

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091819\
 Data File : VX012511.D
 Acq On : 19 Sep 2019 06:34
 Operator : JC/SP
 Sample : K4830-14
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 S13-0281

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\82X091719W.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	1.070	26	30	42	rBV	606770	705241	69.69%	8.395%
2	1.265	59	62	65	rBV	29614	37445	3.70%	0.446%
3	1.302	65	68	77	rVV	23646	67116	6.63%	0.799%
4	2.594	273	280	290	rBV	20957	40761	4.03%	0.485%
5	3.015	344	349	360	rVB7	4005	10592	1.05%	0.126%
6	3.167	369	374	381	rVB4	4896	11568	1.14%	0.138%
7	5.490	741	755	765	rBV	112787	321840	31.81%	3.831%
8	5.655	768	782	805	rVB	218932	650967	64.33%	7.749%
9	5.923	815	826	837	rBV8	7941	28707	2.84%	0.342%
10	6.051	837	847	865	rVV	134575	357217	35.30%	4.252%
11	6.350	890	896	903	rVB8	5170	12737	1.26%	0.152%
12	6.441	904	911	921	rVB5	6682	19256	1.90%	0.229%
13	6.850	967	978	992	rBV	324248	764838	75.58%	9.104%
14	7.453	1066	1077	1085	rBV4	21229	54931	5.43%	0.654%
15	7.843	1134	1141	1148	rVB2	7688	16056	1.59%	0.191%
16	8.026	1166	1171	1181	rVB6	7635	18952	1.87%	0.226%
17	8.386	1224	1230	1237	rVB3	8430	17537	1.73%	0.209%
18	8.660	1268	1275	1278	rBV2	25126	47212	4.67%	0.562%
19	8.709	1278	1283	1295	rVV	631772	1011898	100.00%	12.045%
20	8.831	1299	1303	1308	rVV	20399	35656	3.52%	0.424%
21	8.910	1308	1316	1321	rVV4	8634	20909	2.07%	0.249%
22	9.038	1331	1337	1343	rVB	34664	57851	5.72%	0.689%
23	9.160	1349	1357	1362	rBV2	18790	34277	3.39%	0.408%
24	9.569	1419	1424	1428	rBV3	15000	26656	2.63%	0.317%
25	9.617	1428	1432	1437	rVB	24228	32122	3.17%	0.382%
26	9.672	1437	1441	1446	rBV	32573	48948	4.84%	0.583%
27	9.886	1471	1476	1480	rBV4	8344	14561	1.44%	0.173%
28	10.111	1506	1513	1520	rBV	600968	830685	82.09%	9.888%
29	10.184	1520	1525	1530	rVB	16636	24629	2.43%	0.293%
30	10.233	1530	1533	1540	rVB7	7643	13561	1.34%	0.161%
31	10.337	1544	1550	1551	rBV3	15393	23777	2.35%	0.283%
32	10.507	1573	1578	1583	rVB2	9807	14939	1.48%	0.178%
33	10.654	1593	1602	1608	rBV5	13430	40504	4.00%	0.482%
34	10.831	1628	1631	1639	rVB3	16903	24749	2.45%	0.295%

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35	10.910	1639	1644	1651	rBV8	8527	17710	1.75%	0.211%
36	11.135	1675	1681	1686	rVV	455607	599253	59.22%	7.133%
37	11.178	1686	1688	1693	rVB3	10095	13216	1.31%	0.157%
38	11.276	1700	1704	1708	rVB3	14187	19339	1.91%	0.230%
39	11.446	1725	1732	1737	rBV8	6040	11737	1.16%	0.140%
40	11.672	1763	1769	1775	rBV7	10235	19244	1.90%	0.229%
41	11.806	1787	1791	1796	rVB	15421	20373	2.01%	0.243%
42	11.916	1802	1809	1811	rBV5	7331	15702	1.55%	0.187%
43	11.940	1811	1813	1819	rVB	11945	14409	1.42%	0.172%
44	12.074	1829	1835	1841	rBV	573831	704304	69.60%	8.384%
45	12.141	1841	1846	1850	rVB	11058	16667	1.65%	0.198%
46	12.227	1856	1860	1865	rVB	11982	14356	1.42%	0.171%
47	12.300	1867	1872	1878	rBV	19488	26459	2.61%	0.315%
48	12.361	1878	1882	1891	rVB2	26900	46223	4.57%	0.550%
49	12.458	1893	1898	1902	rBV	27201	33669	3.33%	0.401%
50	12.513	1902	1907	1913	rBV	66021	79648	7.87%	0.948%
51	12.580	1913	1918	1920	rBV	25192	33489	3.31%	0.399%
52	12.605	1920	1922	1926	rVV	37758	42771	4.23%	0.509%
53	12.666	1928	1932	1935	rVV	30130	38009	3.76%	0.452%
54	12.696	1935	1937	1942	rVV5	7397	12449	1.23%	0.148%
55	12.757	1942	1947	1954	rVV5	38217	78388	7.75%	0.933%
56	12.848	1958	1962	1964	rVV2	8568	11931	1.18%	0.142%
57	12.897	1966	1970	1975	rVB2	55236	74588	7.37%	0.888%
58	12.970	1975	1982	1986	rBV2	43104	70500	6.97%	0.839%
59	13.013	1986	1989	1996	rVB2	59106	71539	7.07%	0.852%
60	13.080	1996	2000	2006	rBV3	21941	34021	3.36%	0.405%
61	13.147	2006	2011	2014	rBV	14251	16922	1.67%	0.201%
62	13.190	2014	2018	2025	rBV3	28380	36564	3.61%	0.435%
63	13.257	2025	2029	2033	rVB2	11953	18151	1.79%	0.216%
64	13.300	2033	2036	2039	rBV3	14865	20425	2.02%	0.243%
65	13.342	2039	2043	2047	rVV2	92031	131747	13.02%	1.568%
66	13.476	2061	2065	2072	rVB3	23936	37562	3.71%	0.447%
67	13.556	2074	2078	2081	rBV3	11126	18329	1.81%	0.218%
68	13.598	2081	2085	2087	rVV2	15226	23912	2.36%	0.285%
69	13.629	2087	2090	2096	rVV3	37171	80930	8.00%	0.963%
70	13.696	2098	2101	2102	rVV	23305	30442	3.01%	0.362%
71	13.720	2102	2105	2110	rVV2	32658	49432	4.89%	0.588%

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72	13.806	2114	2119	2122	rBV	15767	20203	2.00%	0.240%
73	13.848	2122	2126	2131	rVB2	22927	31384	3.10%	0.374%
74	13.909	2131	2136	2141	rVB5	19412	29318	2.90%	0.349%
75	13.982	2141	2148	2152	rBV2	34091	49583	4.90%	0.590%
76	14.025	2152	2155	2159	rVV2	12235	17391	1.72%	0.207%
77	14.129	2167	2172	2174	rBV3	9711	15570	1.54%	0.185%
78	14.269	2189	2195	2202	rVB3	25019	51669	5.11%	0.615%
79	14.373	2208	2212	2217	rVB3	14174	17714	1.75%	0.211%
80	14.427	2217	2221	2225	rVB5	11510	15423	1.52%	0.184%
81	14.470	2225	2228	2234	rVB3	8941	12770	1.26%	0.152%
82	14.537	2234	2239	2244	rBV2	30058	45901	4.54%	0.546%
83	14.671	2257	2261	2267	rBV6	8740	19667	1.94%	0.234%
84	14.726	2267	2270	2275	rVB2	8421	11178	1.10%	0.133%
85	14.842	2282	2289	2292	rBV4	12190	22789	2.25%	0.271%
86	15.238	2350	2354	2362	rVB9	7697	17007	1.68%	0.202%

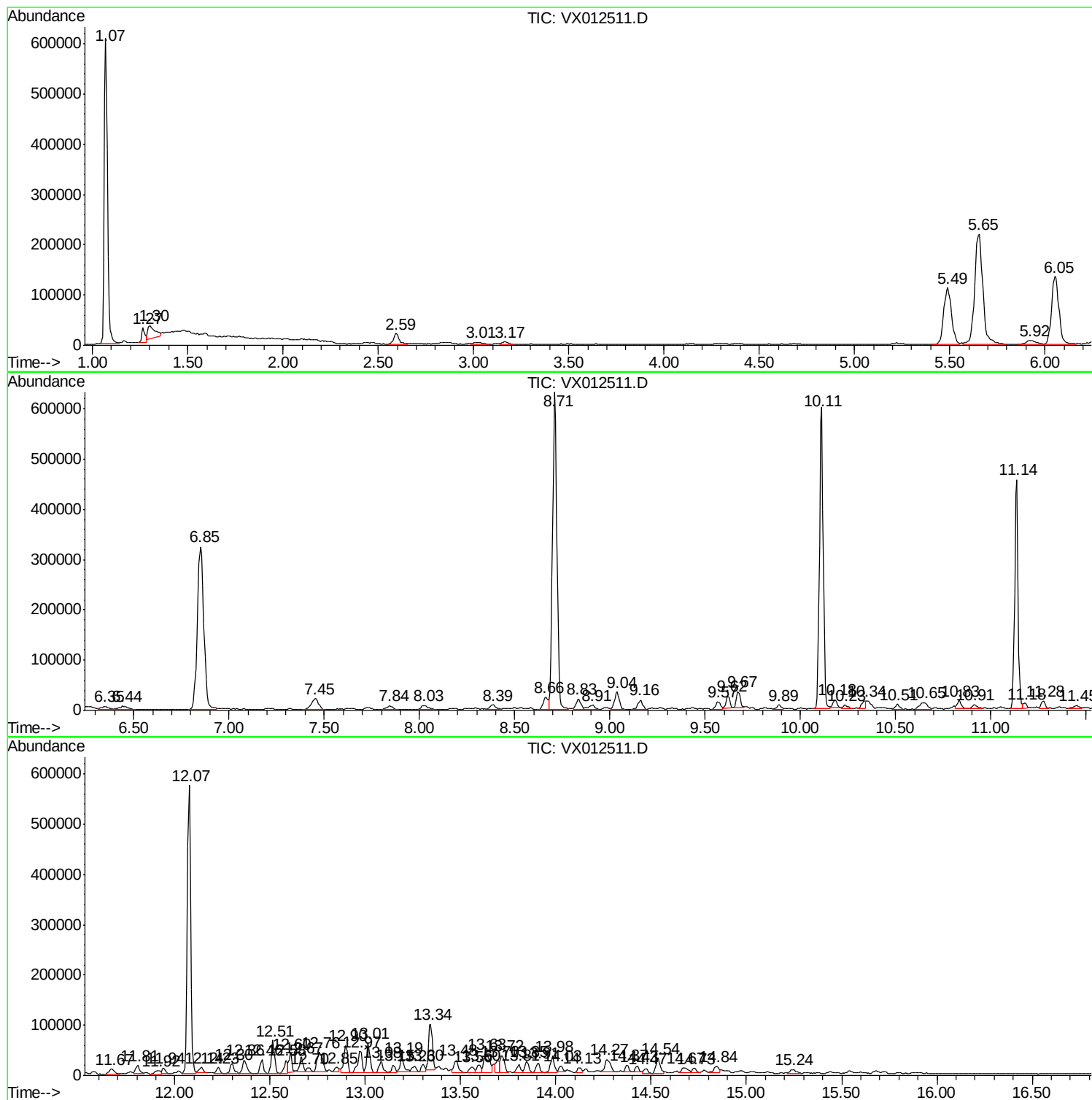
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Quant Title : SW846 8260

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



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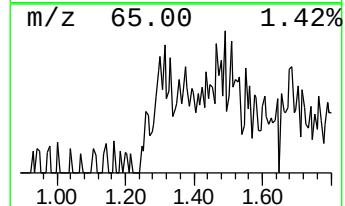
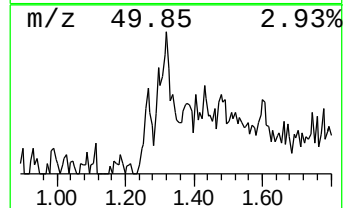
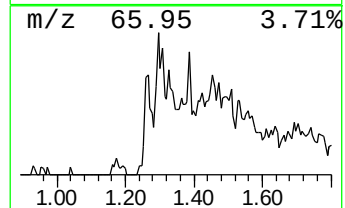
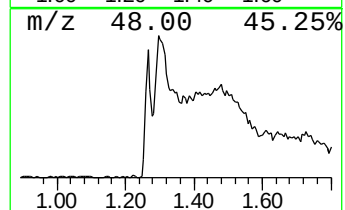
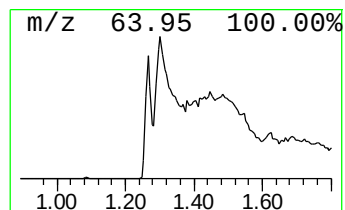
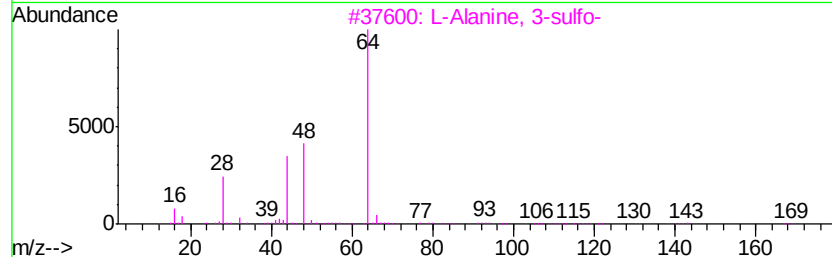
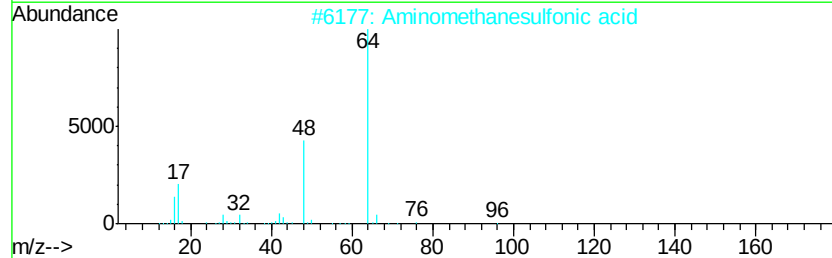
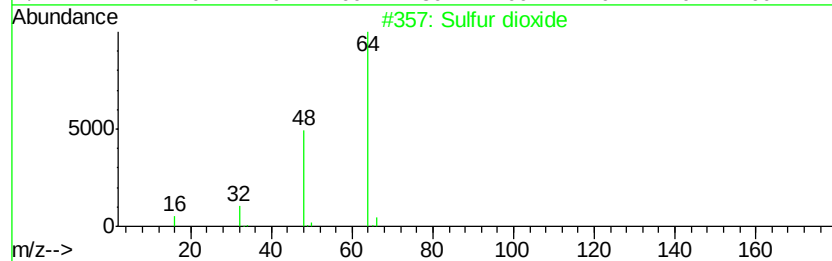
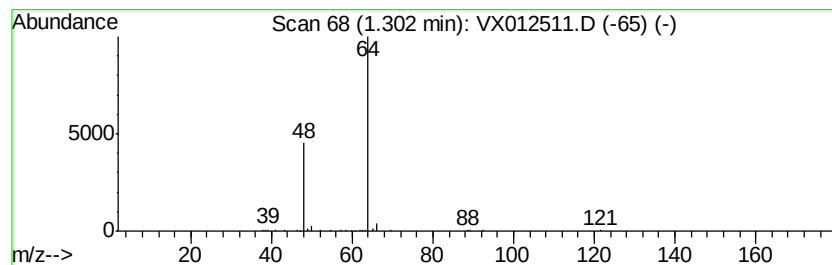
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	5.16 ug/l	67116	Pentafluorobenzene	5.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169 C3H7NO5S	000498-40-8	9
4	(N-(-2-Acetamido))-2-aminoethane...	182 C4H10N2O4S	007365-82-4	9
5	Ethene, 1,1-difluoro-	64 C2H2F2	000075-38-7	5



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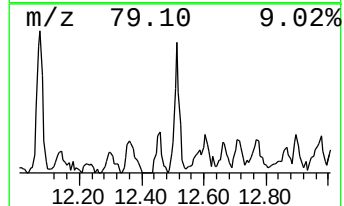
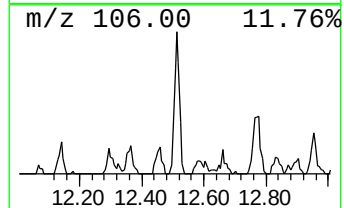
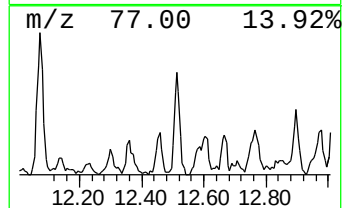
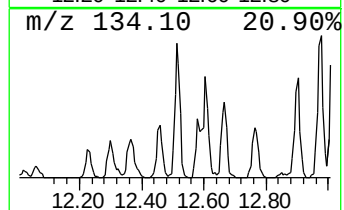
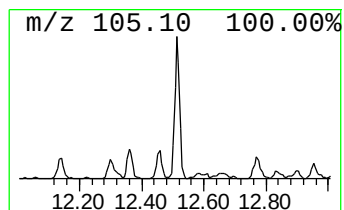
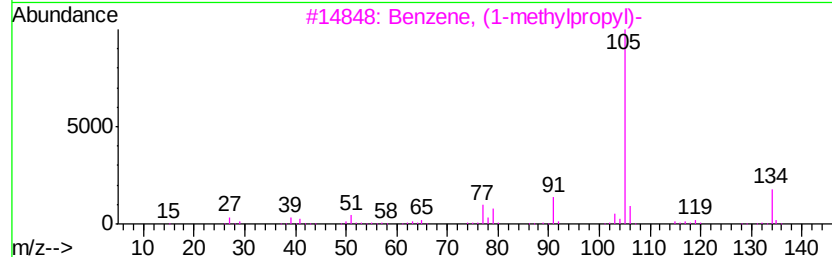
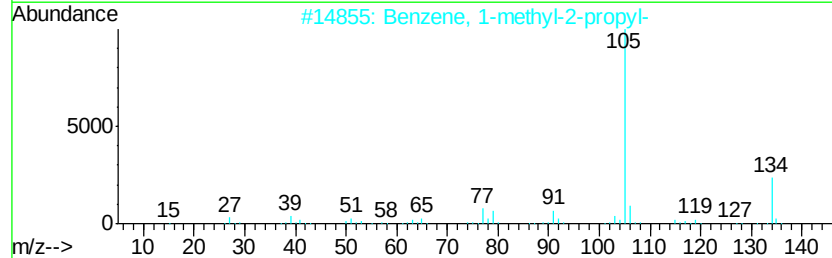
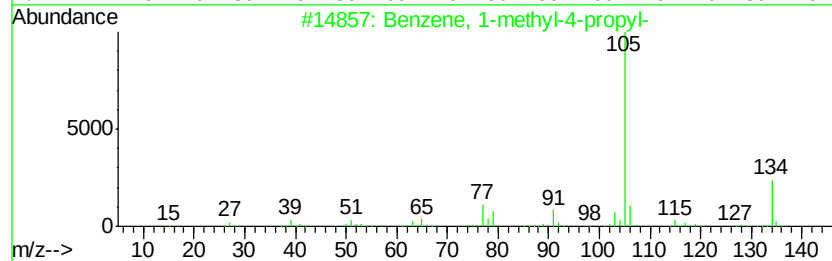
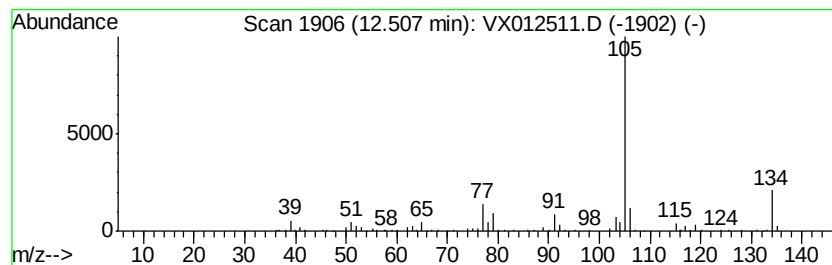
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-methyl-4-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	5.65 ug/l	79648	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-methyl-4-propyl-	134 C10H14	001074-55-1 95
2		Benzene, 1-methyl-2-propyl-	134 C10H14	001074-17-5 91
3		Benzene, (1-methylpropyl)-	134 C10H14	000135-98-8 91
4		Oxirane, 2-methyl-2-phenyl-	134 C9H10O	002085-88-3 80
5		Benzene, 1-methyl-3-propyl-	134 C10H14	001074-43-7 80



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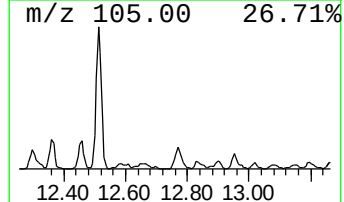
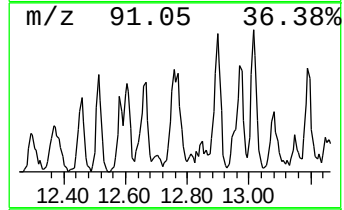
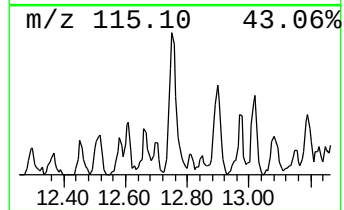
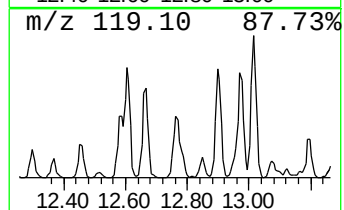
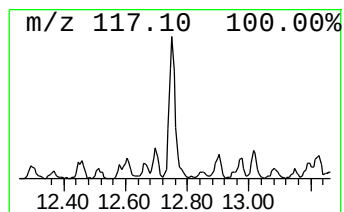
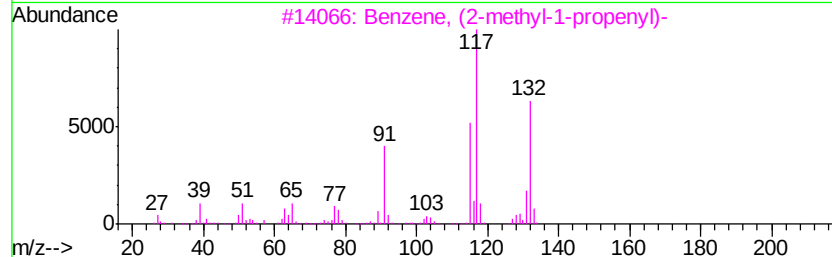
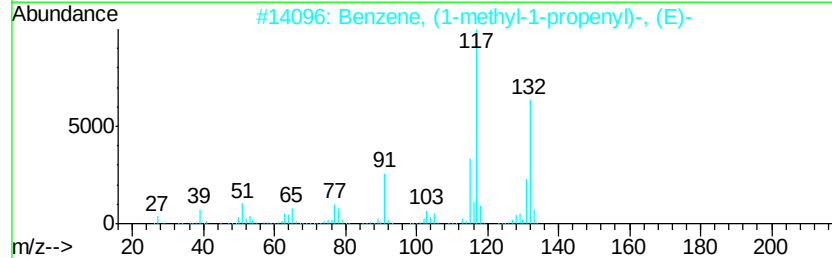
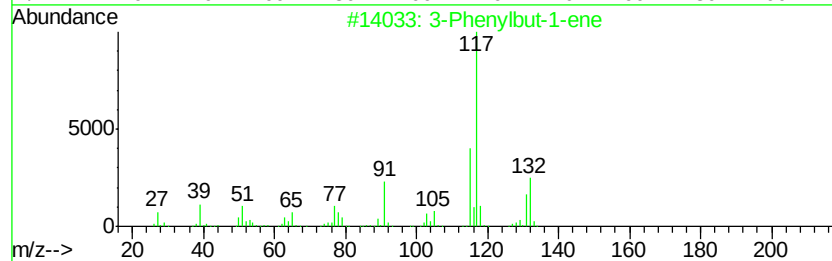
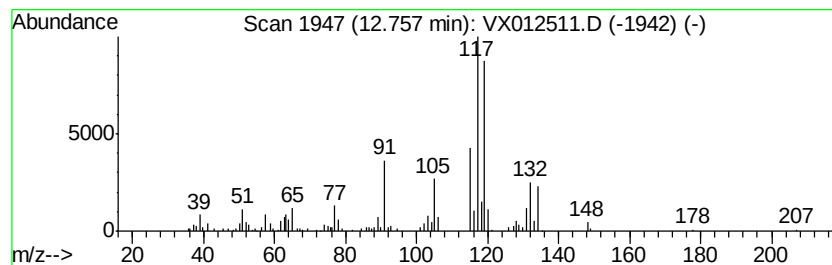
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Phenylbut-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	5.56 ug/l	78388	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
2		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
3		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	55
4		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	55
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	50



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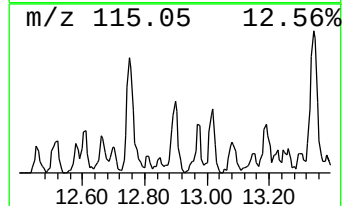
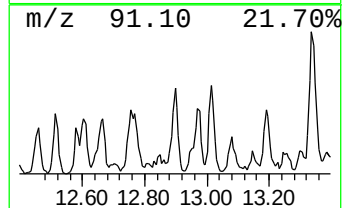
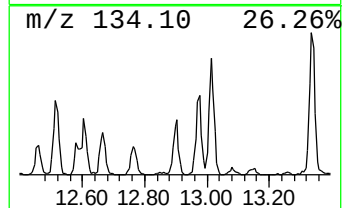
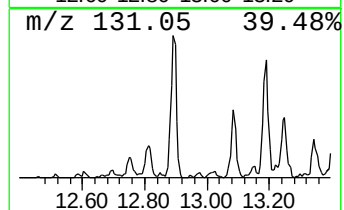
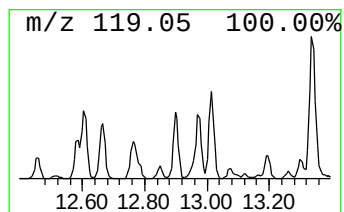
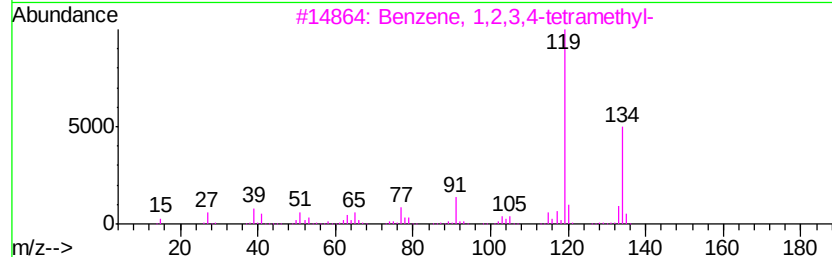
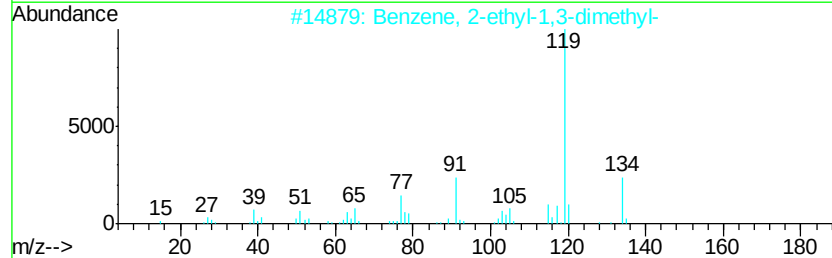
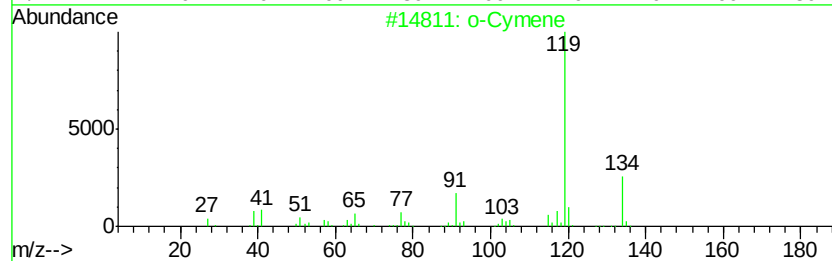
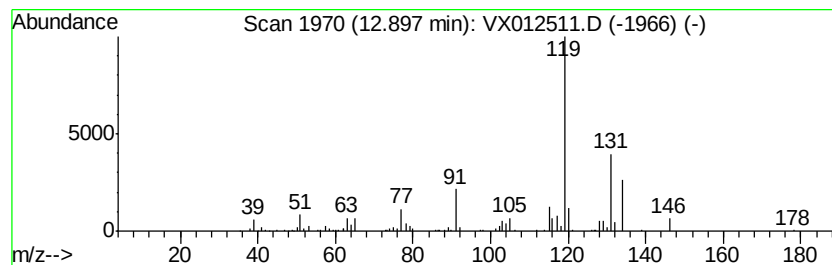
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.90	5.30 ug/l	74588	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	91
2		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	64
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012511.D
Acq On : 19 Sep 2019 06:34
Operator : JC/SP
Sample : K4830-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0281

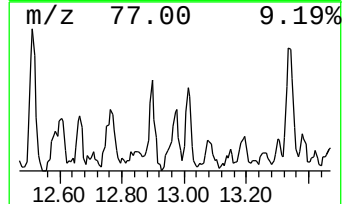
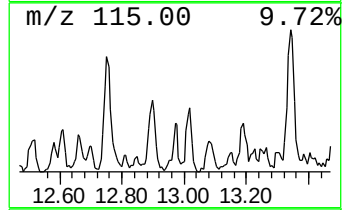
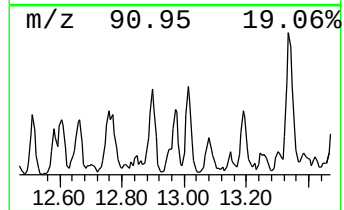
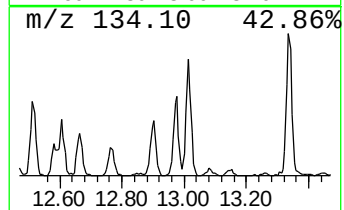
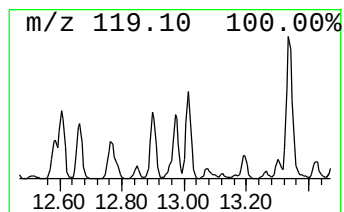
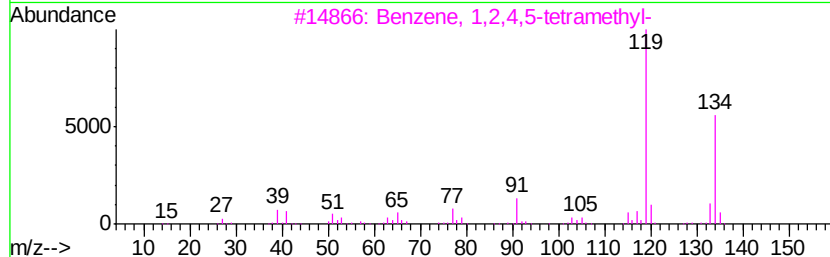
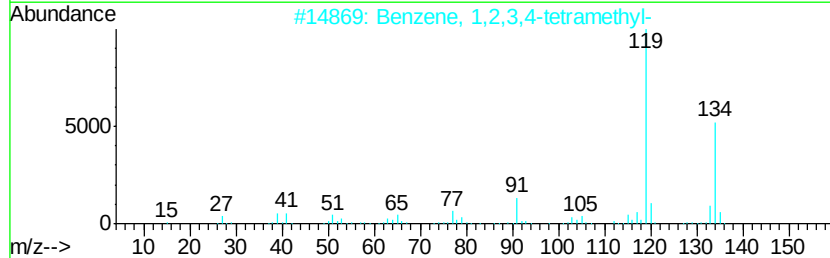
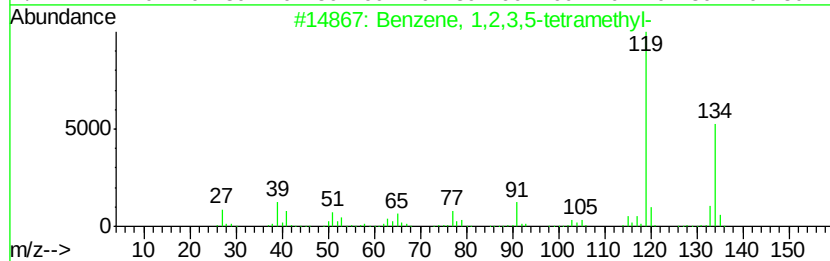
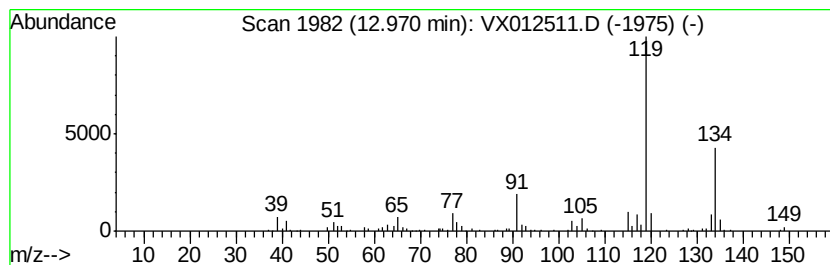
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	5.00 ug/l	70500	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012511.D
Acq On : 19 Sep 2019 06:34
Operator : JC/SP
Sample : K4830-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0281

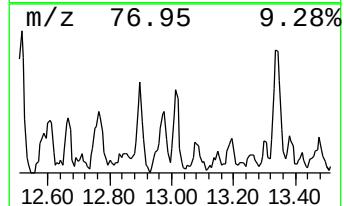
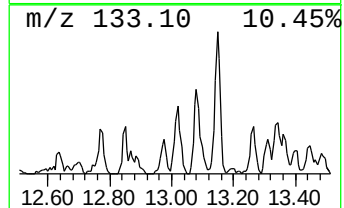
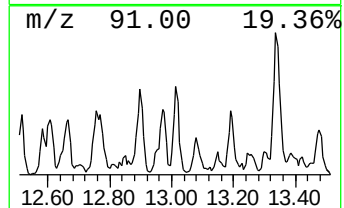
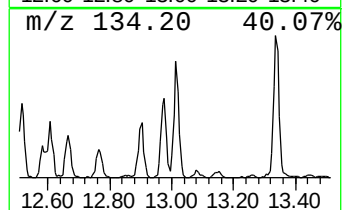
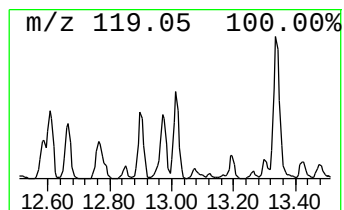
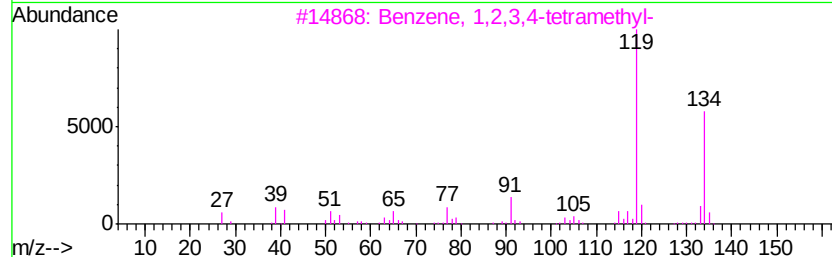
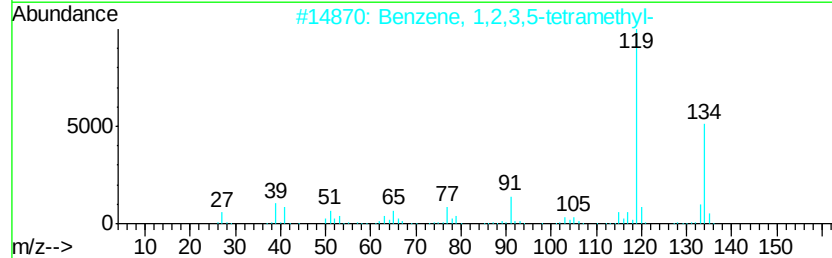
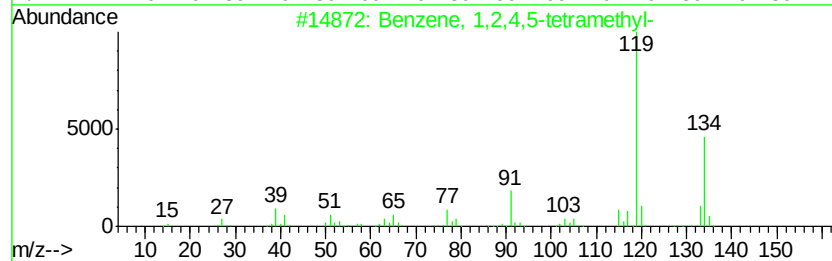
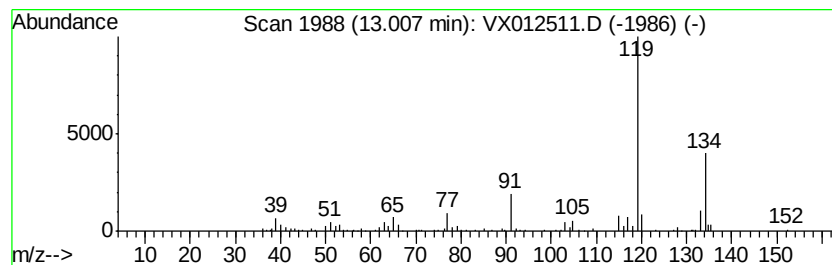
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	5.08 ug/l	71539	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	95
5		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012511.D
Acq On : 19 Sep 2019 06:34
Operator : JC/SP
Sample : K4830-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0281

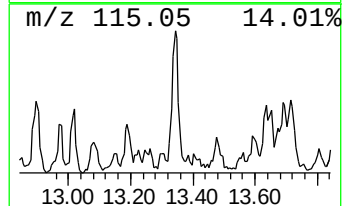
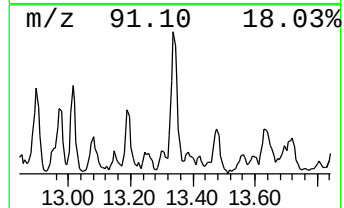
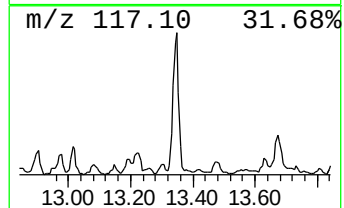
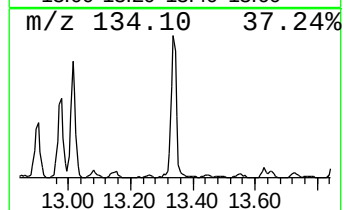
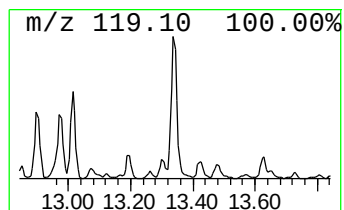
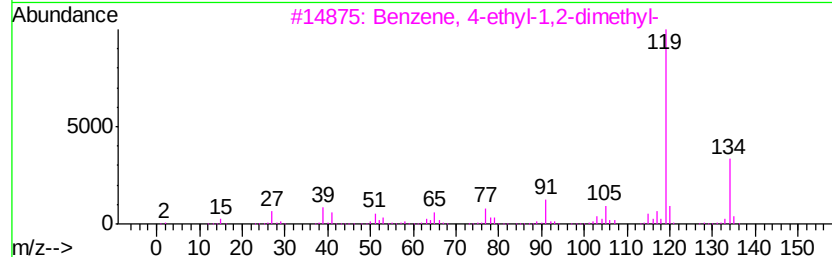
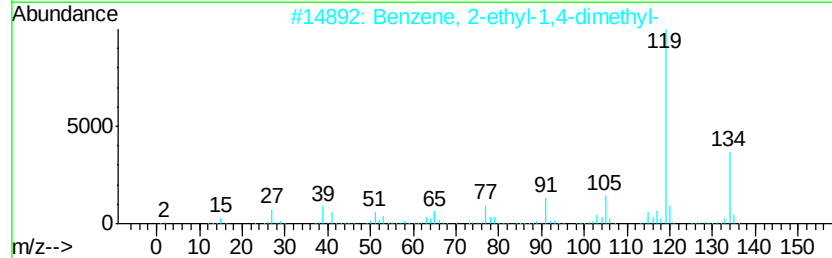
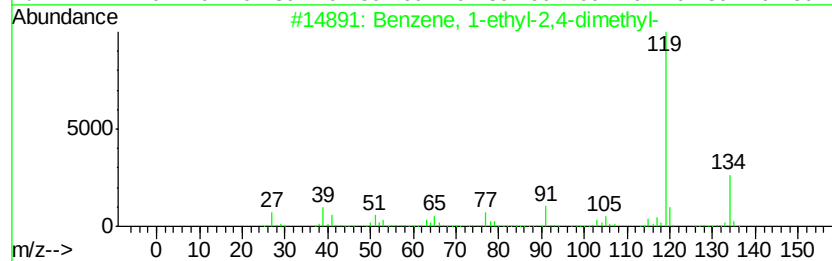
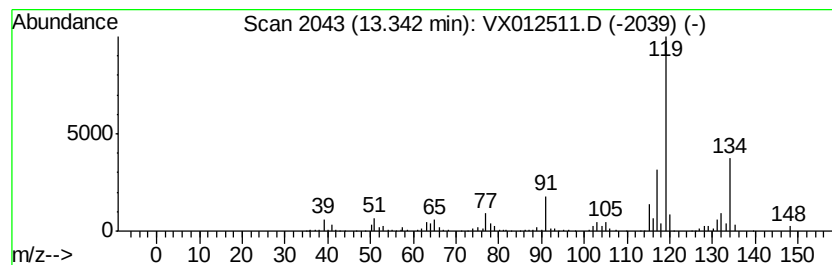
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	9.35 ug/l	131747	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	76
2		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	72
3		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	72
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	72
5		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	70



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012511.D
Acq On : 19 Sep 2019 06:34
Operator : JC/SP
Sample : K4830-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0281

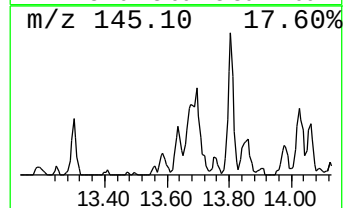
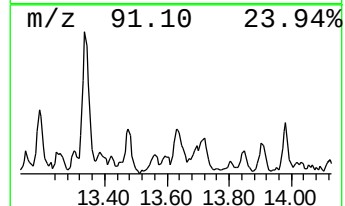
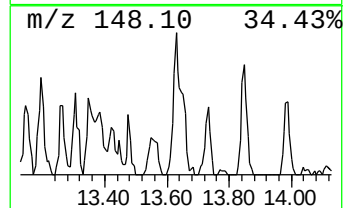
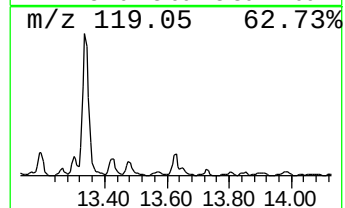
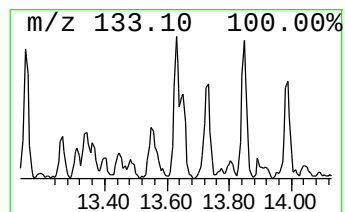
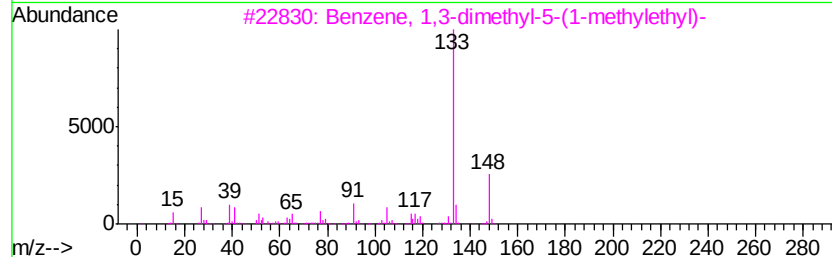
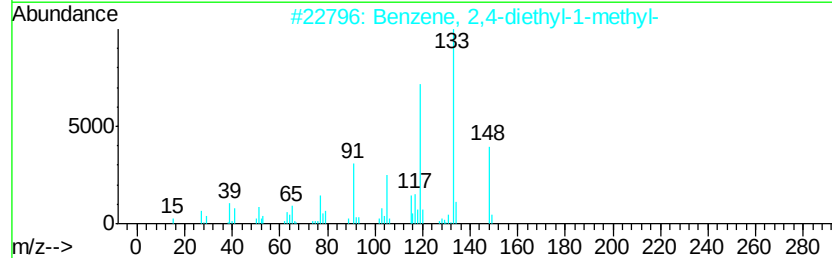
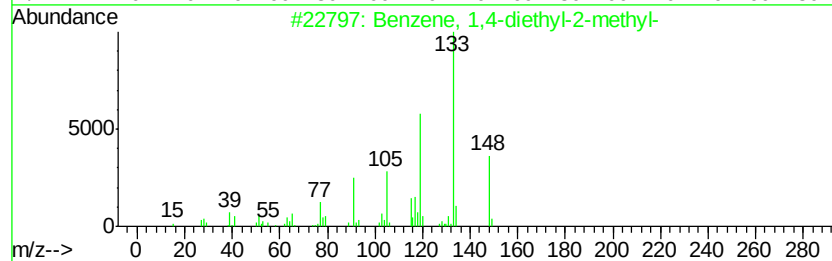
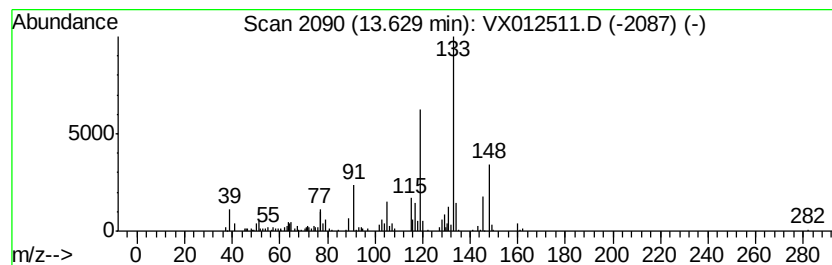
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,4-diethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	5.75 ug/l	80930	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,4-diethyl-2-methyl-	148	C11H16	013632-94-5	83
2		Benzene, 2,4-diethyl-1-methyl-	148	C11H16	001758-85-6	60
3		Benzene, 1,3-dimethyl-5-(1-methyl-...	148	C11H16	004706-90-5	60
4		3,4-Dimethylcumene	148	C11H16	1000370-34-1	60
5		Benzene, pentamethyl-	148	C11H16	000700-12-9	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091819\
Data File : VX012511.D
Acq On : 19 Sep 2019 06:34
Operator : JC/SP
Sample : K4830-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0281

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.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
Sulfur dioxide	1.30	5.2	ug/l	67116	1	5.65	650967	50.0
Benzene, 1-methyl...	12.51	5.7	ug/l	79648	4	12.07	704304	50.0
3-Phenylbut-1-ene	12.76	5.6	ug/l	78388	4	12.07	704304	50.0
o-Cymene	12.90	5.3	ug/l	74588	4	12.07	704304	50.0
Benzene, 1,2,3,5-...	12.97	5.0	ug/l	70500	4	12.07	704304	50.0
Benzene, 1,2,4,5-...	13.01	5.1	ug/l	71539	4	12.07	704304	50.0
Benzene, 1-ethyl-...	13.34	9.3	ug/l	131747	4	12.07	704304	50.0
Benzene, 1,4-diet...	13.63	5.8	ug/l	80930	4	12.07	704304	50.0