

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082318\
 Data File : VX004226.D
 Acq On : 23 Aug 2018 15:00
 Operator : JC/MD
 Sample : J4579-09
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0553

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	1363833	1795754	5.00%	1.206%
2	1.788	191	197	210	rVB	766172	1083190	3.02%	0.728%
3	1.995	226	231	246	rVB	540231	764900	2.13%	0.514%
4	2.837	362	369	373	rBV	238774	536799	1.50%	0.361%
5	2.885	373	377	380	rVV	412168	797247	2.22%	0.536%
6	2.928	380	384	399	rVB	357575	744056	2.07%	0.500%
7	3.166	414	423	436	rBV	769750	1734820	4.83%	1.165%
8	3.513	471	480	493	rBV	349147	777233	2.17%	0.522%
9	4.391	614	624	638	rVB	928460	2706449	7.54%	1.818%
10	5.501	791	806	810	rBV	214976	586086	1.63%	0.394%
11	5.574	810	818	827	rVV	697286	2142324	5.97%	1.439%
12	5.659	827	832	839	rVB	230485	554836	1.55%	0.373%
13	5.934	864	877	889	rBV3	161183	560458	1.56%	0.377%
14	6.068	889	899	913	rVV	231374	595131	1.66%	0.400%
15	6.257	917	930	939	rVV3	135211	463557	1.29%	0.311%
16	6.354	939	946	954	rVV	130500	363149	1.01%	0.244%
17	6.860	1019	1029	1039	rBV	483444	1150327	3.20%	0.773%
18	7.458	1114	1127	1139	rBV	887336	2040588	5.69%	1.371%
19	8.714	1328	1333	1339	rVB	1184967	1883156	5.25%	1.265%
20	8.787	1339	1345	1350	rBV	2396748	3611584	10.06%	2.426%
21	10.116	1557	1563	1569	rVB	940886	1261583	3.51%	0.848%
22	10.256	1579	1586	1592	rBV	10576669	13879867	38.67%	9.325%
23	10.366	1595	1604	1609	rBV	25564527	35892819	100.00%	24.113%
24	10.701	1653	1659	1671	rVB	13407918	16612910	46.28%	11.161%
25	11.018	1706	1711	1717	rBV	1237755	1536885	4.28%	1.032%
26	11.140	1725	1731	1736	rBV	1041319	1329852	3.71%	0.893%
27	11.360	1762	1767	1774	rBV	1539767	1811326	5.05%	1.217%
28	11.439	1774	1780	1787	rVV	3782011	7275596	20.27%	4.888%
29	11.506	1787	1791	1800	rVB	2295281	2797585	7.79%	1.879%
30	11.670	1812	1818	1827	rBV	3194269	3913529	10.90%	2.629%
31	11.811	1836	1841	1846	rVB	9927946	12291780	34.25%	8.258%
32	12.024	1870	1876	1880	rBV	321026	412286	1.15%	0.277%
33	12.079	1880	1885	1890	rVB2	1405672	1868262	5.21%	1.255%
34	12.146	1890	1896	1901	rBV	4400788	5314453	14.81%	3.570%

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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	12.298	1916	1921	1929	rBV2	2322068	3350264	9.33%	2.251%
36	12.372	1929	1933	1943	rVB3	721703	1065404	2.97%	0.716%
37	12.585	1963	1968	1970	rBV	443432	537257	1.50%	0.361%
38	12.609	1970	1972	1976	rVB	492913	533117	1.49%	0.358%
39	12.670	1977	1982	1985	rBV	700028	816048	2.27%	0.548%
40	12.756	1992	1996	2004	rVB3	509263	861535	2.40%	0.579%
41	12.902	2016	2020	2025	rVB2	324696	436038	1.21%	0.293%
42	12.981	2025	2033	2036	rBV	499532	664217	1.85%	0.446%
43	13.018	2036	2039	2046	rVB	797883	934143	2.60%	0.628%
44	13.347	2088	2093	2098	rVB2	1410534	1872019	5.22%	1.258%
45	13.481	2110	2115	2122	rVB	678968	839640	2.34%	0.564%
46	13.835	2165	2173	2181	rVB	2935928	3735100	10.41%	2.509%
47	14.694	2307	2314	2319	rBV	819652	1112286	3.10%	0.747%
48	14.841	2333	2338	2347	rBV	817322	1004575	2.80%	0.675%

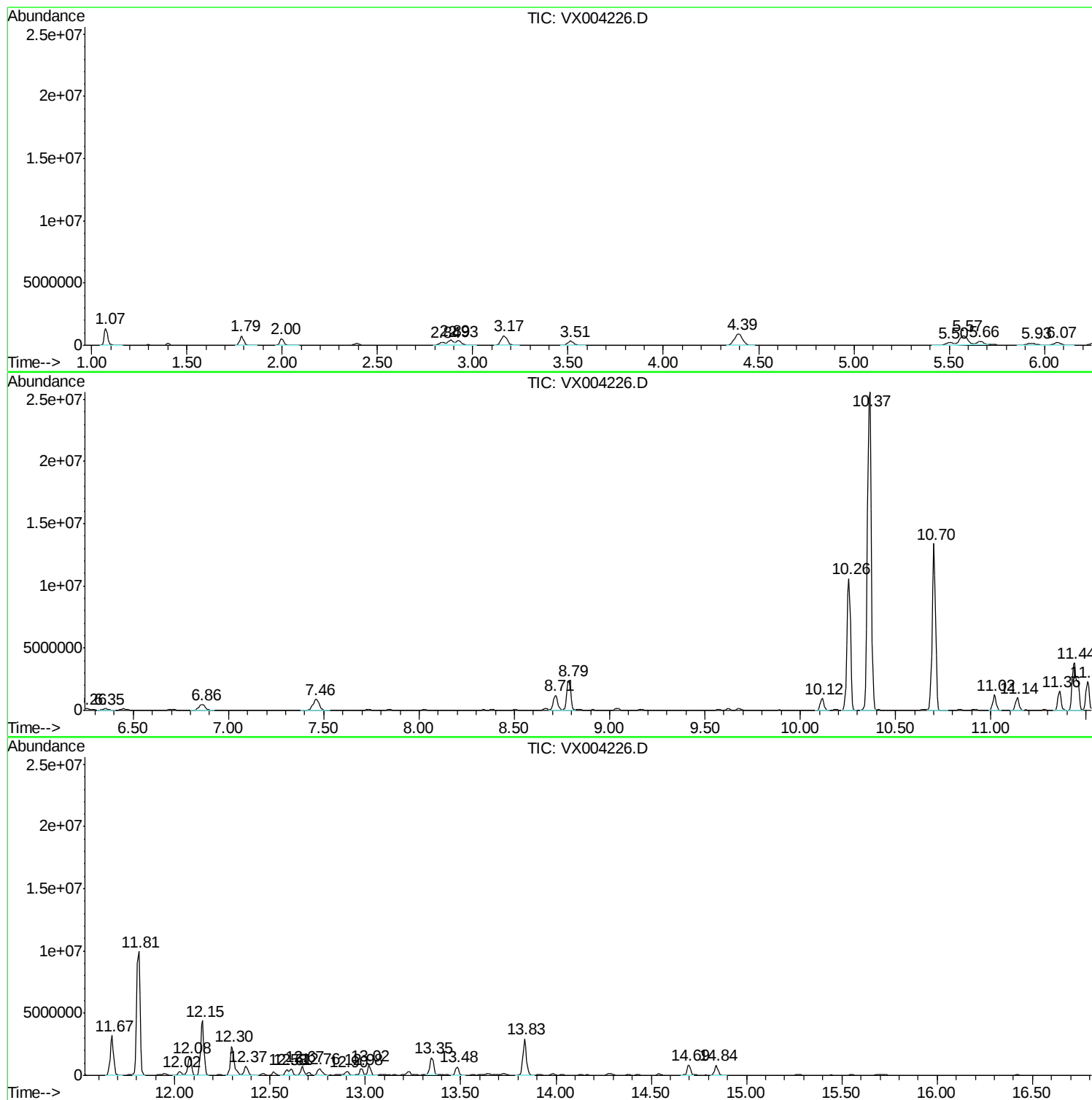
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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



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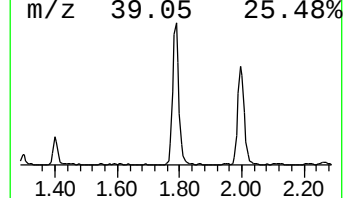
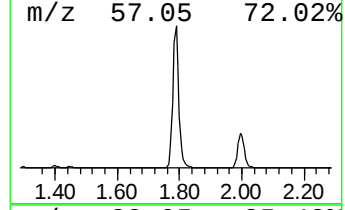
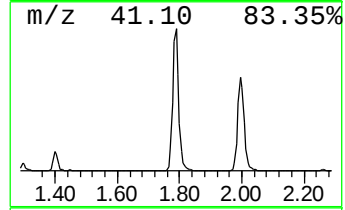
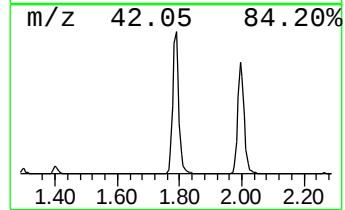
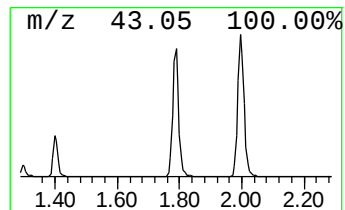
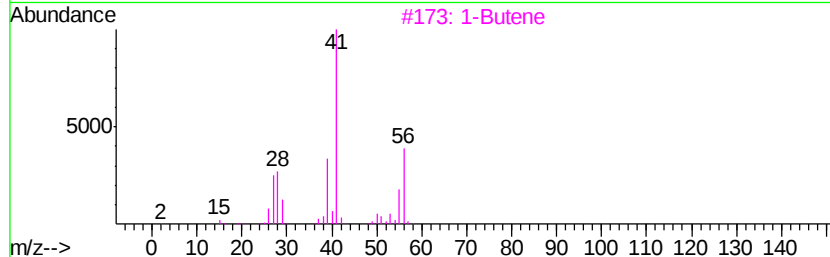
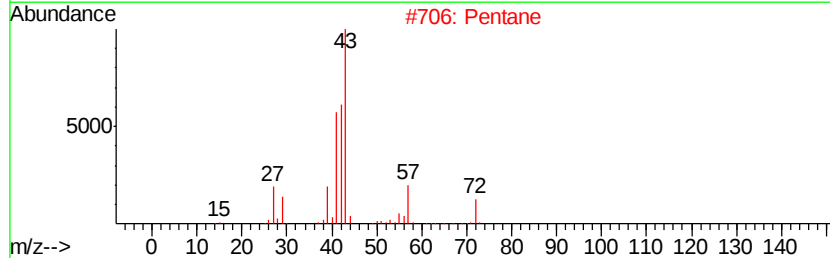
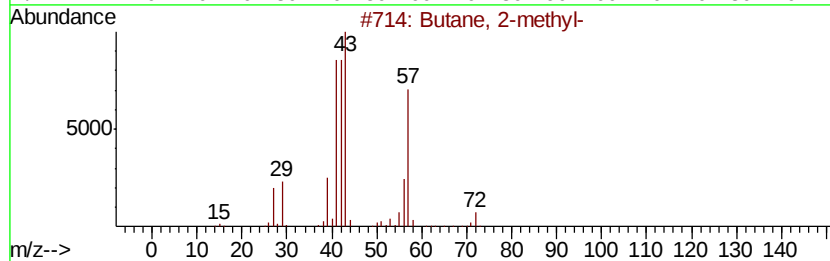
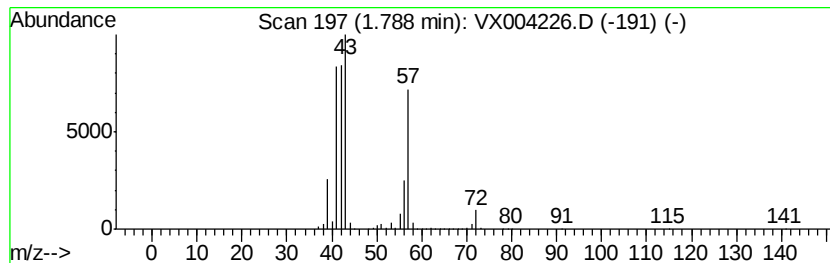
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	97.61 ug/l	1083190	Pentafluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	94
2			Pentane	72	C5H12	000109-66-0	43
3			1-Butene	56	C4H8	000106-98-9	10
4			Methane, isocyanato-	57	C2H3NO	000624-83-9	9
5			Cyclobutane	56	C4H8	000287-23-0	9



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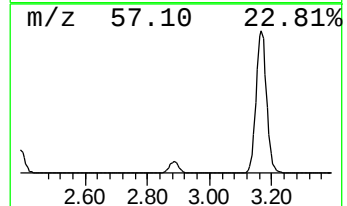
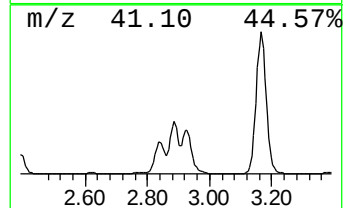
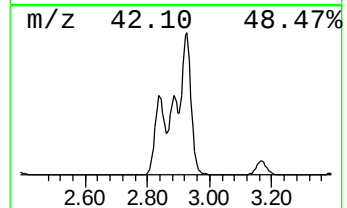
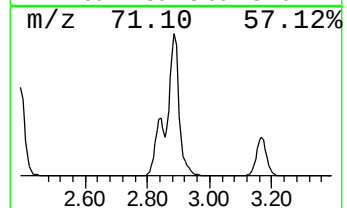
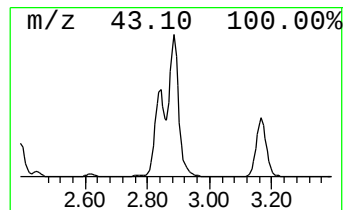
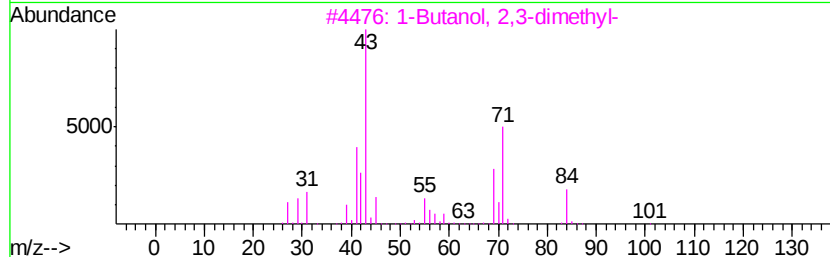
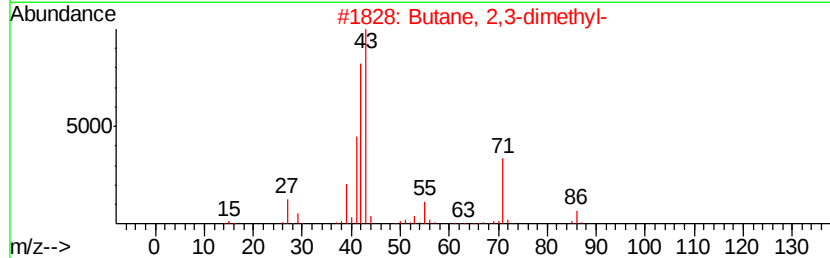
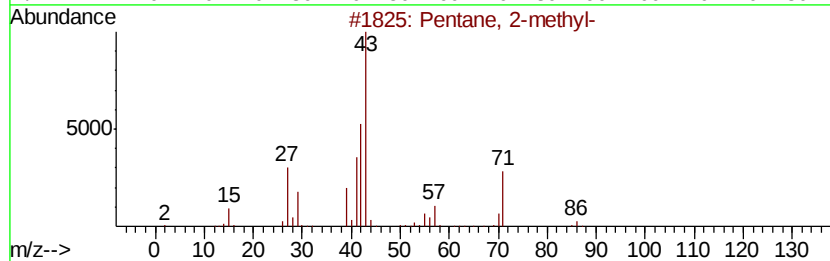
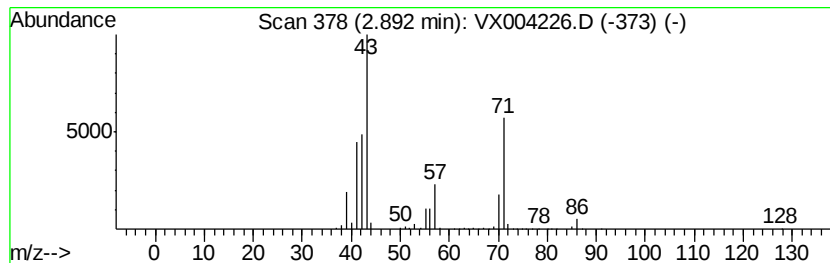
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	71.85 ug/l	797247	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

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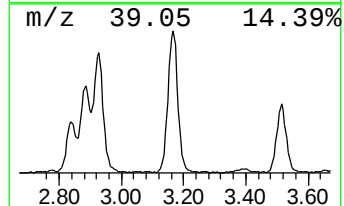
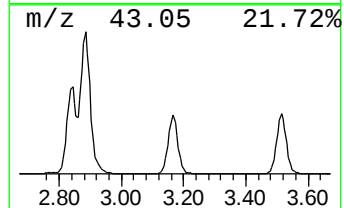
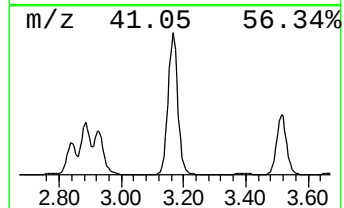
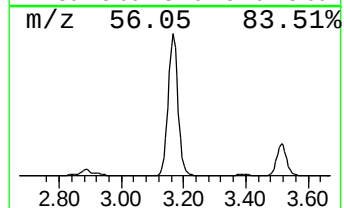
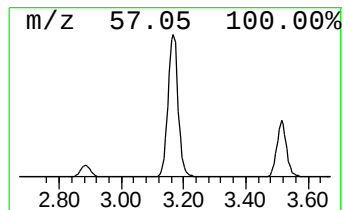
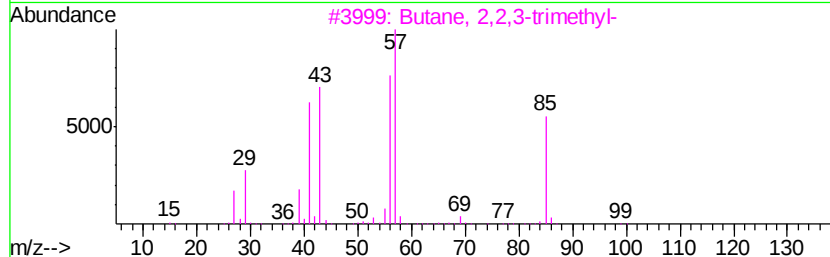
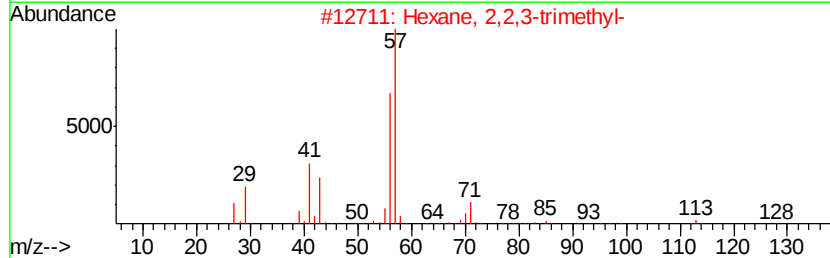
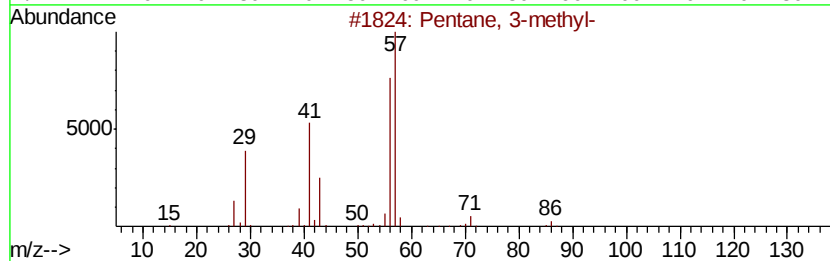
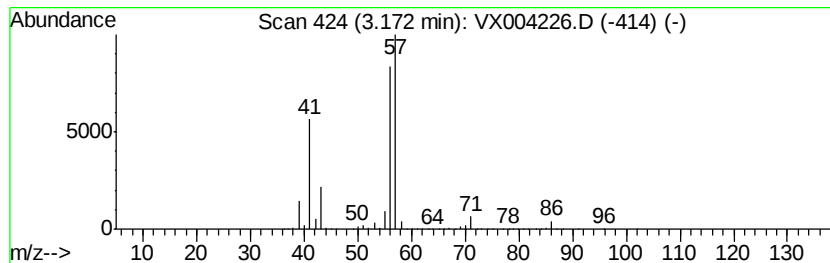
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	156.34 ug/l	1734820	Pentafluorobenzene	5.66

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		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
4		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
5		n-Hexane	86	C6H14	000110-54-3	47



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampled :
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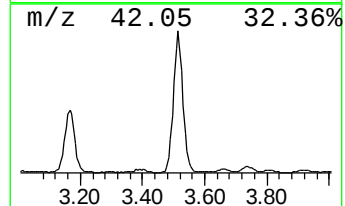
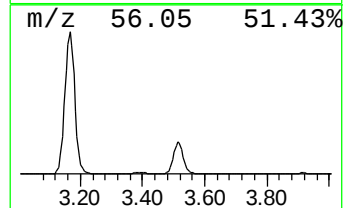
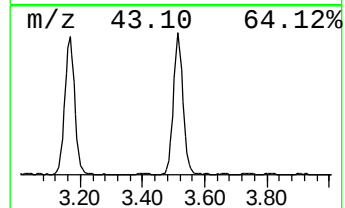
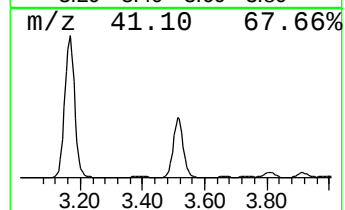
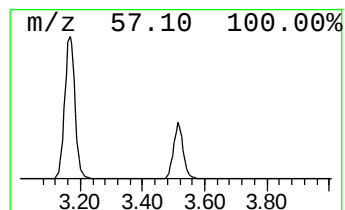
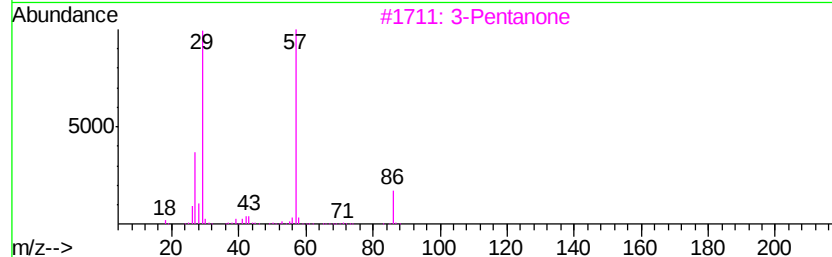
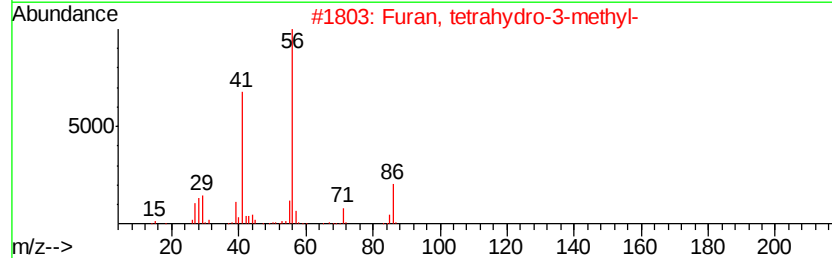
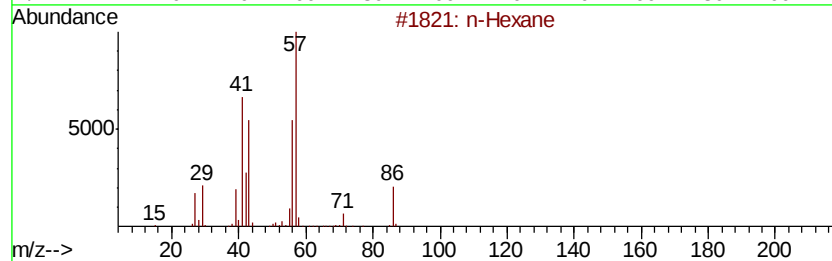
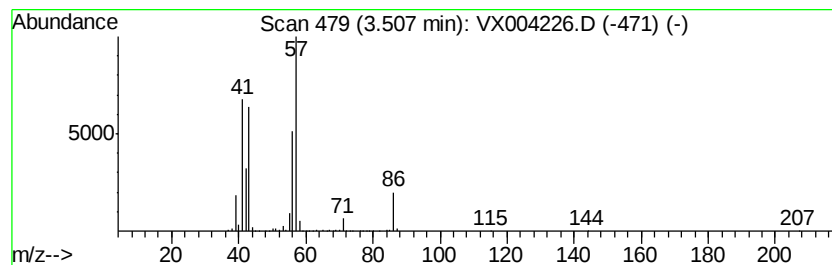
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Quant Title : SW846 8260

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

Peak Number 5 n-Hexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.51	70.04 ug/l	777233	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	47
3		3-Pentanone	86	C5H10O	000096-22-0	38
4		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
5		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35



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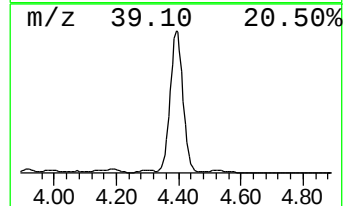
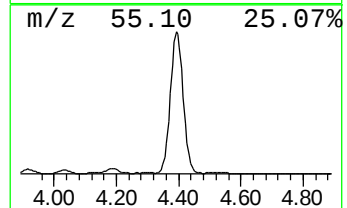
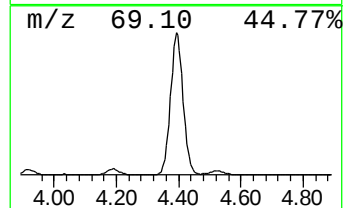
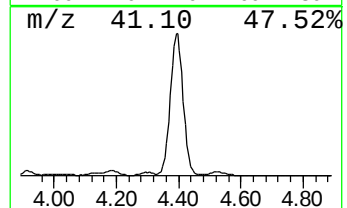
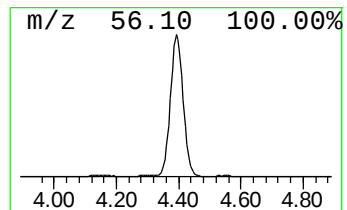
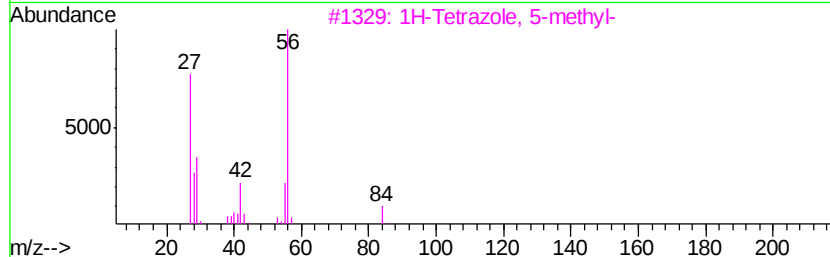
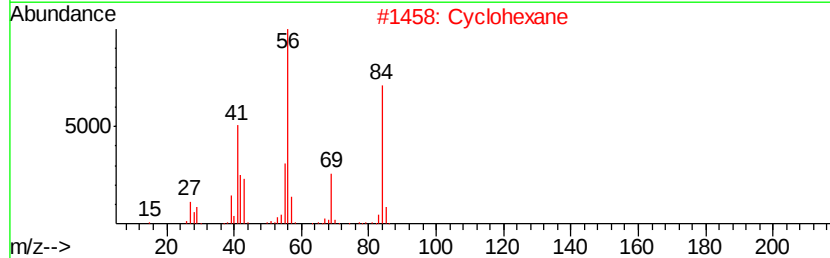
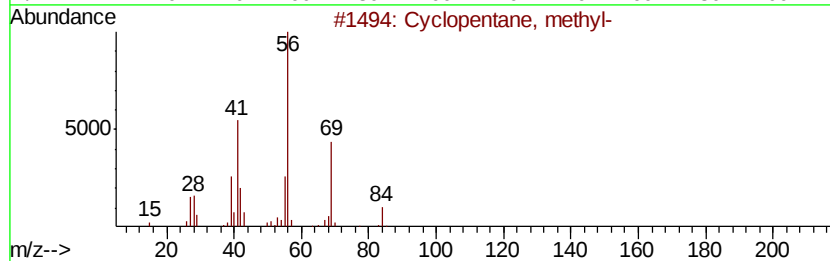
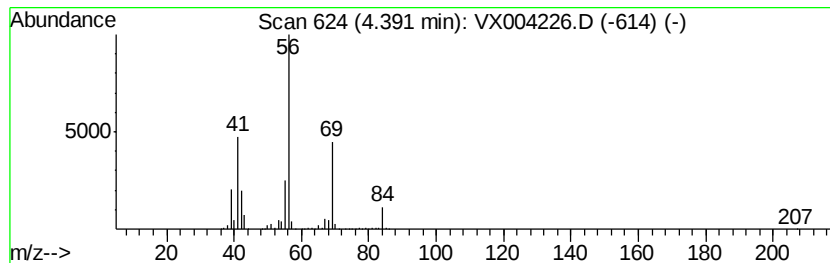
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	243.90 ug/l	2706450	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclohexane	84	C6H12	000110-82-7	78
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		Cyclobutane, butyl-	112	C8H16	013152-44-8	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082318\
Data File : VX004226.D
Acq On : 23 Aug 2018 15:00
Operator : JC/MD
Sample : J4579-09
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0553

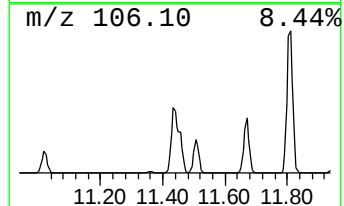
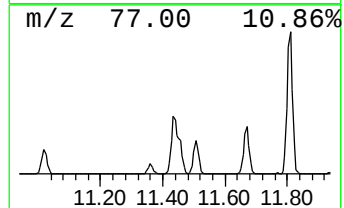
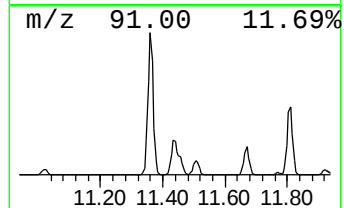
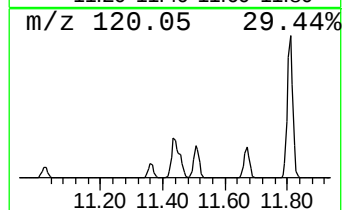
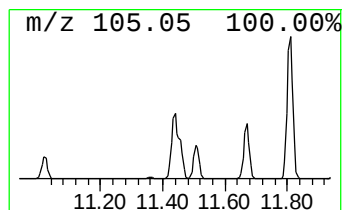
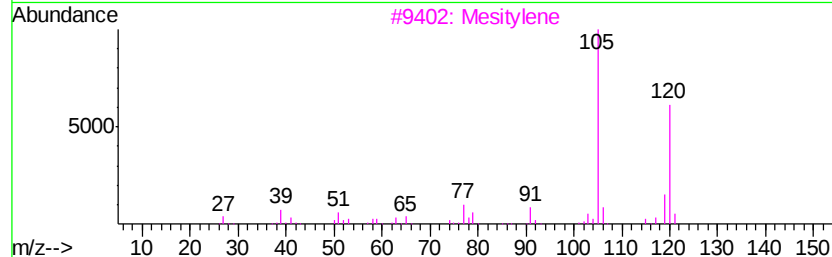
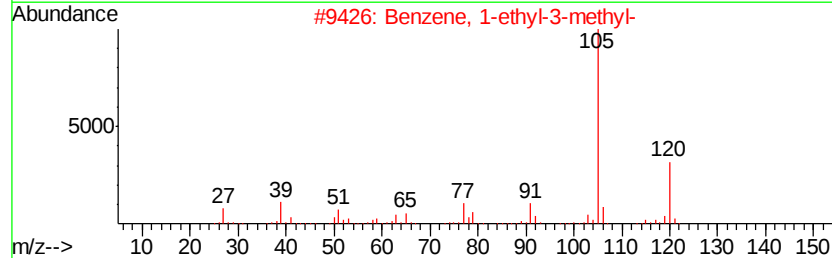
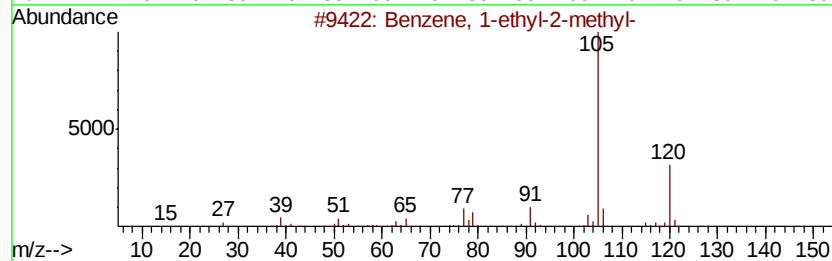
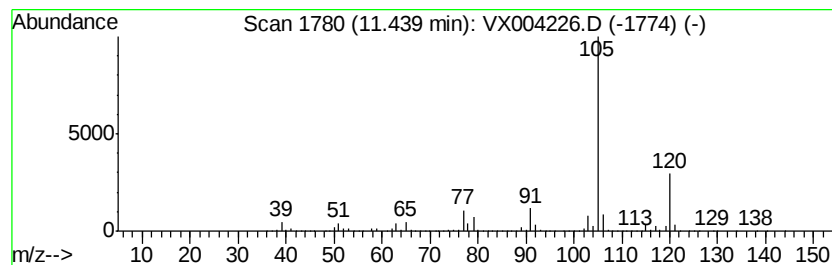
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	194.72 ug/l	7275600	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	95
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
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\VX082318\
Data File : VX004226.D
Acq On : 23 Aug 2018 15:00
Operator : JC/MD
Sample : J4579-09
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0553

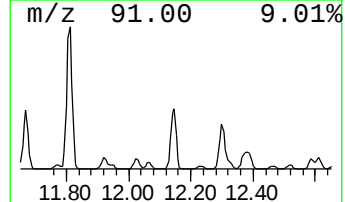
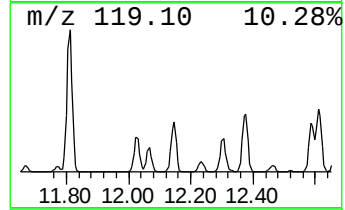
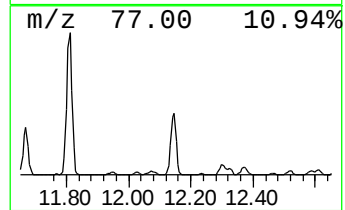
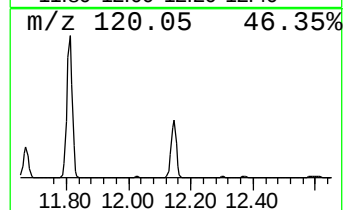
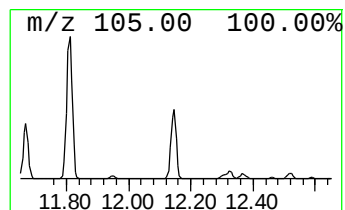
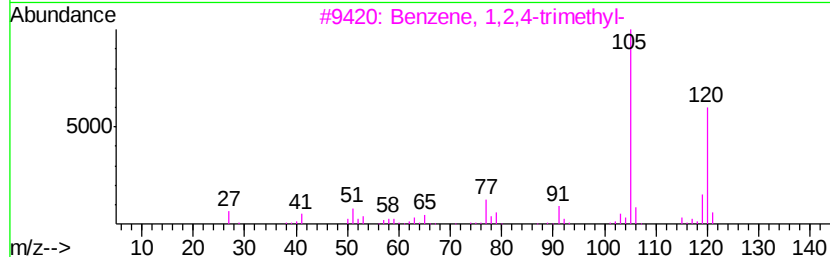
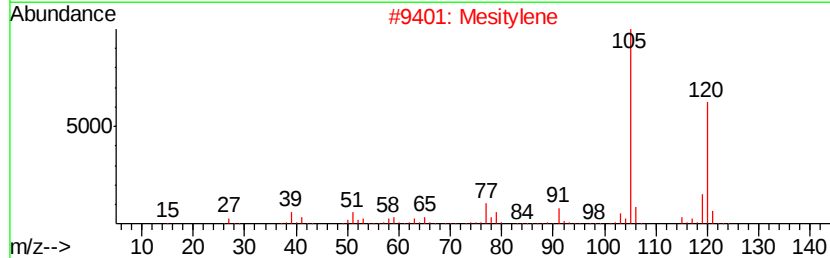
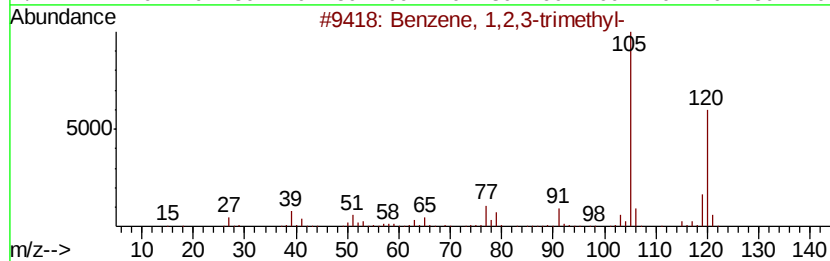
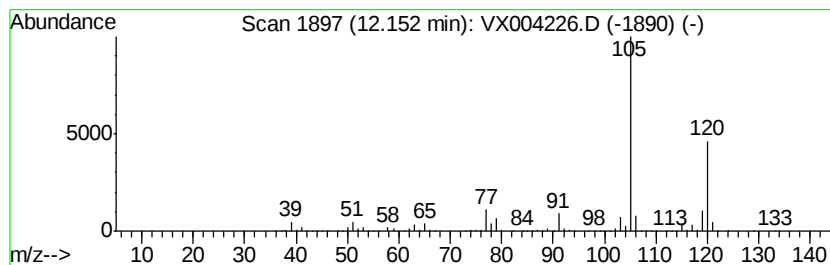
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	142.23 ug/l	5314450	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082318\
Data File : VX004226.D
Acq On : 23 Aug 2018 15:00
Operator : JC/MD
Sample : J4579-09
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0553

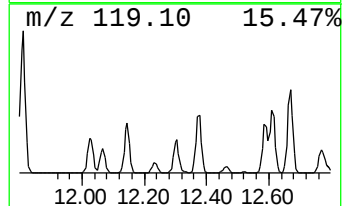
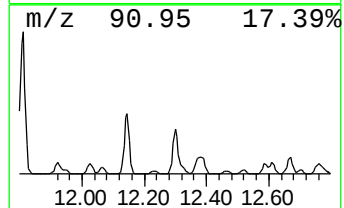
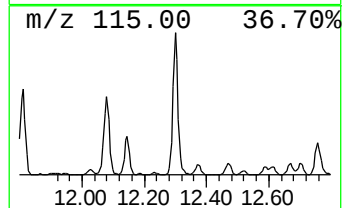
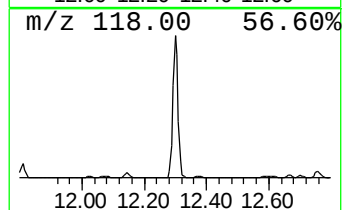
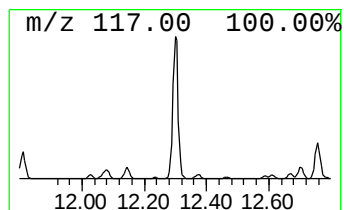
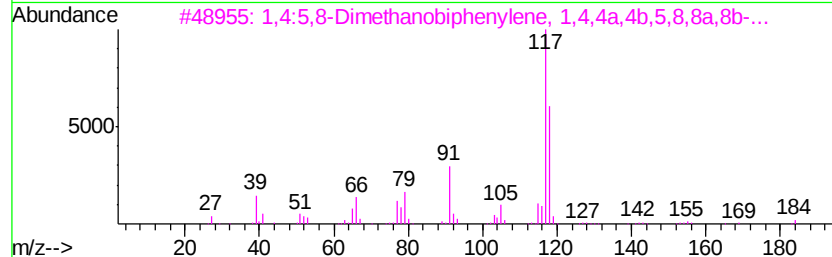
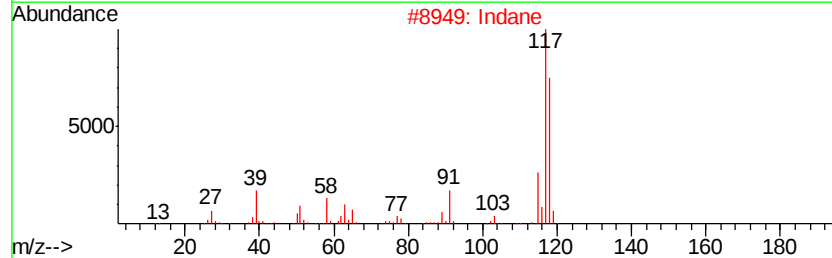
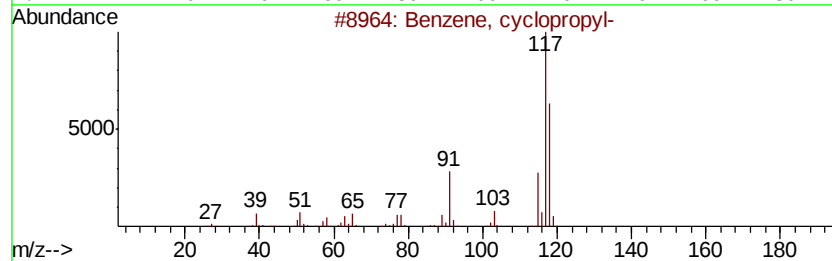
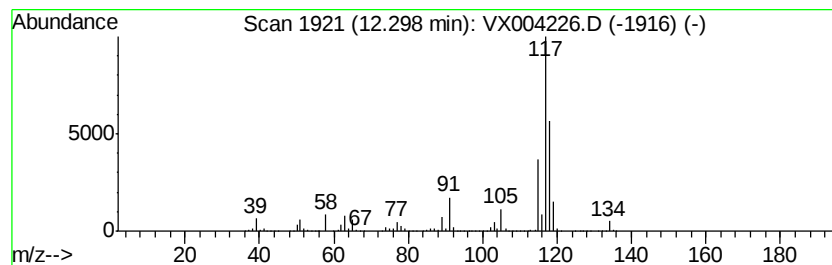
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, cyclopropyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	89.66 ug/l	3350260	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, cvclopropyl-	118	C9H10	000873-49-4	76
2		Indane	118	C9H10	000496-11-7	76
3		1,4:5,8-Dimethanobiphenylene, 1,...	184	C14H16	001624-13-1	72
4		Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5		Deltacyclene	118	C9H10	007785-10-6	58



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082318\
Data File : VX004226.D
Acq On : 23 Aug 2018 15:00
Operator : JC/MD
Sample : J4579-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0553

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	97.6	ug/l	1083190	1	5.66	554836	50.0
Pentane, 2-methyl-	2.89	71.8	ug/l	797247	1	5.66	554836	50.0
Pentane, 3-methyl-	3.17	156.3	ug/l	1734820	1	5.66	554836	50.0
n-Hexane	3.51	70.0	ug/l	777233	1	5.66	554836	50.0
Cyclopentane, met...	4.39	243.9	ug/l	2706450	1	5.66	554836	50.0
Benzene, 1-ethyl-...	11.44	194.7	ug/l	7275600	4	12.08	1868260	50.0
Benzene, 1,2,3-tr...	12.15	142.2	ug/l	5314450	4	12.08	1868260	50.0
Benzene, cyclopro...	12.30	89.7	ug/l	3350260	4	12.08	1868260	50.0