

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082318\
 Data File : VX004228.D
 Acq On : 23 Aug 2018 15:53
 Operator : JC/MD
 Sample : J4579-11
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0552

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	94	rBV	1297036	1758795	2.61%	0.583%
2	1.788	191	197	212	rVB	1753324	2474396	3.68%	0.820%
3	1.995	226	231	246	rVB	1987306	2794278	4.15%	0.926%
4	2.392	288	296	303	rBV	384586	752954	1.12%	0.249%
5	2.837	362	369	372	rBV	590800	1215722	1.81%	0.403%
6	2.886	372	377	401	rVB	2438738	5762908	8.56%	1.909%
7	3.166	413	423	446	rVB	2163049	4861159	7.22%	1.611%
8	3.513	470	480	497	rBV	2290165	5200437	7.73%	1.723%
9	4.397	614	625	639	rVB	3730424	10877075	16.17%	3.604%
10	5.574	809	818	829	rVV2	2535720	7815516	11.62%	2.589%
11	5.720	838	842	861	rVB2	286648	805683	1.20%	0.267%
12	5.928	863	876	890	rBV4	720239	2345506	3.49%	0.777%
13	6.257	914	930	939	rBV2	337125	1139200	1.69%	0.377%
14	6.354	939	946	954	rVV	326520	900552	1.34%	0.298%
15	6.452	954	962	974	rVB	528127	1428383	2.12%	0.473%
16	6.702	991	1003	1012	rBV	446839	1055112	1.57%	0.350%
17	6.860	1020	1029	1037	rBV	499062	1158327	1.72%	0.384%
18	7.464	1113	1128	1140	rBV	3570599	8175731	12.15%	2.709%
19	8.714	1328	1333	1341	rVB	1254980	2104290	3.13%	0.697%
20	10.116	1557	1563	1569	rVB	984004	1310498	1.95%	0.434%
21	10.256	1580	1586	1595	rVB	17950210	24030592	35.71%	7.962%
22	10.372	1595	1605	1610	rBV2	43044926	67287703	100.00%	22.293%
23	10.701	1653	1659	1665	rVB	24426369	33316392	49.51%	11.038%
24	11.018	1706	1711	1724	rVB	1692026	2110139	3.14%	0.699%
25	11.140	1725	1731	1736	rBV	1083665	1365199	2.03%	0.452%
26	11.360	1759	1767	1774	rBV	2507539	3059244	4.55%	1.014%
27	11.439	1774	1780	1787	rVV	10007435	18168176	27.00%	6.019%
28	11.506	1787	1791	1801	rVB	6423723	7866982	11.69%	2.606%
29	11.671	1812	1818	1827	rBV	5442480	6647664	9.88%	2.202%
30	11.811	1836	1841	1846	rVB	18680265	21916261	32.57%	7.261%
31	12.030	1871	1877	1880	rBV	578787	745630	1.11%	0.247%
32	12.079	1880	1885	1890	rVB2	1476281	2127692	3.16%	0.705%
33	12.146	1890	1896	1901	rBV	8732810	10395237	15.45%	3.444%
34	12.298	1915	1921	1929	rBV2	4149824	6151421	9.14%	2.038%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

35	12.372	1929	1933	1943	rVB4	1648079	2435722	3.62%	0.807%
36	12.585	1963	1968	1970	rBV	859406	1034643	1.54%	0.343%
37	12.609	1970	1972	1977	rVB	958065	1073694	1.60%	0.356%
38	12.670	1977	1982	1985	rBV	1224606	1442283	2.14%	0.478%
39	12.762	1992	1997	2004	rBV4	830925	1450921	2.16%	0.481%
40	12.902	2015	2020	2025	rVB2	630901	841050	1.25%	0.279%
41	12.981	2025	2033	2036	rVV	908236	1165737	1.73%	0.386%
42	13.018	2036	2039	2045	rVB	1459743	1734301	2.58%	0.575%
43	13.225	2069	2073	2077	rVB	687384	815276	1.21%	0.270%
44	13.347	2089	2093	2099	rVB2	2503832	3355152	4.99%	1.112%
45	13.481	2110	2115	2124	rVB	1236113	1512999	2.25%	0.501%
46	13.835	2165	2173	2181	rBV	8016435	10013013	14.88%	3.317%
47	14.700	2307	2315	2325	rBV	2692988	3511369	5.22%	1.163%
48	14.841	2332	2338	2347	rBV	1915284	2321528	3.45%	0.769%

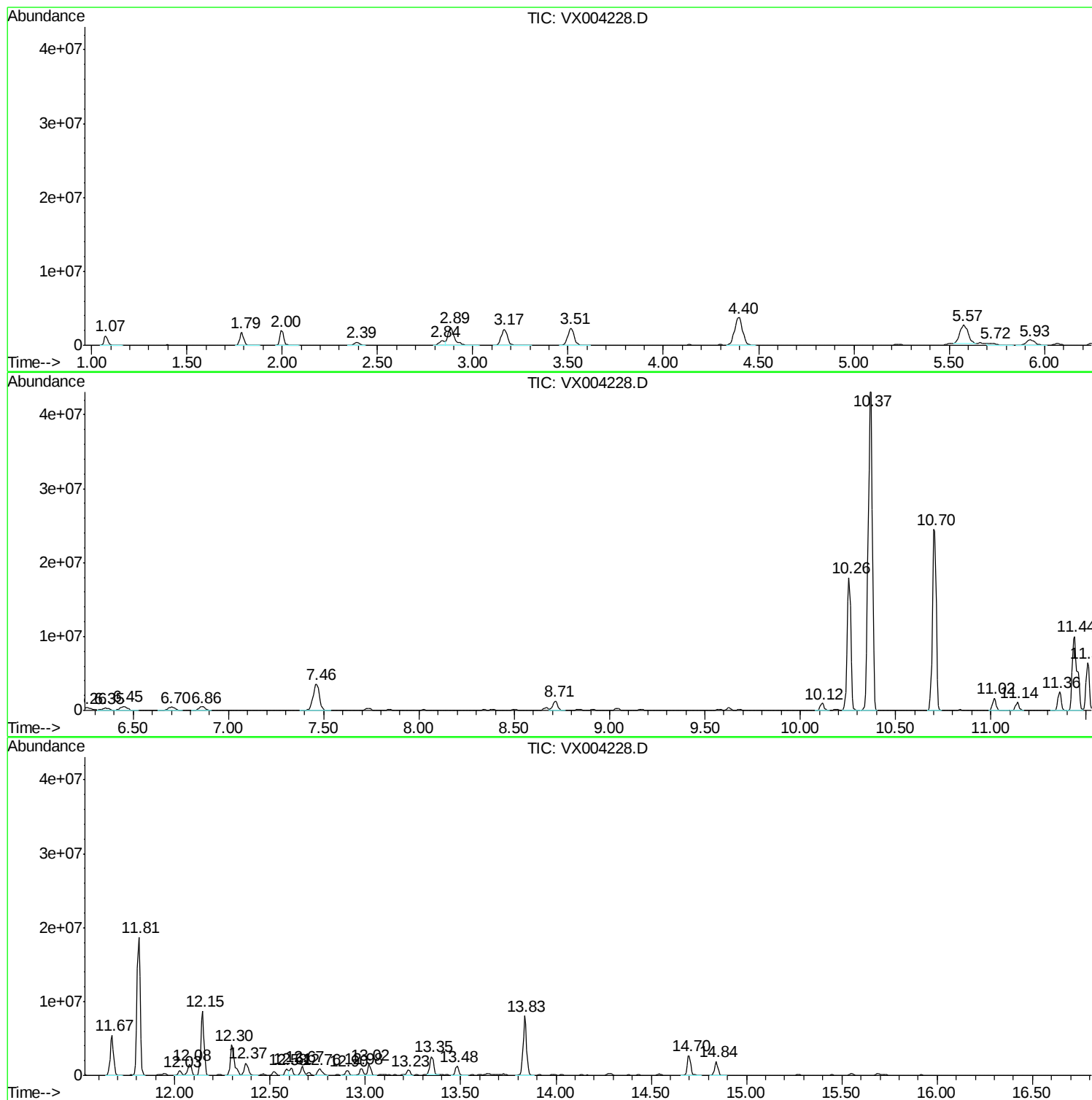
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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



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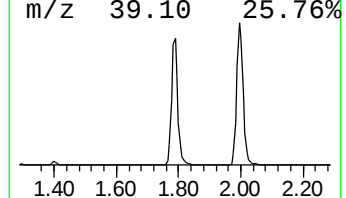
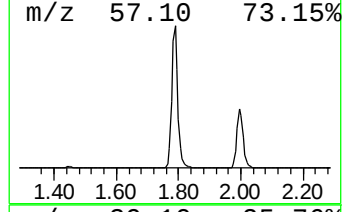
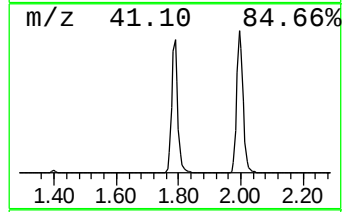
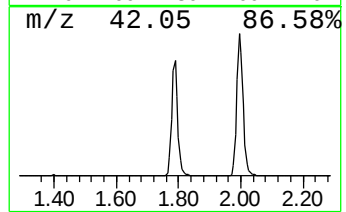
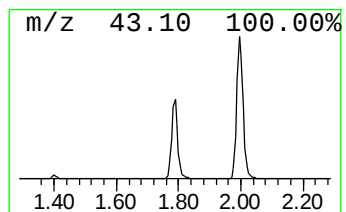
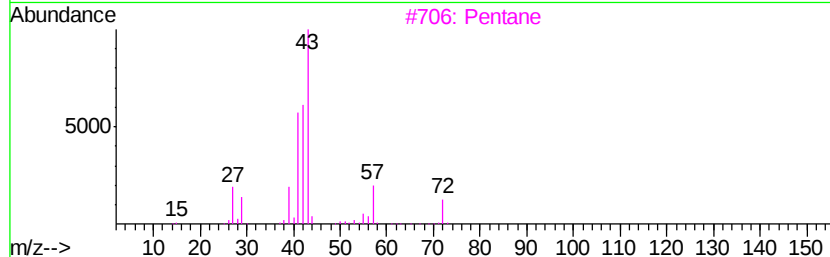
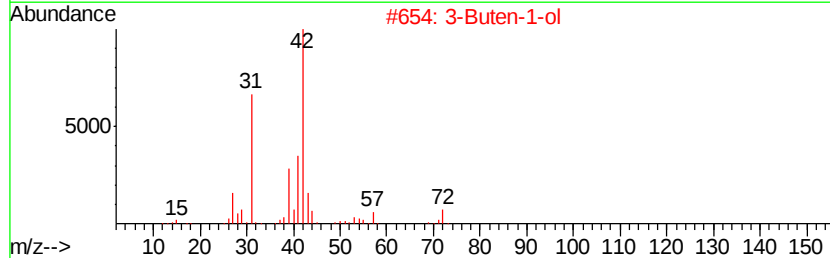
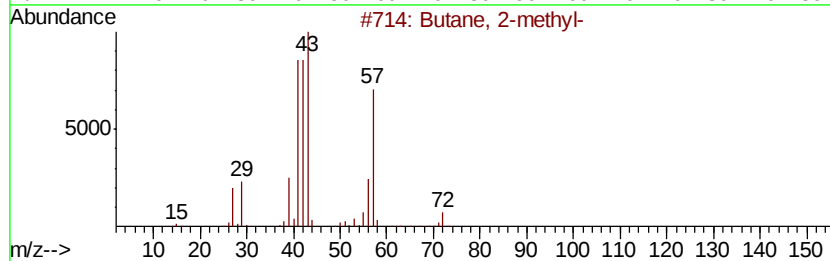
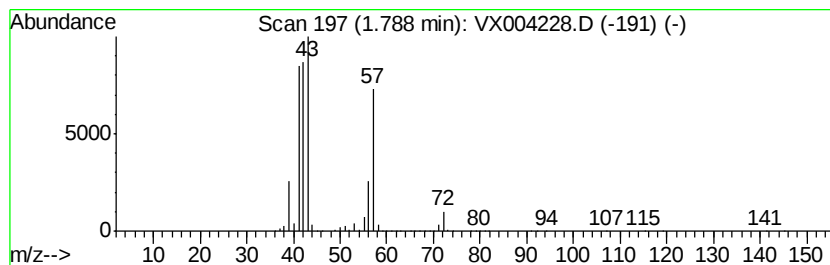
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	153.56 ug/l	2474400	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		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10
5		Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

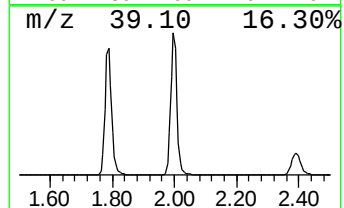
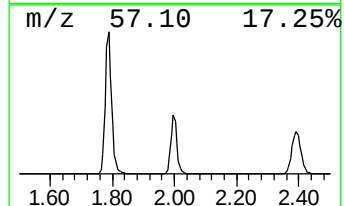
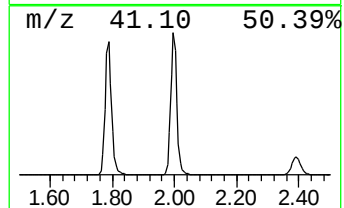
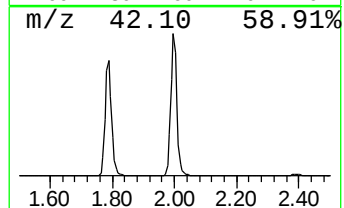
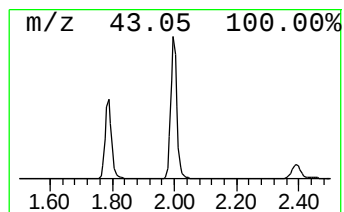
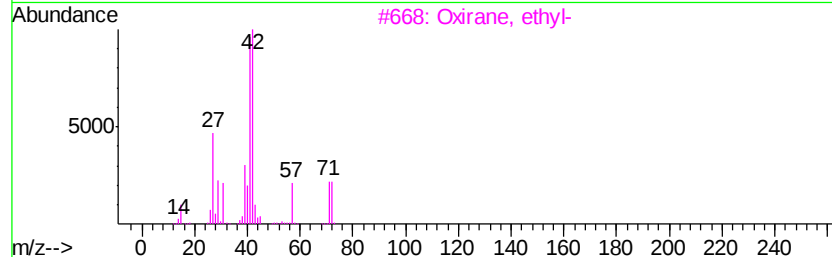
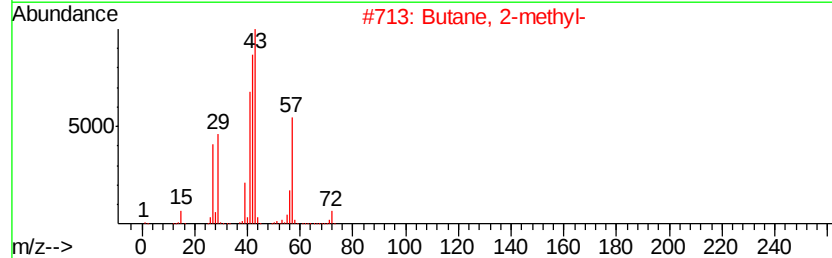
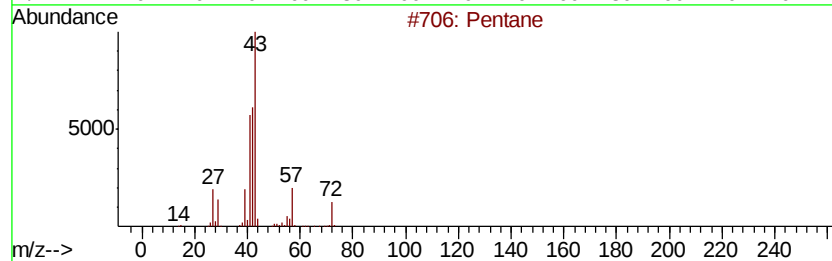
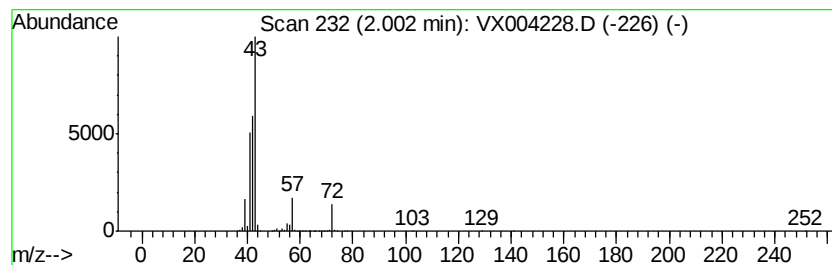
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	173.41 ug/l	2794280	Pentafluorobenzene	5.67

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		Oxirane, ethyl-	72	C4H8O	000106-88-7	33
4		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	25
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0552

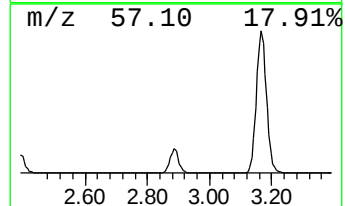
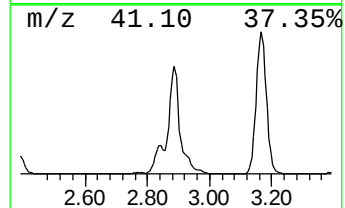
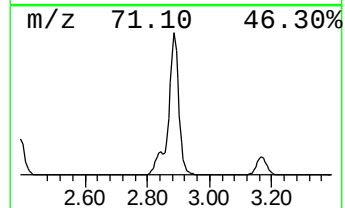
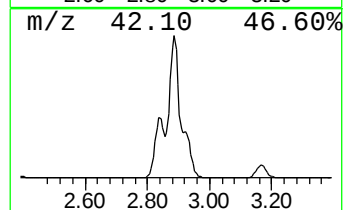
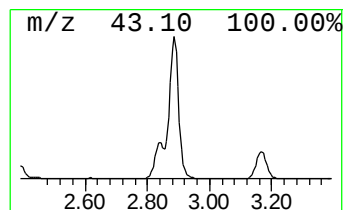
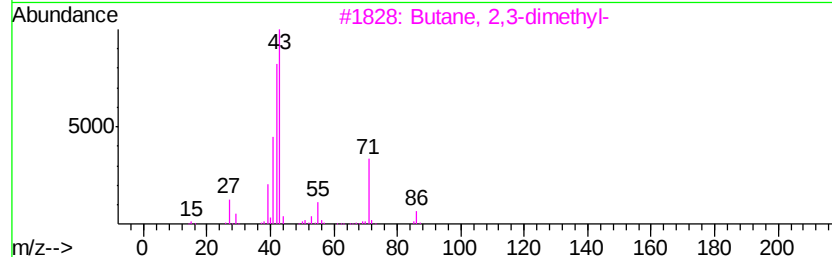
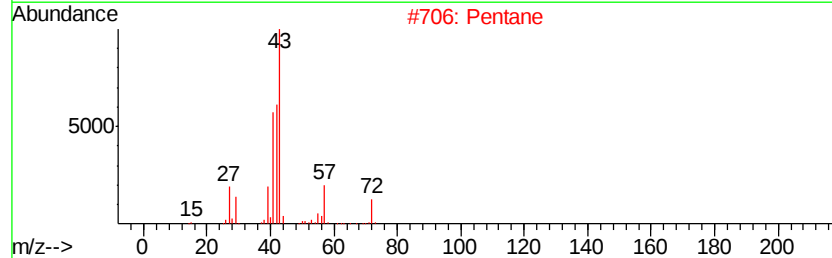
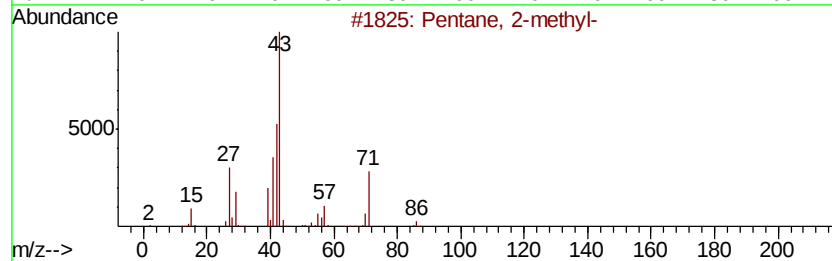
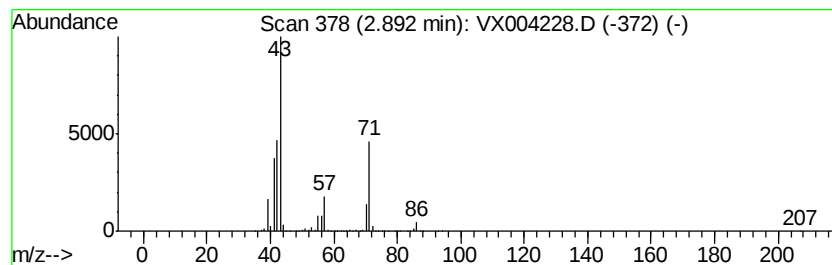
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	357.64 ug/l	5762910	Pentafluorobenzene	5.67

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	45
4		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40
5		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38



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Instrument :
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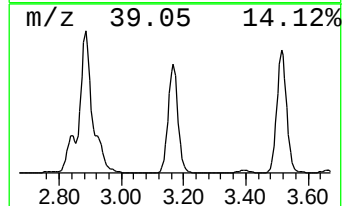
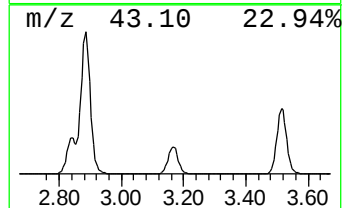
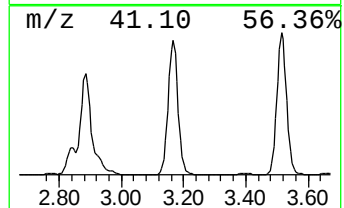
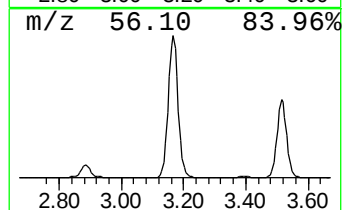
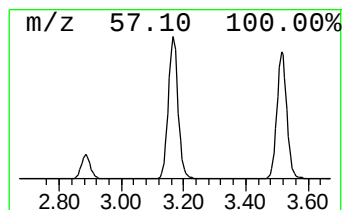
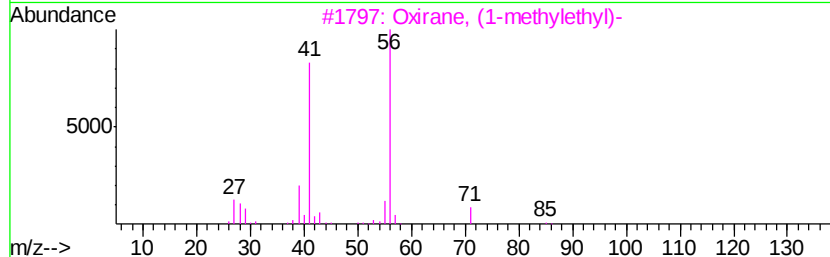
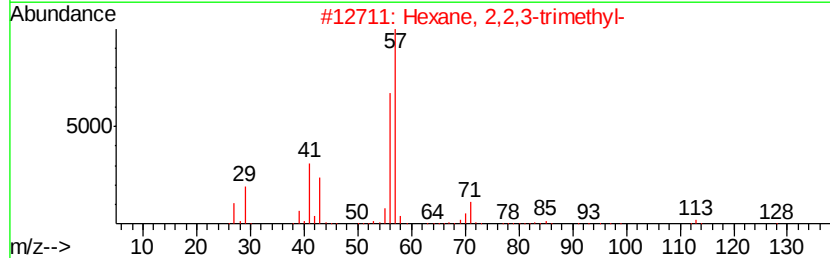
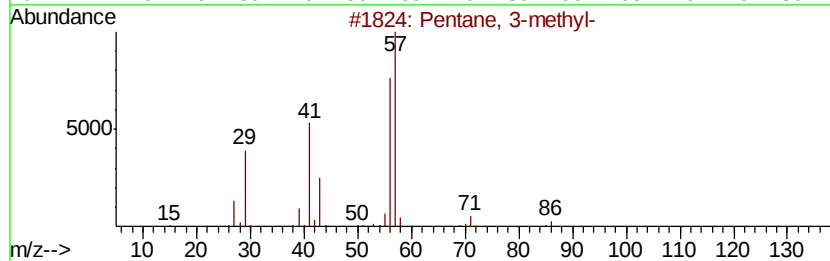
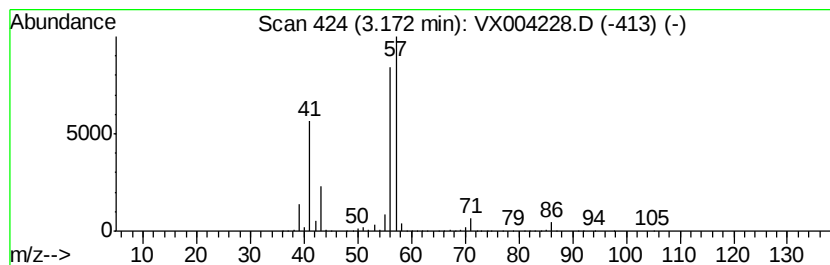
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	301.68 ug/l	4861160	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91	
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64	
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	64	
4	n-Hexane	86	C6H14	000110-54-3	47	
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40	



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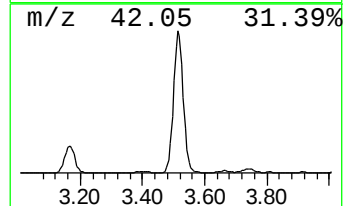
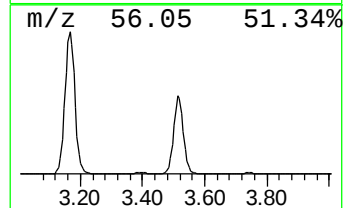
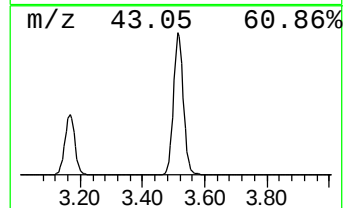
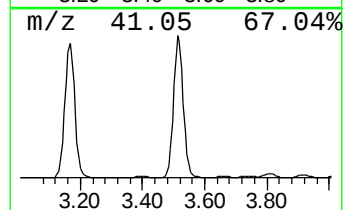
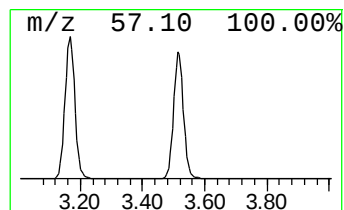
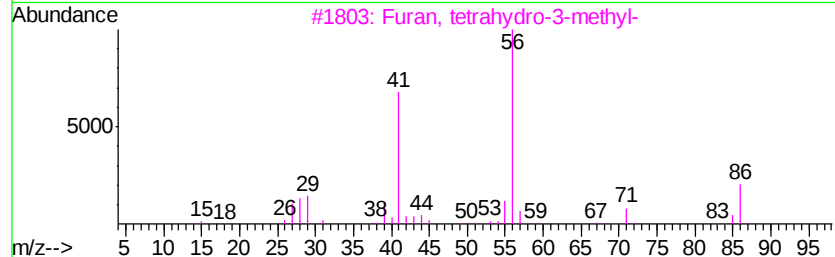
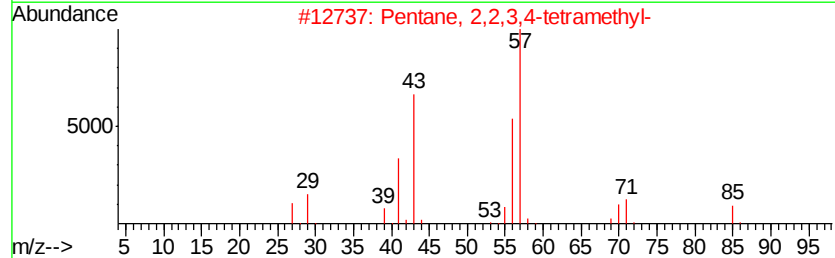
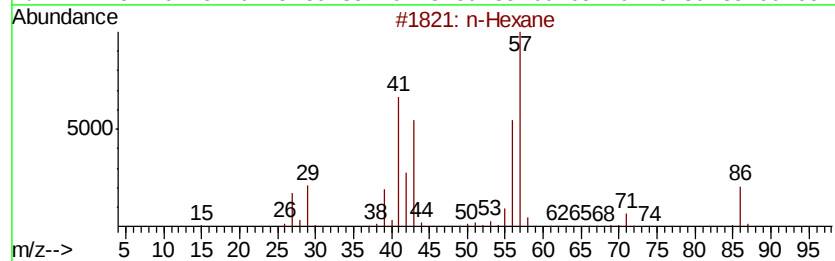
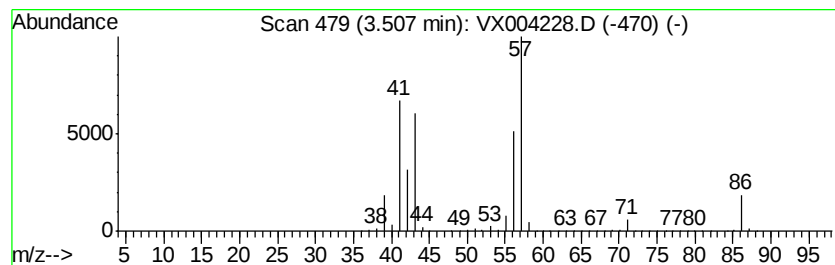
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Quant Title : SW846 8260

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

Peak Number 5 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.51	322.74 ug/l	5200440	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	94
2		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	50
3		Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	50
4		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
5		Methane, isocyanato-	57	C2H3NO	000624-83-9	32



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082318\
Data File : VX004228.D
Acq On : 23 Aug 2018 15:53
Operator : JC/MD
Sample : J4579-11
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

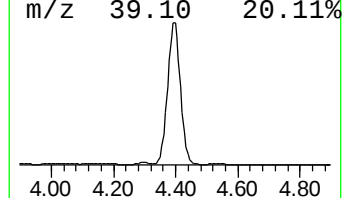
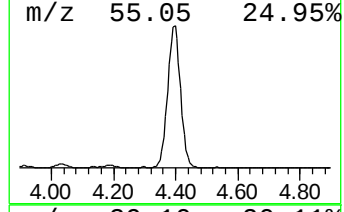
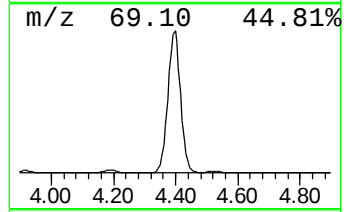
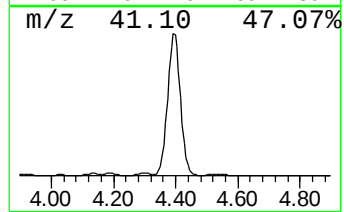
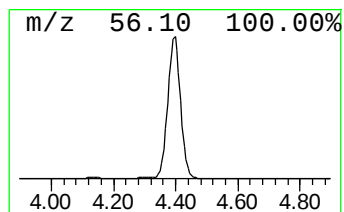
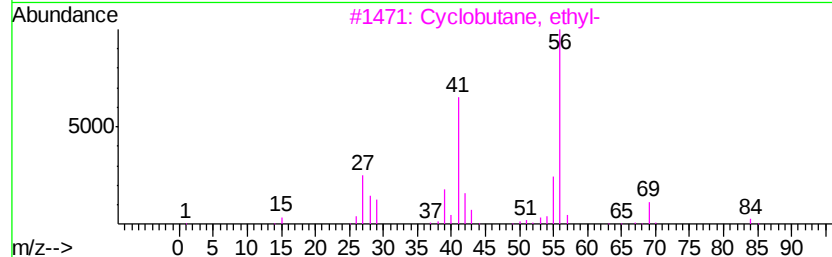
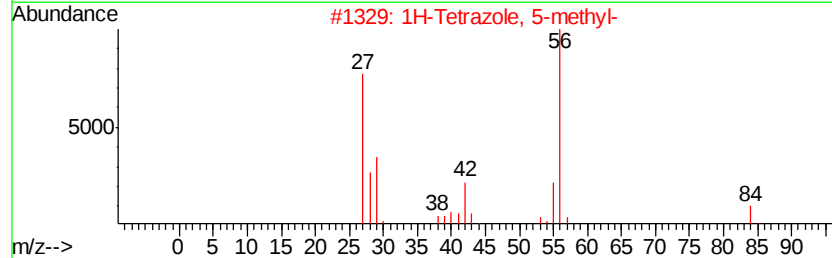
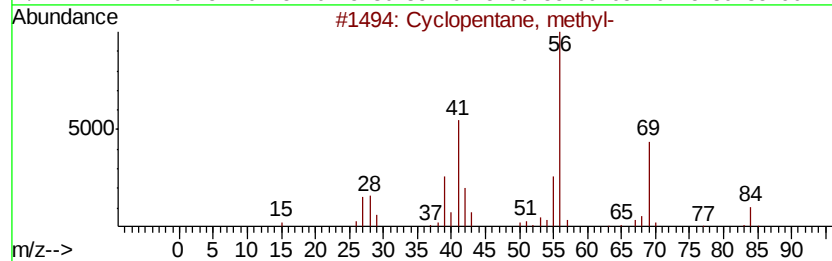
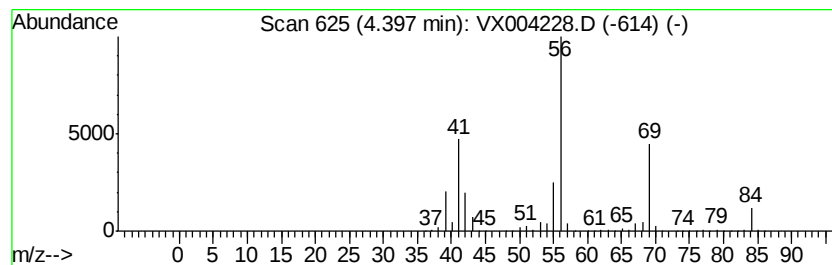
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	675.02 ug/l	10877100	Pentafluorobenzene	5.67

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	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4		Cyclohexane	84	C6H12	000110-82-7	56
5		Cyclobutane, butyl-	112	C8H16	013152-44-8	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082318\
Data File : VX004228.D
Acq On : 23 Aug 2018 15:53
Operator : JC/MD
Sample : J4579-11
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

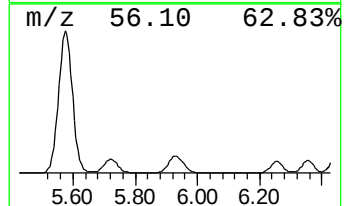
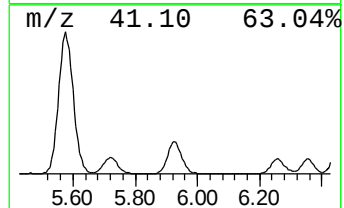
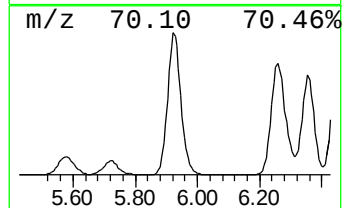
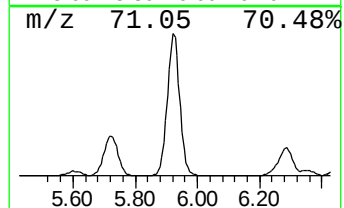
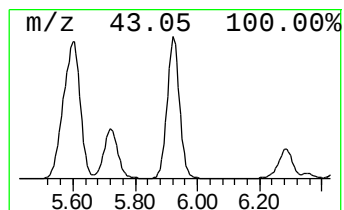
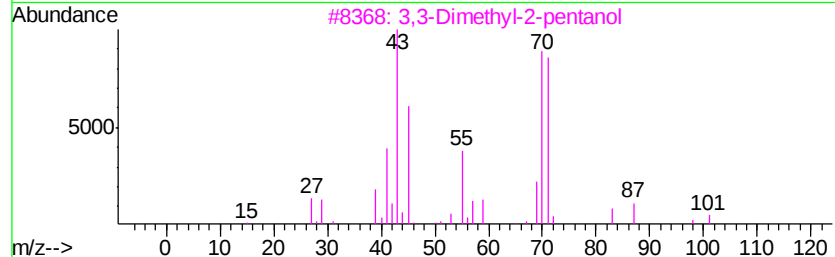
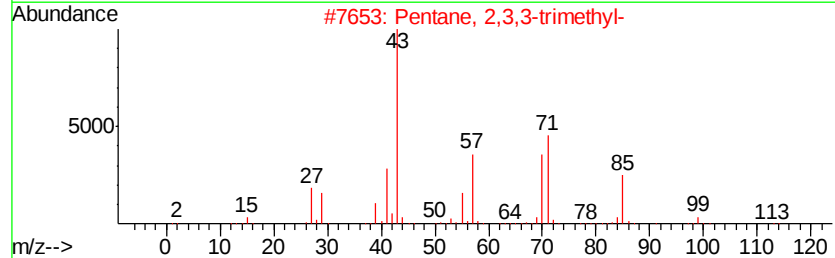
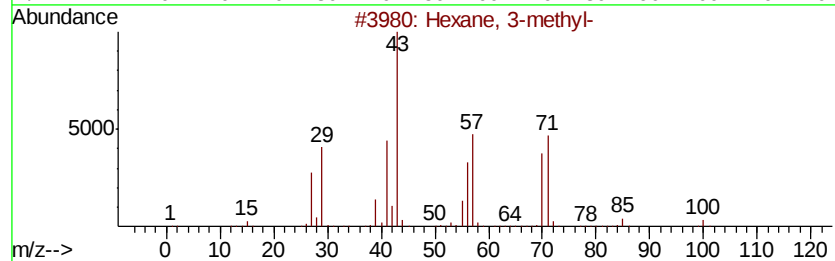
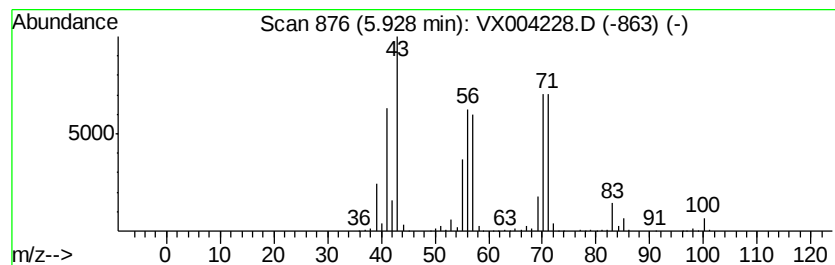
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	145.56 ug/l	2345510	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 3-methyl-	100	C7H16	000589-34-4	72
2		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	50
3		3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	50
4		Sulfurous acid, isobutyl 2-pentyl...	208	C9H20O3S	1000309-15-2	50
5		Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082318\
Data File : VX004228.D
Acq On : 23 Aug 2018 15:53
Operator : JC/MD
Sample : J4579-11
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

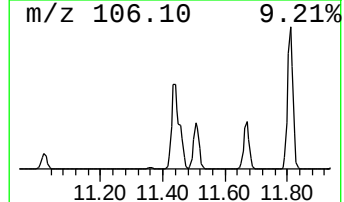
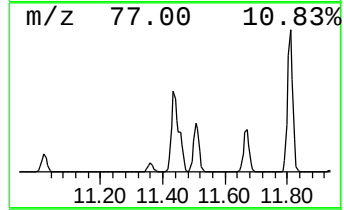
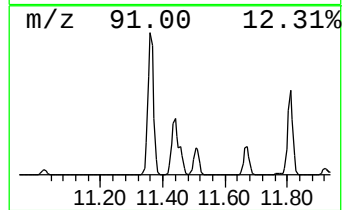
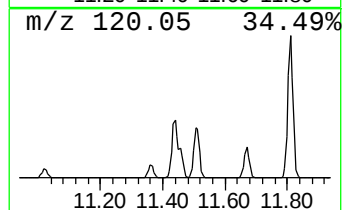
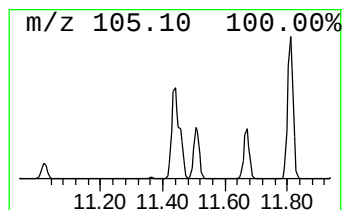
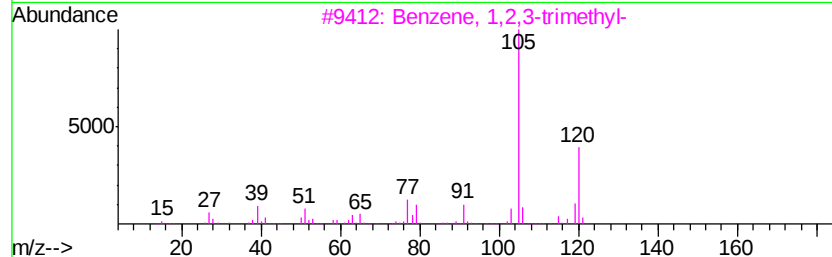
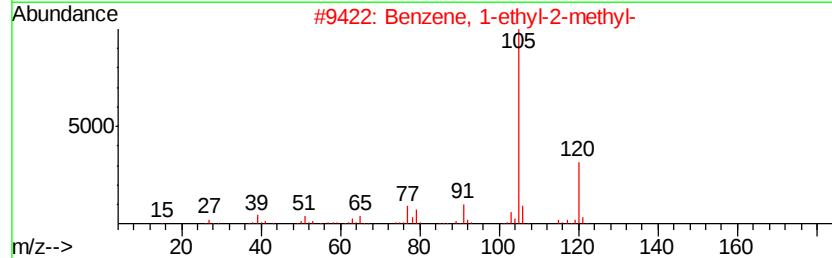
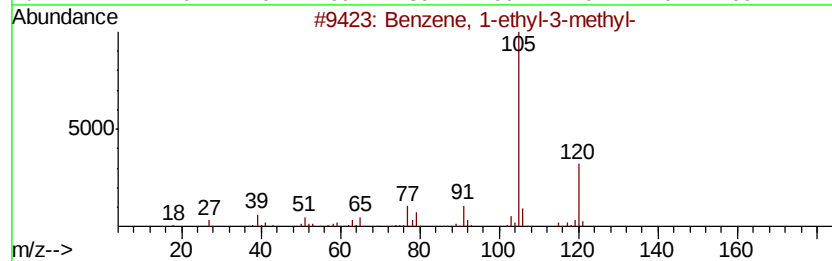
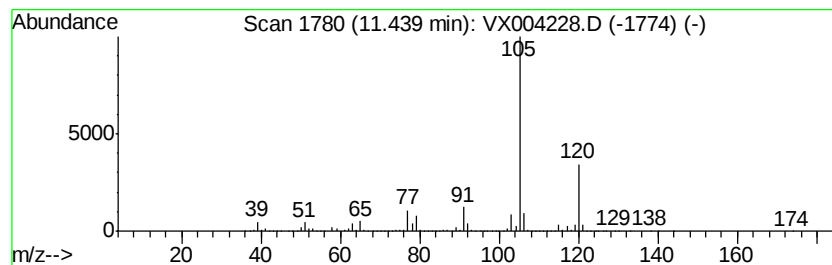
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	426.95 ug/l	18168200	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
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\VX082318\
Data File : VX004228.D
Acq On : 23 Aug 2018 15:53
Operator : JC/MD
Sample : J4579-11
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

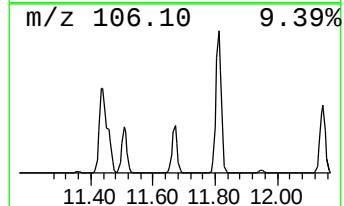
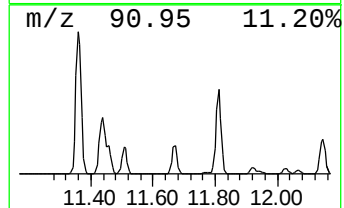
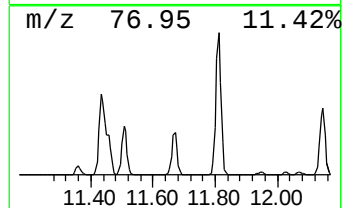
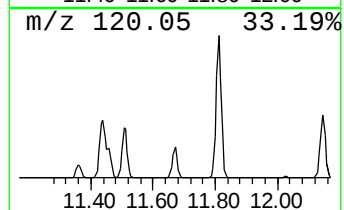
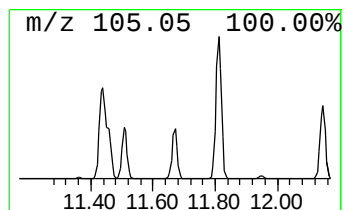
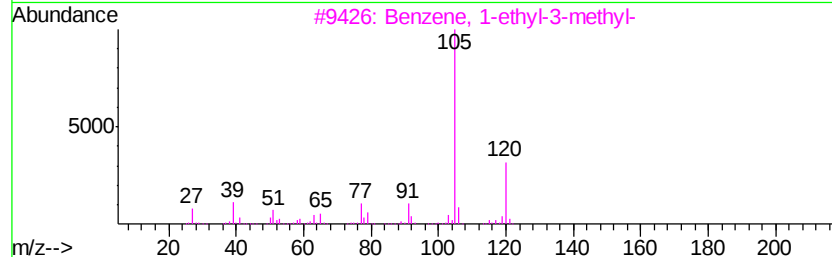
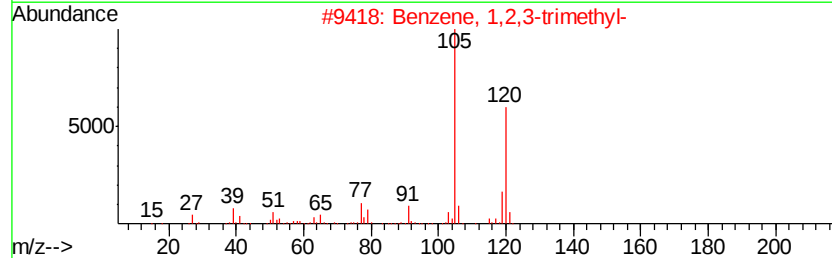
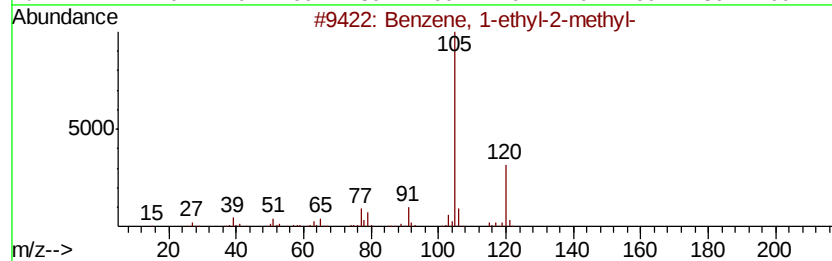
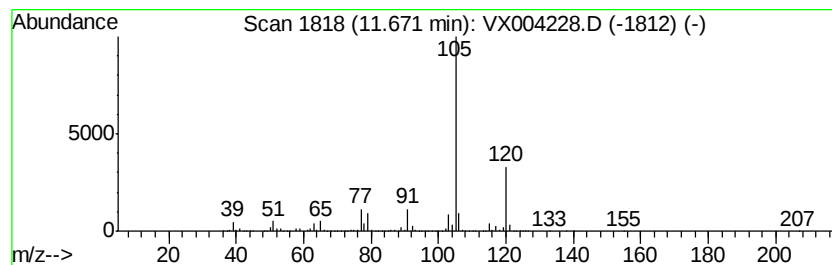
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	156.22 ug/l	6647660	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082318\
Data File : VX004228.D
Acq On : 23 Aug 2018 15:53
Operator : JC/MD
Sample : J4579-11
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

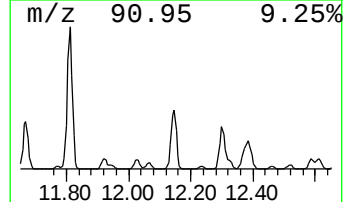
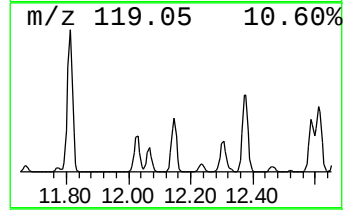
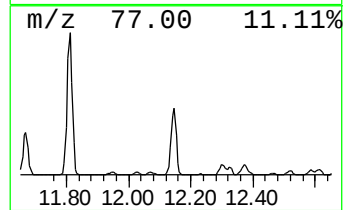
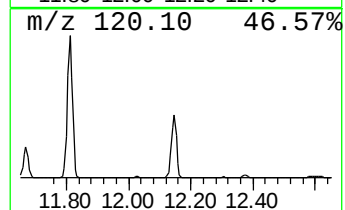
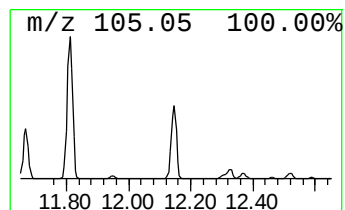
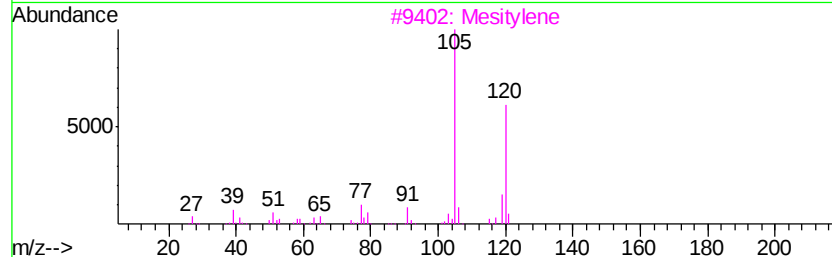
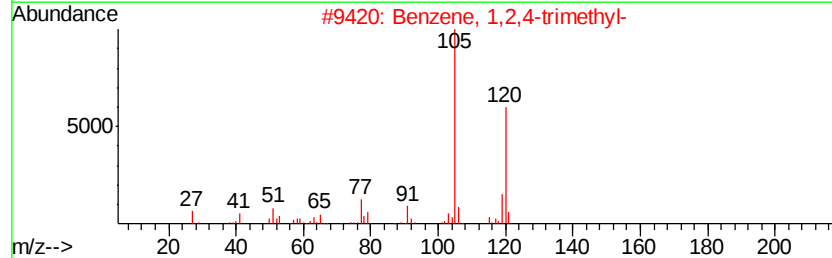
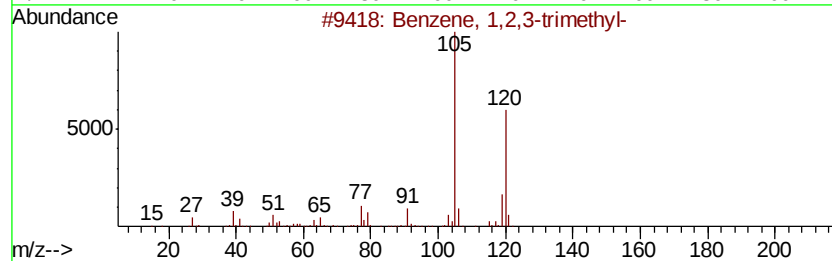
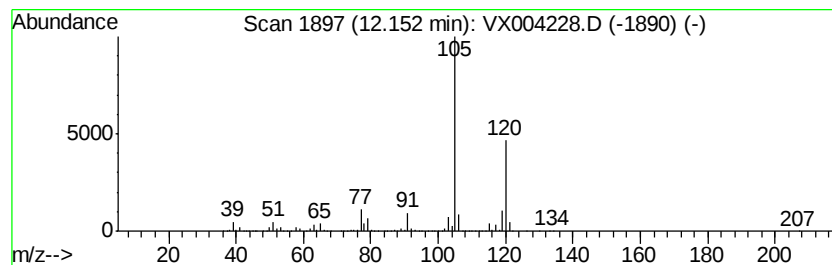
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	244.28 ug/l	10395200	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082318\
Data File : VX004228.D
Acq On : 23 Aug 2018 15:53
Operator : JC/MD
Sample : J4579-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0552

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	153.6	ug/l	2474400	1	5.67	805683	50.0
Pentane	2.00	173.4	ug/l	2794280	1	5.67	805683	50.0
Pentane, 2-methyl-	2.89	357.6	ug/l	5762910	1	5.67	805683	50.0
Pentane, 3-methyl-	3.17	301.7	ug/l	4861160	1	5.67	805683	50.0
n-Hexane	3.51	322.7	ug/l	5200440	1	5.67	805683	50.0
Cyclopentane, met...	4.40	675.0	ug/l	10877100	1	5.67	805683	50.0
Hexane, 3-methyl-	5.93	145.6	ug/l	2345510	1	5.67	805683	50.0
Benzene, 1-ethyl-...	11.44	426.9	ug/l	18168200	4	12.08	2127690	50.0
Benzene, 1-ethyl-...	11.67	156.2	ug/l	6647660	4	12.08	2127690	50.0
Benzene, 1,2,3-tr...	12.15	244.3	ug/l	10395200	4	12.08	2127690	50.0