

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX120319\
 Data File : VX013728.D
 Acq On : 03 Dec 2019 16:34
 Operator : JC/SP
 Sample : K5984-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 S39-0191

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\82X112619W.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	39	rBV	2364249	2681432	85.23%	10.570%
2	1.265	59	62	69	rBV	196495	232826	7.40%	0.918%
3	1.600	110	117	125	rVB	38190	86102	2.74%	0.339%
4	2.594	273	280	286	rBV	52751	97738	3.11%	0.385%
5	5.490	744	755	768	rBV	347521	998827	31.75%	3.937%
6	5.655	771	782	794	rVV	652049	1789825	56.89%	7.056%
7	6.057	839	848	859	rVB	397301	1014424	32.24%	3.999%
8	6.849	968	978	989	rBV	983890	2280302	72.48%	8.989%
9	8.544	1253	1256	1263	rVB2	24751	45574	1.45%	0.180%
10	8.709	1276	1283	1292	rBV	2063590	3146271	100.00%	12.403%
11	9.331	1377	1385	1391	rBV	438381	657517	20.90%	2.592%
12	10.111	1504	1513	1519	rBV	1884905	2639014	83.88%	10.403%
13	10.648	1594	1601	1608	rBV	14574	36912	1.17%	0.146%
14	11.013	1657	1661	1664	rBV	25275	32506	1.03%	0.128%
15	11.135	1675	1681	1686	rBV	1574305	2027222	64.43%	7.992%
16	11.275	1701	1704	1710	rVB7	25747	36877	1.17%	0.145%
17	11.355	1714	1717	1721	rBV	39898	46461	1.48%	0.183%
18	11.452	1726	1733	1737	rVV2	47226	80601	2.56%	0.318%
19	11.501	1737	1741	1749	rVB	75033	99458	3.16%	0.392%
20	11.666	1763	1768	1775	rVB2	73957	108159	3.44%	0.426%
21	11.763	1780	1784	1787	rVV2	29991	40194	1.28%	0.158%
22	11.806	1787	1791	1796	rVB	240998	311358	9.90%	1.227%
23	11.916	1803	1809	1811	rBV3	47822	82443	2.62%	0.325%
24	11.940	1811	1813	1820	rVB	93065	110384	3.51%	0.435%
25	12.019	1820	1826	1830	rBV	69009	98291	3.12%	0.387%
26	12.074	1830	1835	1840	rBV	2020684	2452652	77.95%	9.669%
27	12.141	1840	1846	1849	rBV	70428	86462	2.75%	0.341%
28	12.227	1856	1860	1867	rVB	46634	62906	2.00%	0.248%
29	12.300	1867	1872	1878	rBV2	175652	305813	9.72%	1.206%
30	12.367	1878	1883	1892	rVB3	282527	454744	14.45%	1.793%
31	12.458	1894	1898	1904	rBV3	42723	64016	2.03%	0.252%
32	12.513	1904	1907	1912	rVB	31058	40328	1.28%	0.159%
33	12.580	1913	1918	1921	rBV	108404	148828	4.73%	0.587%
34	12.665	1928	1932	1935	rBV2	173118	191232	6.08%	0.754%

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ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE
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Sampling : 1
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Max Peaks: 100
Peak Location: TOP

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

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35	12.714	1935	1940	1943	rVV2	258792	410955	13.06%	1.620%
36	12.751	1943	1946	1953	rVV4	116027	188463	5.99%	0.743%
37	12.812	1953	1956	1960	rVV3	36224	39210	1.25%	0.155%
38	12.867	1960	1965	1967	rVV	138550	195668	6.22%	0.771%
39	12.891	1967	1969	1975	rVB	168258	192262	6.11%	0.758%
40	12.952	1975	1979	1980	rBV2	57876	68884	2.19%	0.272%
41	12.976	1980	1983	1986	rVB2	149479	173543	5.52%	0.684%
42	13.013	1986	1989	1996	rVB2	223361	279364	8.88%	1.101%
43	13.080	1996	2000	2006	rBV2	92082	131158	4.17%	0.517%
44	13.147	2006	2011	2015	rBV	58624	78409	2.49%	0.309%
45	13.190	2015	2018	2021	rBV	62156	65348	2.08%	0.258%
46	13.245	2025	2027	2033	rVB2	23568	40571	1.29%	0.160%
47	13.300	2033	2036	2039	rBV3	44747	58954	1.87%	0.232%
48	13.342	2039	2043	2050	rVV2	185434	274107	8.71%	1.081%
49	13.458	2059	2062	2063	rVV2	31960	38590	1.23%	0.152%
50	13.476	2063	2065	2071	rVB2	52224	60573	1.93%	0.239%
51	13.562	2074	2079	2081	rBV3	21657	36166	1.15%	0.143%
52	13.635	2087	2091	2095	rVV5	38320	63910	2.03%	0.252%
53	13.696	2095	2101	2102	rVV4	32514	59715	1.90%	0.235%
54	13.714	2102	2104	2111	rVB2	39648	55193	1.75%	0.218%
55	13.806	2115	2119	2120	rBV2	33269	36853	1.17%	0.145%
56	13.830	2120	2123	2130	rVB	102252	144460	4.59%	0.569%
57	14.690	2259	2264	2268	rBV	25084	32517	1.03%	0.128%
58	14.836	2282	2288	2297	rVB	39990	54604	1.74%	0.215%

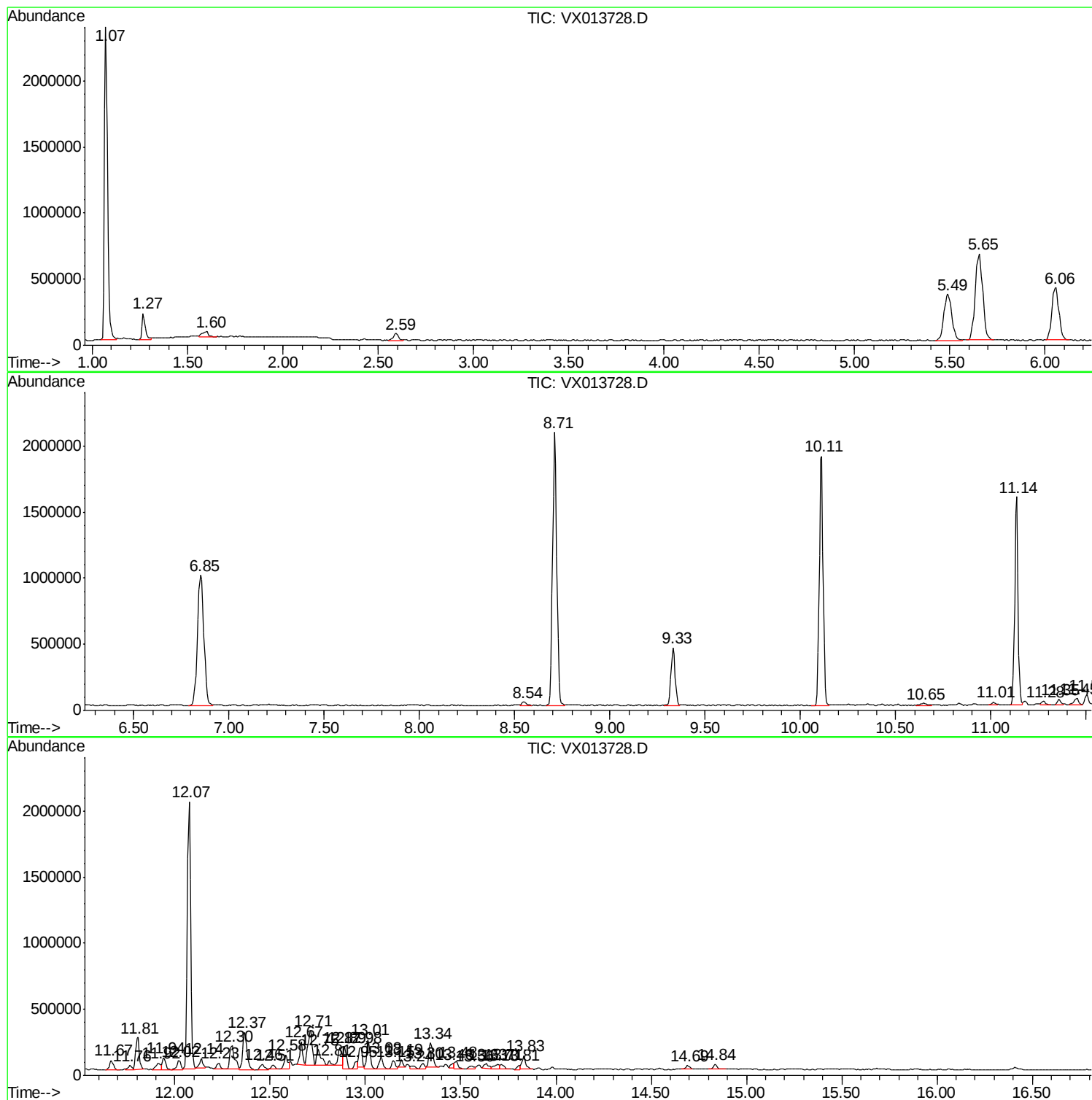
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Quant Title : SW846 8260

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



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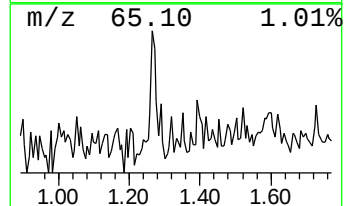
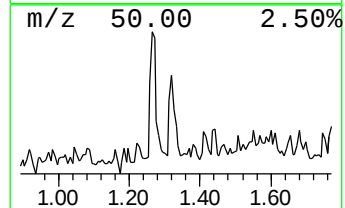
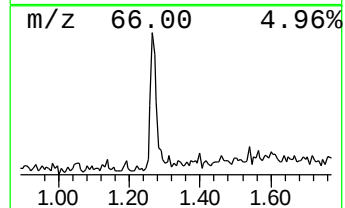
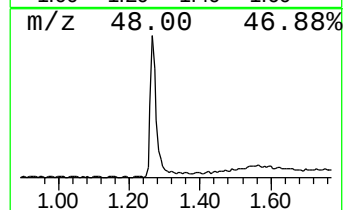
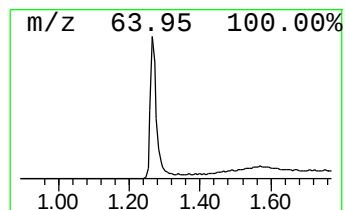
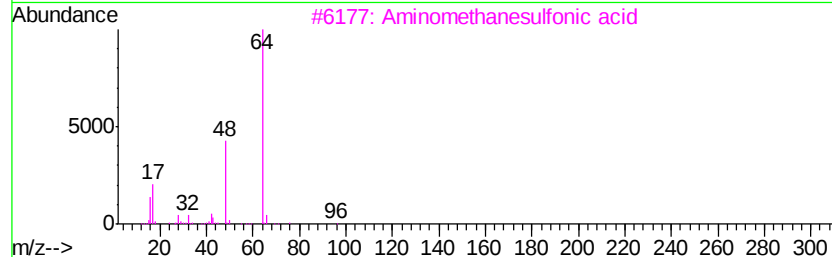
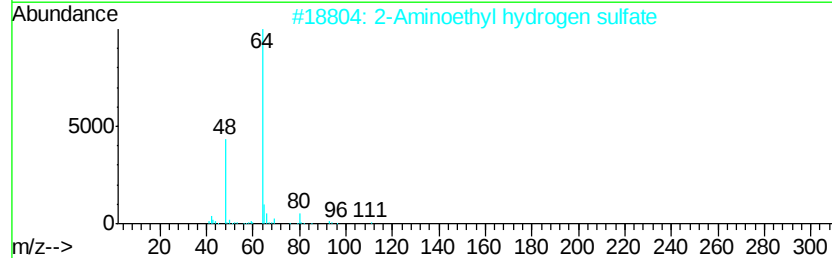
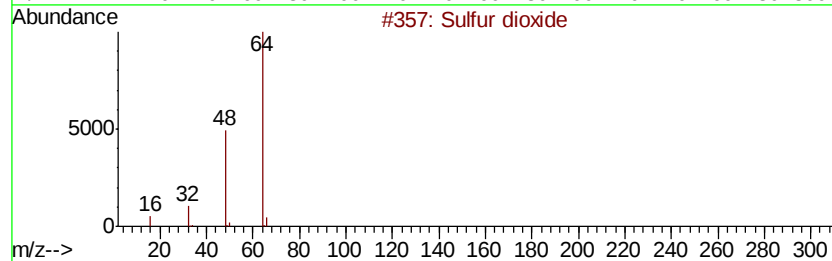
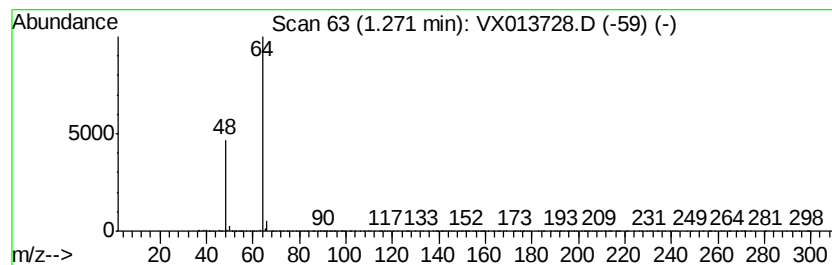
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	6.50 ug/l	232826	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	83
2		2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
3		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4		4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	74
5		(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
S39-0191

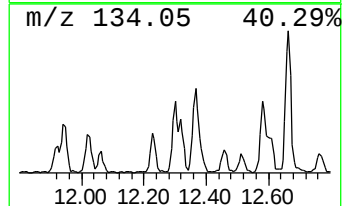
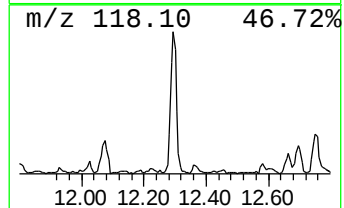
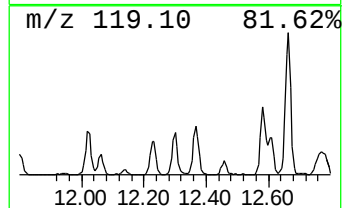
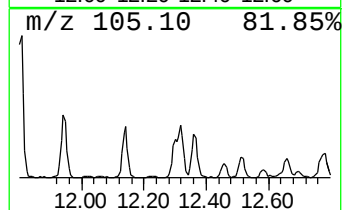
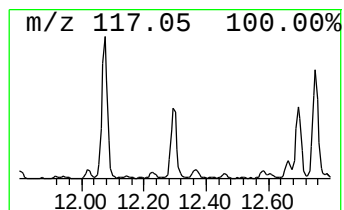
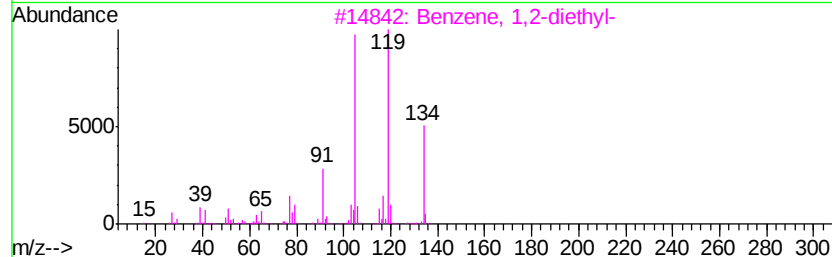
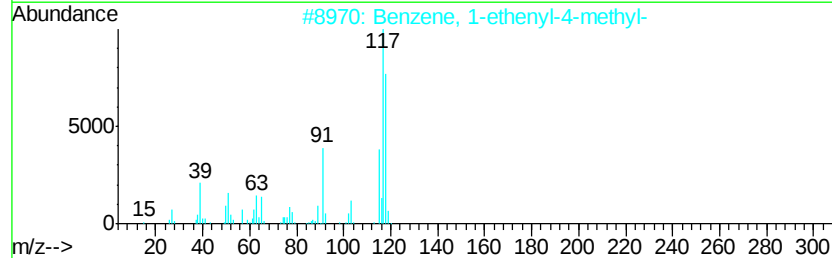
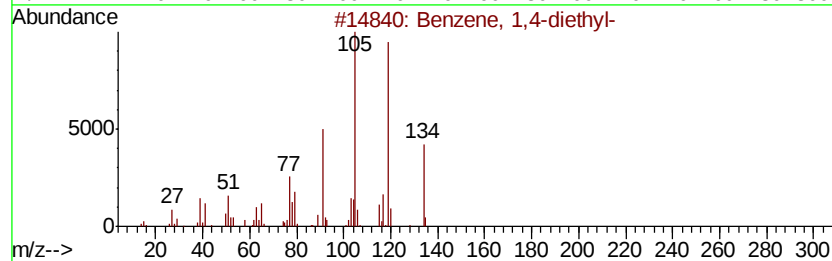
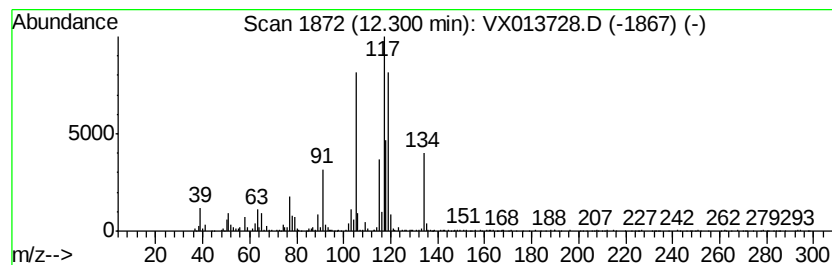
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,4-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	6.23 ug/l	305813	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	70
2		Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	64
3		Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	55
4		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	55
5		7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	46



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

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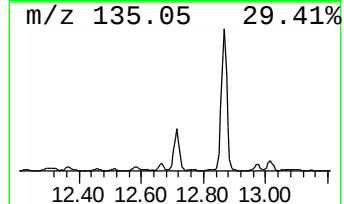
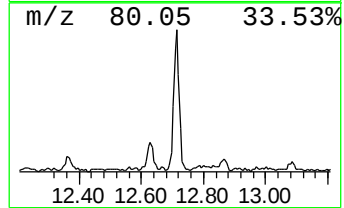
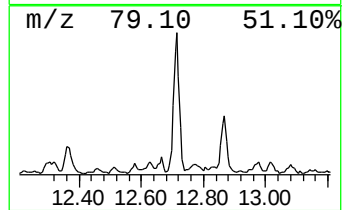
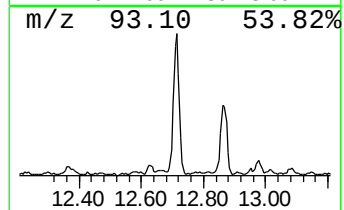
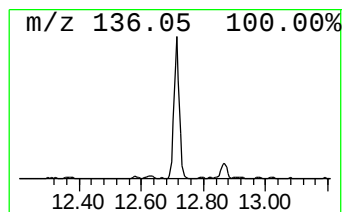
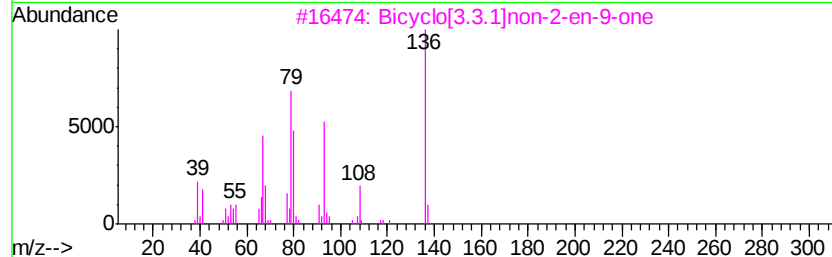
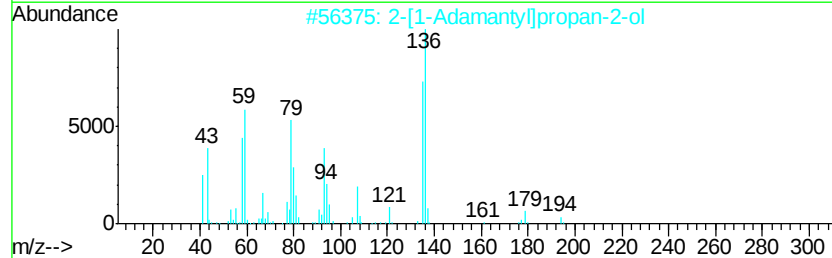
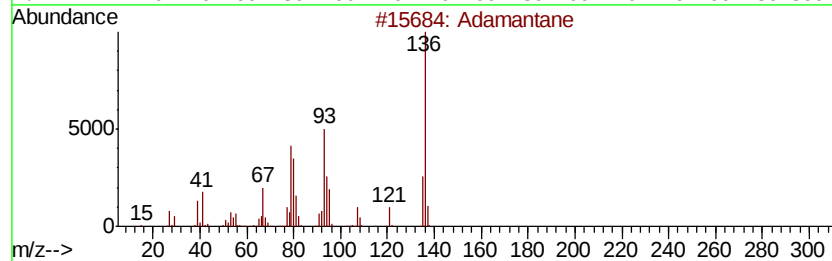
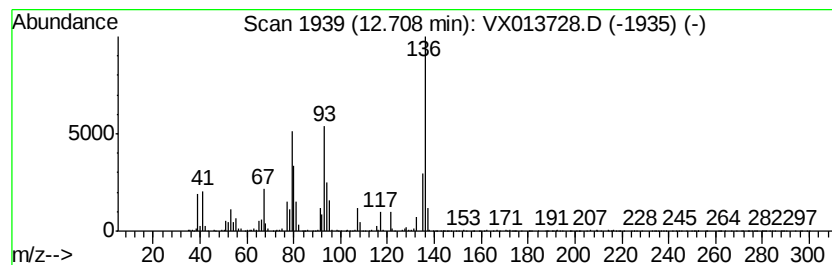
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Adamantane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	8.38 ug/l	410955	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adamantane	136	C10H16	000281-23-2	98
2		2-[1-Adamantyl]propan-2-ol	194	C13H22O	000775-64-4	80
3		Bicyclo[3.3.1]non-2-en-9-one	136	C9H12O	004844-11-5	68
4		1-(6-Methyl-2-pyrazinyl)-1-ethanone	136	C7H8N2O	022047-26-3	46
5		2-Purinol	136	C5H4N4O	002308-57-8	43



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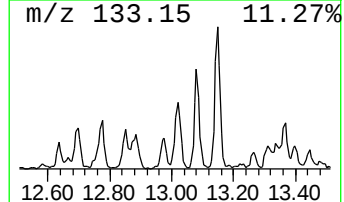
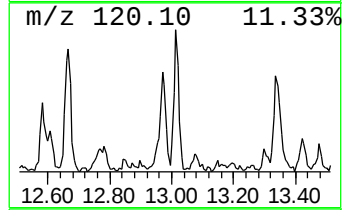
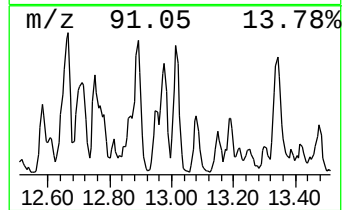
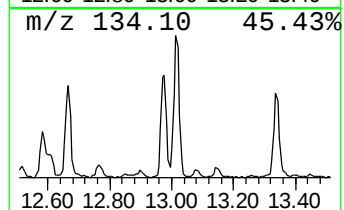
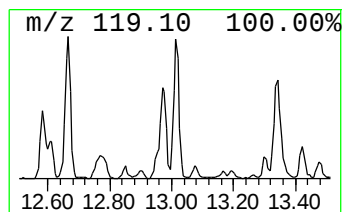
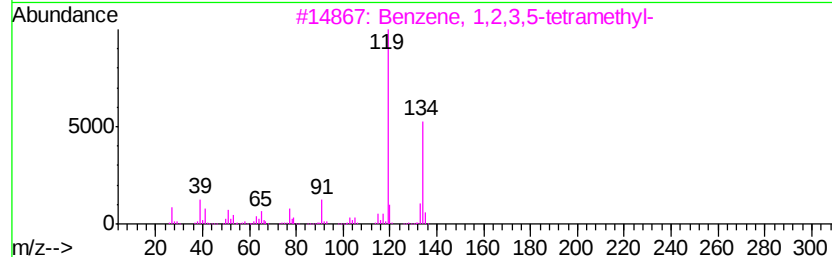
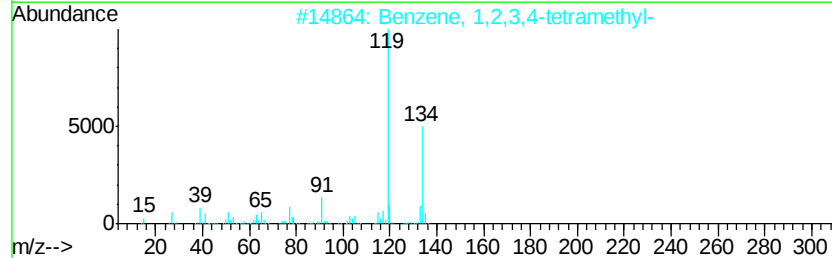
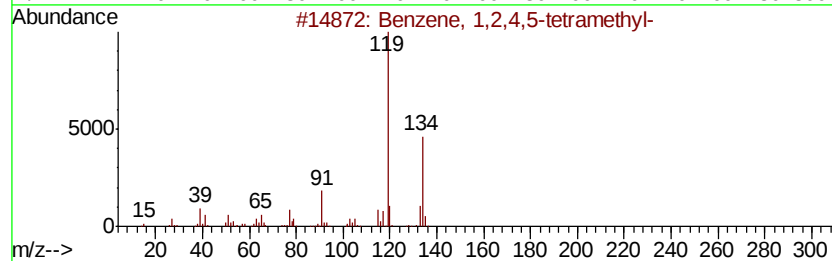
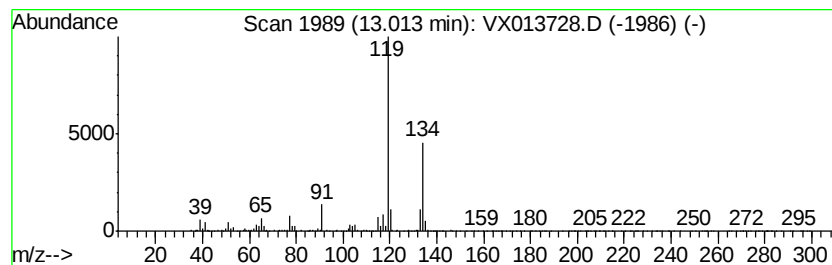
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	5.70 ug/l	279364	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	95
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4		o-Cymene	134	C10H14	000527-84-4	94
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



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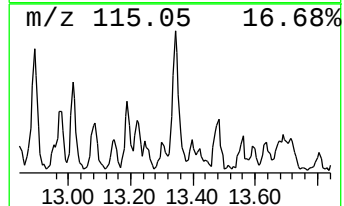
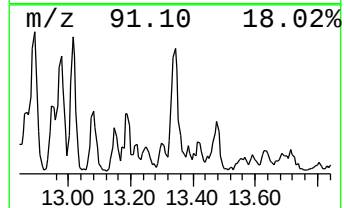
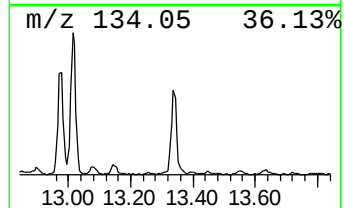
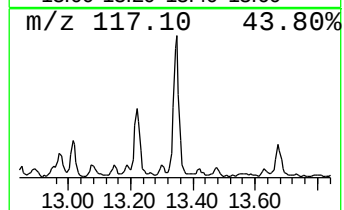
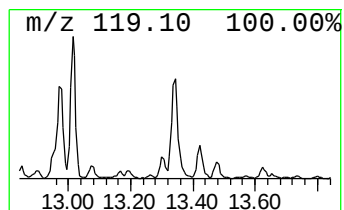
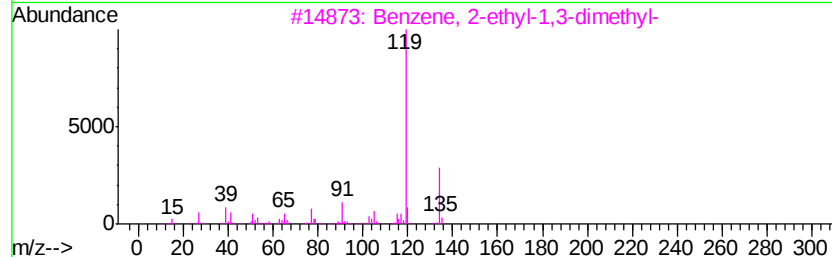
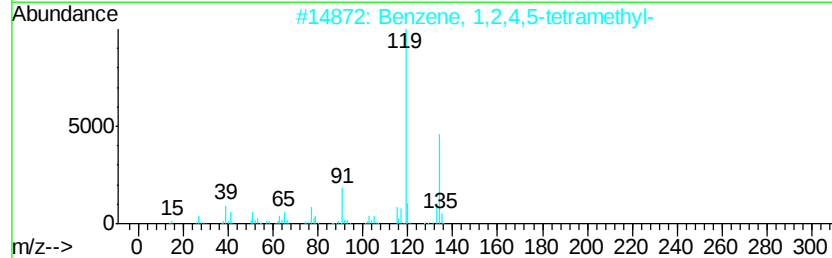
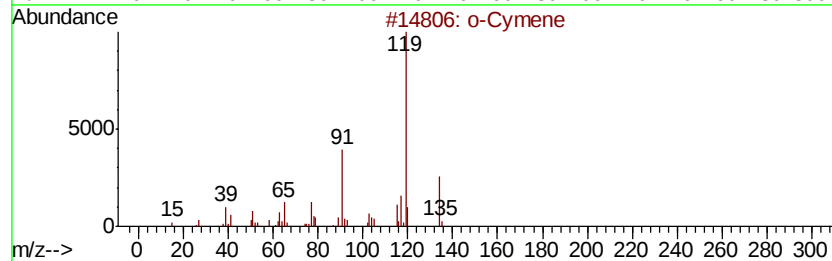
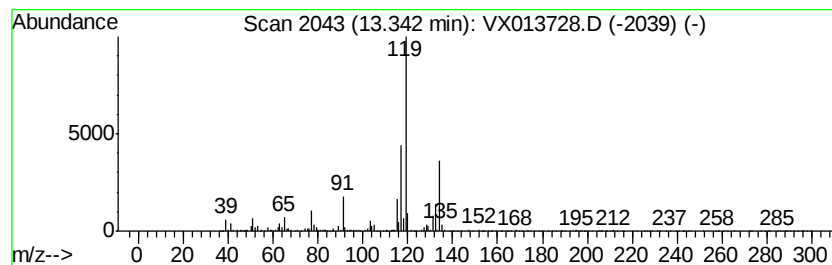
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	5.59 ug/l	274107	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	76
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
3		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	62
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	62
5		p-Cymene	134	C10H14	000099-87-6	62



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX120319\
Data File : VX013728.D
Acq On : 03 Dec 2019 16:34
Operator : JC/SP
Sample : K5984-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S39-0191

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.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	1.27	6.5	ug/l	232826	1	5.65	1789830	50.0
Benzene, 1,4-diet...	12.30	6.2	ug/l	305813	4	12.07	2452650	50.0
Adamantane	12.71	8.4	ug/l	410955	4	12.07	2452650	50.0
Benzene, 1,2,4,5-...	13.01	5.7	ug/l	279364	4	12.07	2452650	50.0
o-Cymene	13.34	5.6	ug/l	274107	4	12.07	2452650	50.0