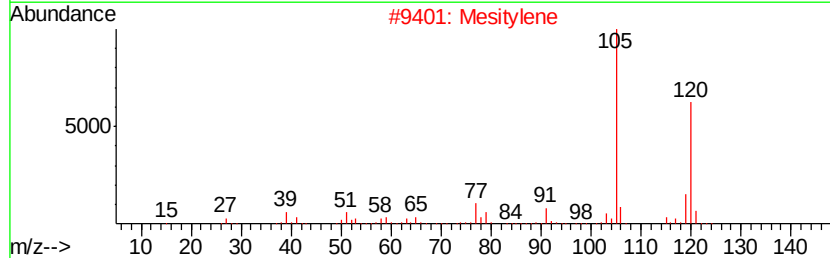
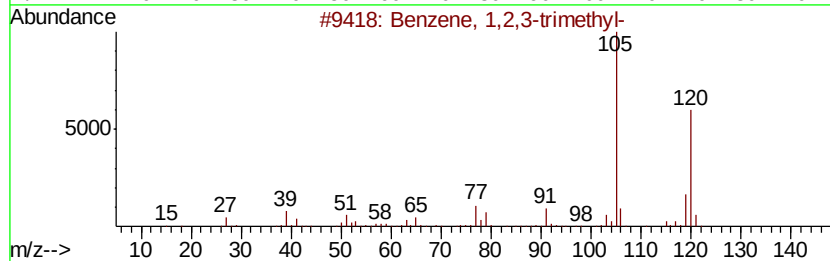
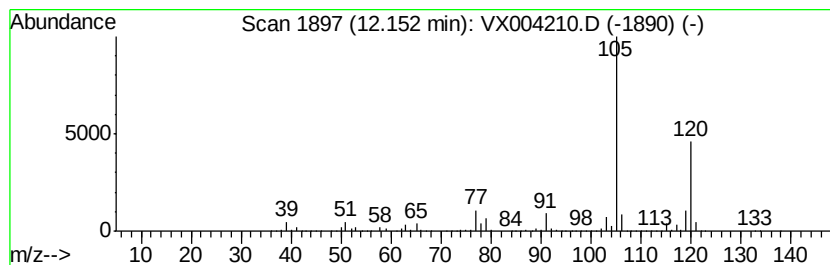
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	105.41 ug/l	4053420	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		Mesitylene	120	C9H12	000108-67-8	94
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082218\
Data File : VX004210.D
Acq On : 22 Aug 2018 20:23
Operator : JC/MD
Sample : J4579-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0548

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.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	156.2	ug/l	1502440	1	5.66	480975	50.0
Pentane	2.00	135.6	ug/l	1304720	1	5.66	480975	50.0
Pentane, 2-methyl-	2.89	163.5	ug/l	1572470	1	5.66	480975	50.0
Pentane, 3-methyl-	3.17	151.9	ug/l	1461350	1	5.66	480975	50.0
n-Hexane	3.51	159.0	ug/l	1529690	1	5.66	480975	50.0
Cyclopentane, met...	4.39	472.1	ug/l	4541090	1	5.66	480975	50.0
Hexane, 3-methyl-	5.93	145.4	ug/l	1398950	1	5.66	480975	50.0
Benzene, 1-ethyl-...	11.43	215.3	ug/l	8279580	4	12.08	1922780	50.0
Benzene, 1,2,3-tr...	12.15	105.4	ug/l	4053420	4	12.08	1922780	50.0