

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
 Data File : VX027245.D
 Acq On : 01 Mar 2022 13:56
 Operator : JC/MD
 Sample : N1688-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-27

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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
 Title : SW846 8260

Signal : TIC: VX027245.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	21	27	42	rBV	22909	43816	8.55%	1.000%
2	2.386	207	213	218	rBV	7360	12153	2.37%	0.277%
3	2.538	230	238	246	rBV	3918	7890	1.54%	0.180%
4	2.752	268	273	279	rBV	3412	5738	1.12%	0.131%
5	2.959	299	307	316	rVB2	3878	8710	1.70%	0.199%
6	3.117	326	333	343	rVB2	6714	15417	3.01%	0.352%
7	5.391	695	706	718	rBV2	51084	148010	28.87%	3.377%
8	5.562	724	734	749	rVB	87701	248229	48.41%	5.663%
9	5.964	790	800	805	rBV	55227	140587	27.42%	3.207%
10	6.044	805	813	829	rVV	195743	512751	100.00%	11.698%
11	6.763	920	931	946	rBV	135224	323777	63.15%	7.387%
12	8.580	1223	1229	1234	rBV	4449	6915	1.35%	0.158%
13	8.653	1234	1241	1248	rVV	301636	445768	86.94%	10.170%
14	8.720	1248	1252	1262	rVB	19888	30954	6.04%	0.706%
15	10.055	1465	1471	1481	rBV	286461	380274	74.16%	8.676%
16	10.195	1488	1494	1505	rVB	192478	246779	48.13%	5.630%
17	10.305	1507	1512	1524	rVB	131059	163393	31.87%	3.728%
18	10.640	1562	1567	1580	rVB	111874	144053	28.09%	3.286%
19	10.964	1615	1620	1626	rVB	13125	15812	3.08%	0.361%
20	11.079	1634	1639	1650	rBV	228395	293367	57.21%	6.693%
21	11.305	1671	1676	1682	rBV	23867	29062	5.67%	0.663%
22	11.403	1684	1692	1697	rVV	23068	35743	6.97%	0.815%
23	11.616	1722	1727	1734	rVB	48360	61780	12.05%	1.409%
24	11.750	1744	1749	1755	rBV	113185	140687	27.44%	3.210%
25	12.024	1788	1794	1800	rBV	298936	369894	72.14%	8.439%
26	12.085	1800	1804	1812	rVB	53925	69367	13.53%	1.583%
27	12.244	1823	1830	1838	rBV2	60884	76949	15.01%	1.756%
28	12.317	1838	1842	1849	rVB3	3914	6287	1.23%	0.143%
29	12.463	1862	1866	1872	rVB	6108	6795	1.33%	0.155%
30	12.530	1872	1877	1880	rBV	7859	10359	2.02%	0.236%
31	12.616	1885	1891	1894	rVV	16747	20444	3.99%	0.466%
32	12.646	1894	1896	1900	rVB2	4994	5340	1.04%	0.122%
33	12.701	1900	1905	1913	rBV2	16585	23398	4.56%	0.534%
34	12.847	1925	1929	1935	rVB2	6373	8563	1.67%	0.195%
35	12.921	1935	1941	1945	rBV	12923	16604	3.24%	0.379%
36	12.963	1945	1948	1956	rVB	18342	21252	4.14%	0.485%

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Integration Parameters: RTEINT.P

Integrator: RTE

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Sampling : 1

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Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Title : SW846 8260

37	13.171	1979	1982	1987	rVB	9748	11008	2.15%	0.251%
38	13.292	1997	2002	2008	rVB2	33770	46950	9.16%	1.071%
39	13.427	2020	2024	2029	rVB2	9040	11637	2.27%	0.265%
40	13.585	2046	2050	2055	rVV4	5595	9253	1.80%	0.211%
41	13.664	2061	2063	2073	rVB2	4854	8057	1.57%	0.184%
42	13.774	2073	2081	2088	rBV	36054	50965	9.94%	1.163%
43	14.219	2147	2154	2163	rVB3	6111	12194	2.38%	0.278%
44	14.481	2193	2197	2203	rBV4	4609	7428	1.45%	0.169%
45	14.640	2216	2223	2227	rBV	13775	20078	3.92%	0.458%
46	14.780	2239	2246	2255	rBV	36577	48734	9.50%	1.112%
47	15.115	2293	2301	2309	rBV4	4526	7816	1.52%	0.178%
48	15.481	2355	2361	2369	rBV2	9350	16016	3.12%	0.365%
49	15.615	2378	2383	2387	rBV2	13669	20813	4.06%	0.475%
50	15.652	2387	2389	2395	rVB2	4890	6565	1.28%	0.150%
51	15.841	2411	2420	2431	rBV5	3136	8773	1.71%	0.200%

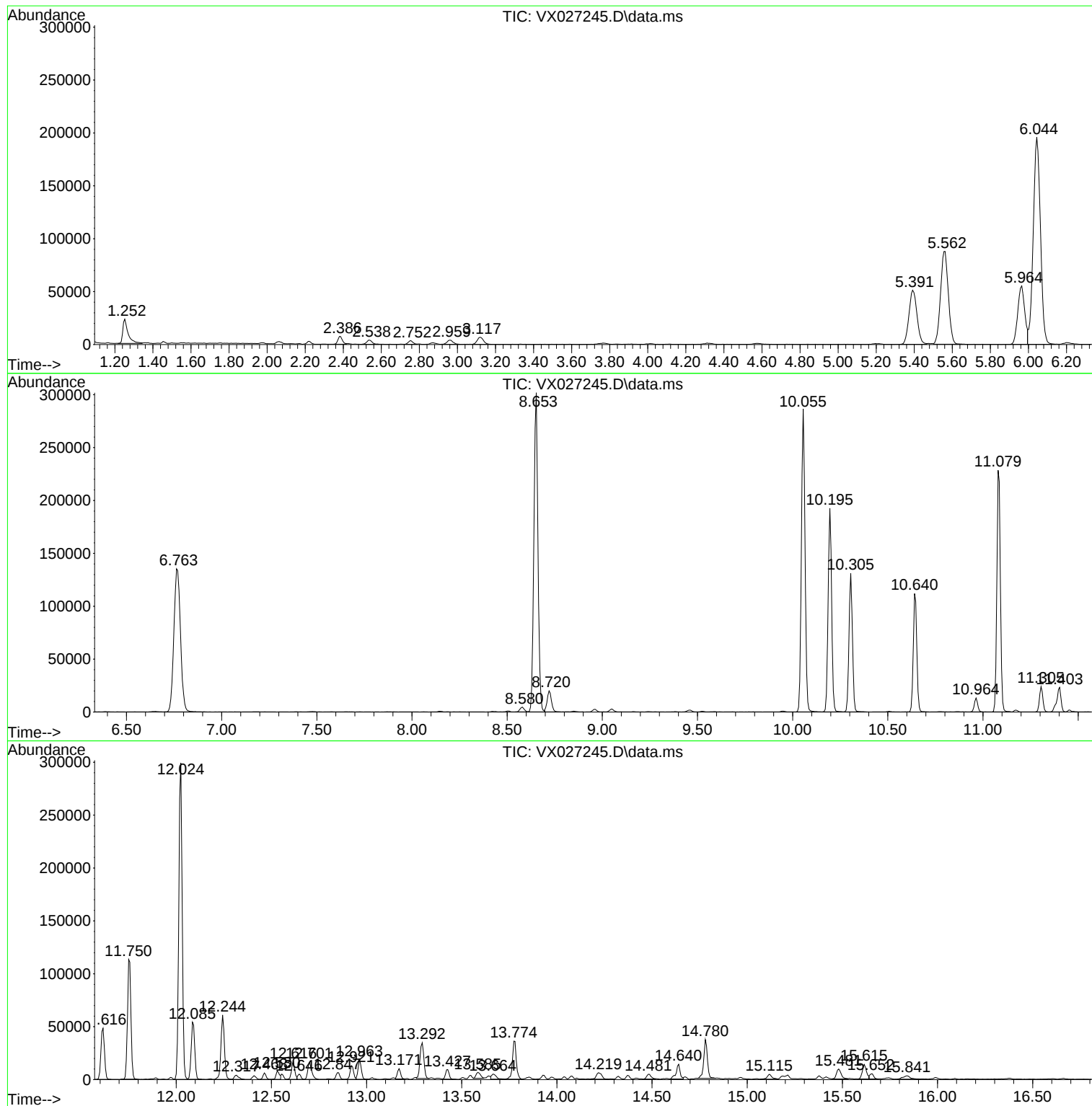
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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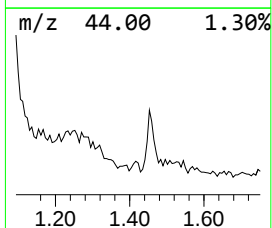
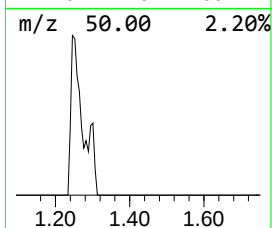
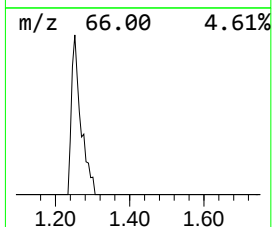
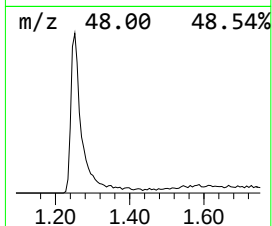
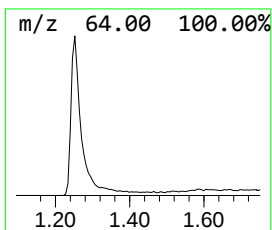
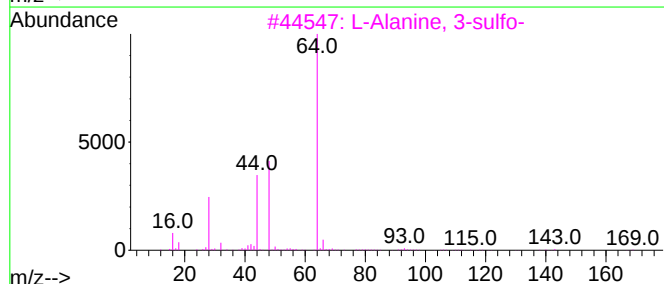
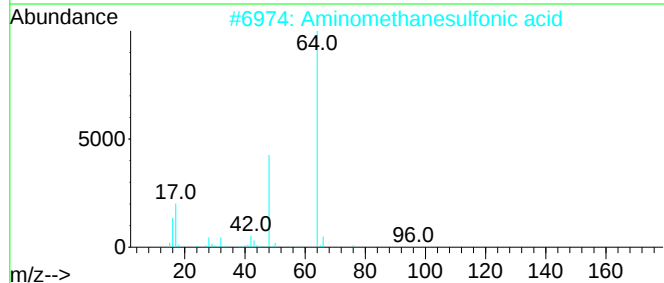
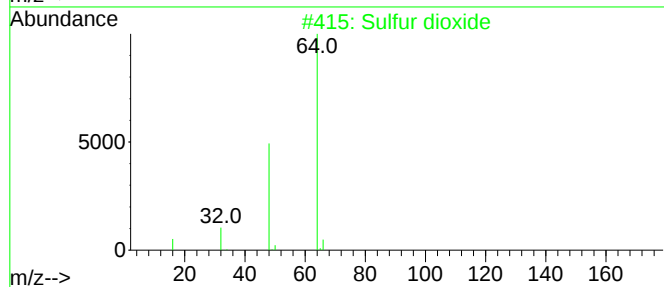
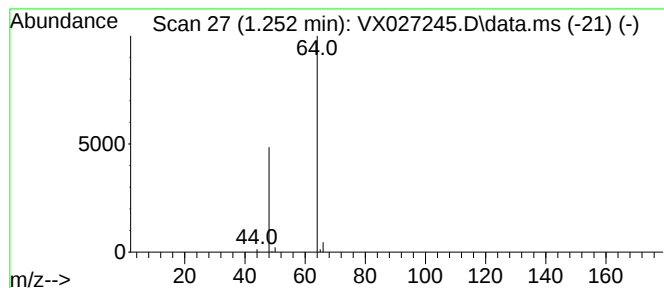
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	8.83 ug/l	43816	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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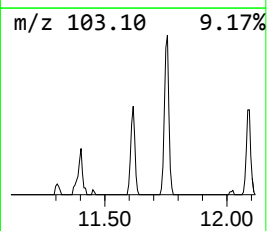
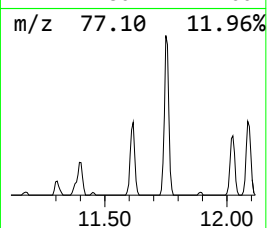
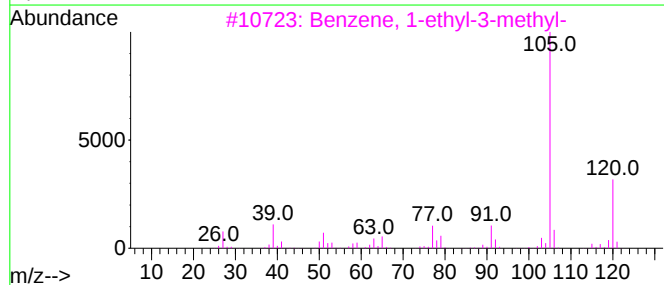
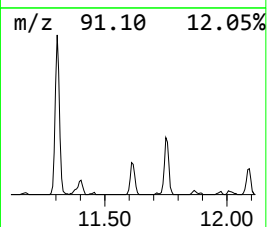
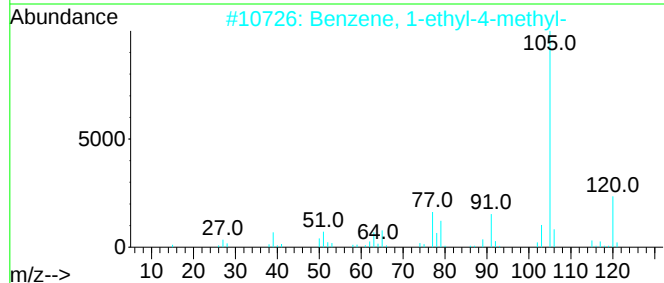
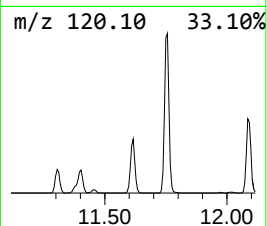
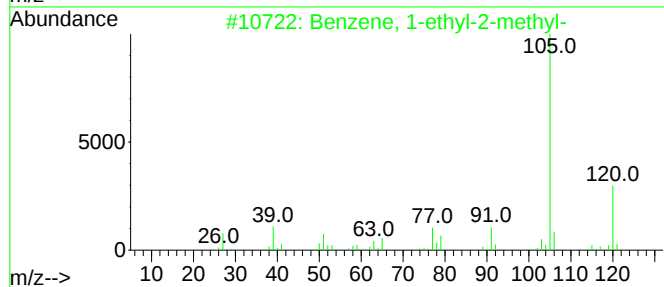
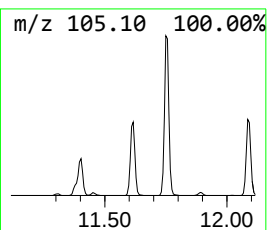
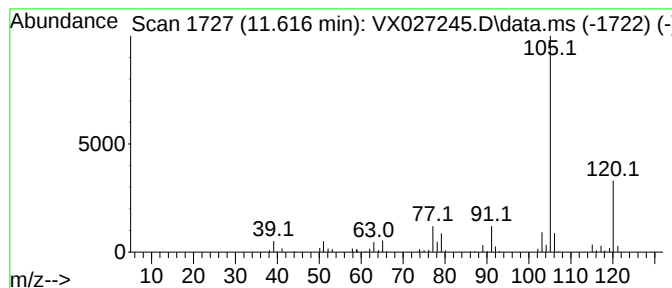
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	8.35 ug/l	61780	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Mesitylene	120	C9H12	000108-67-8	90



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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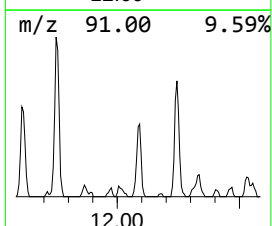
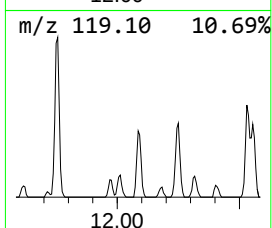
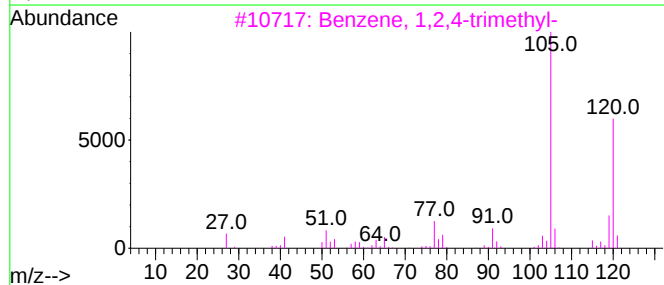
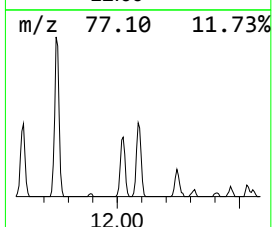
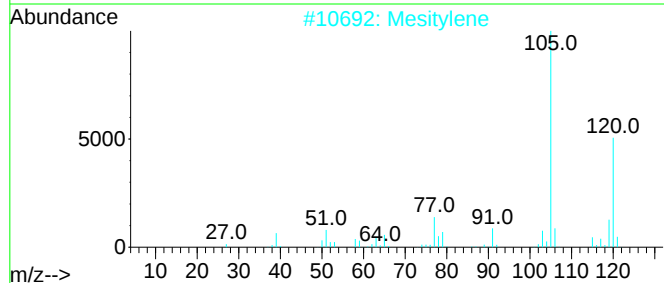
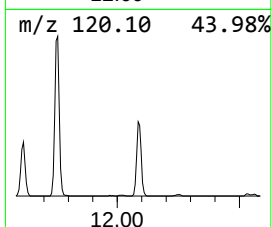
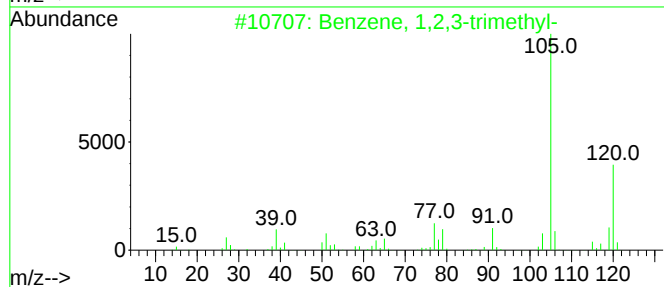
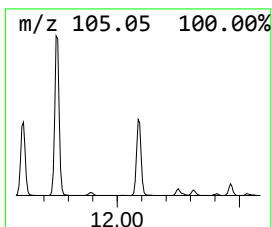
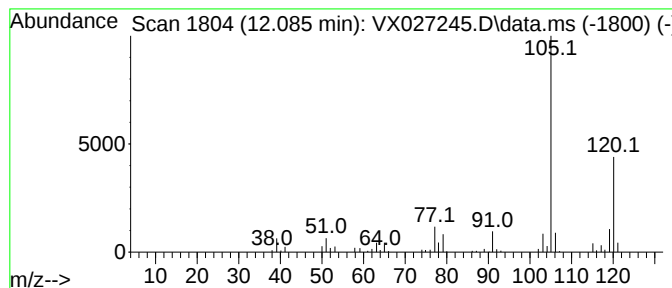
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	9.38 ug/l	69367	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	97
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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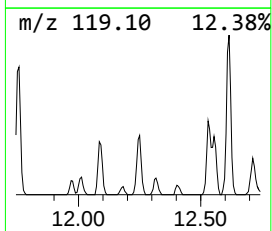
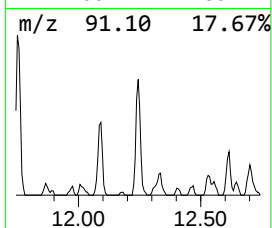
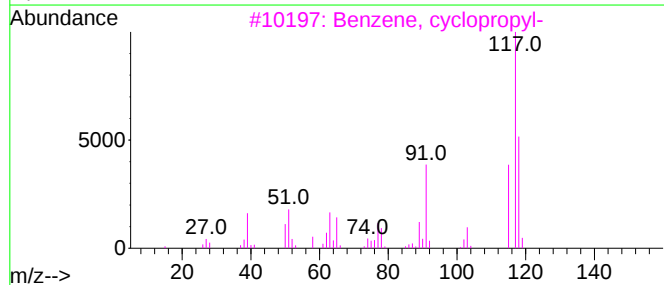
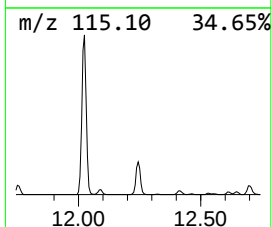
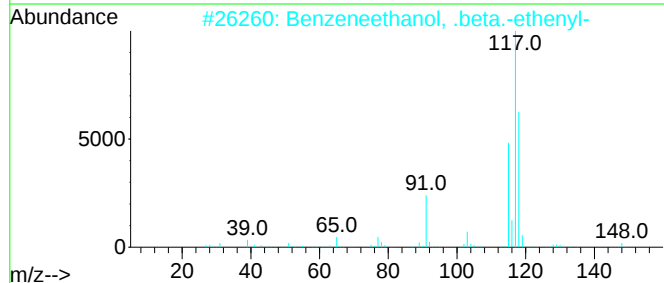
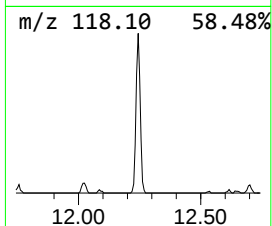
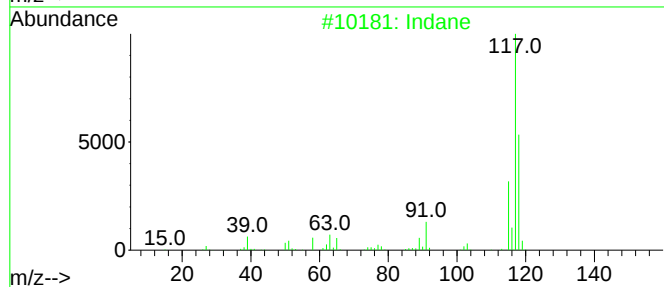
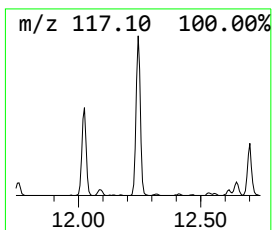
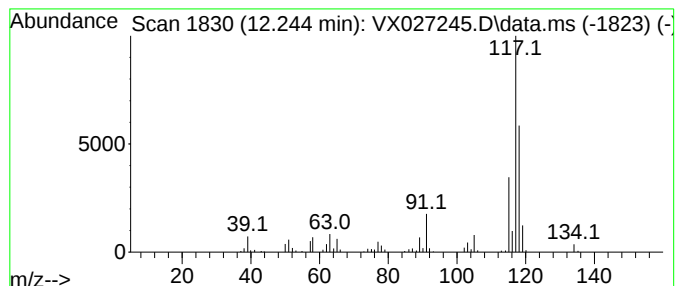
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	10.40 ug/l	76949	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	86
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74



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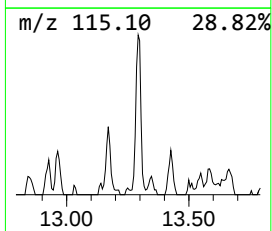
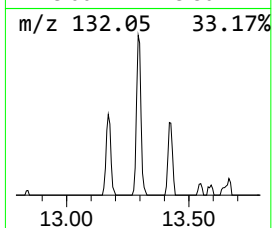
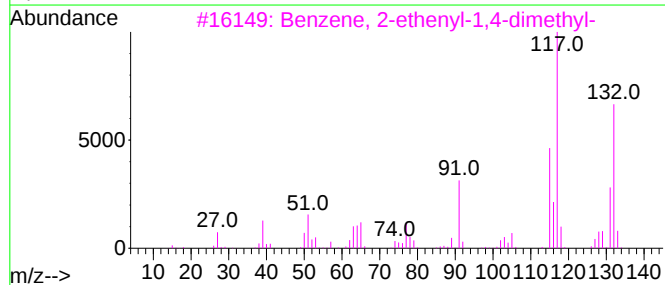
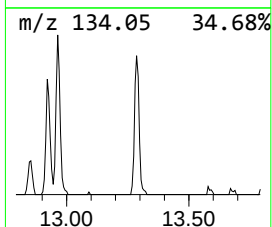
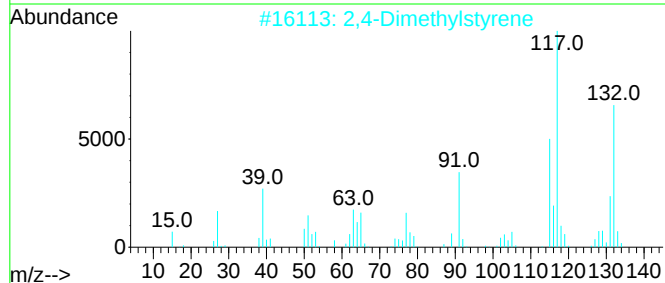
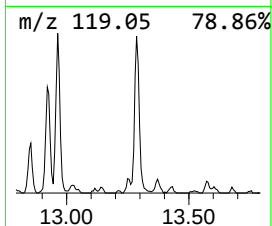
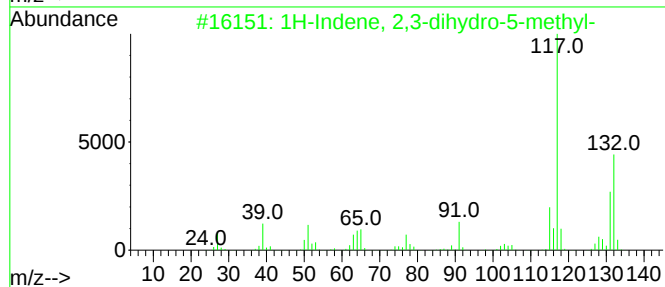
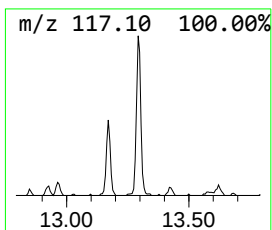
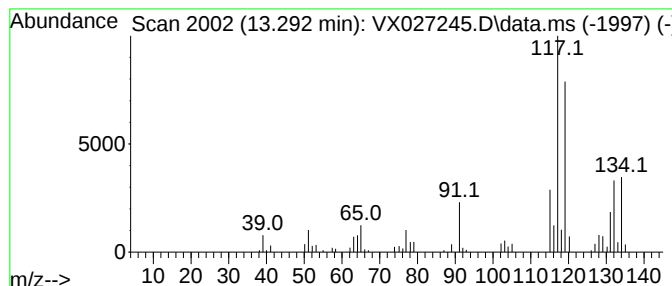
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.35 ug/l	46950	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	86
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	83
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	60
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027245.D
Acq On : 01 Mar 2022 13:56
Operator : JC/MD
Sample : N1688-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

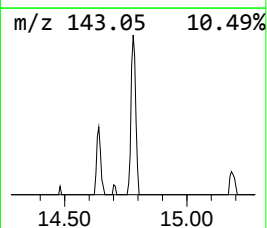
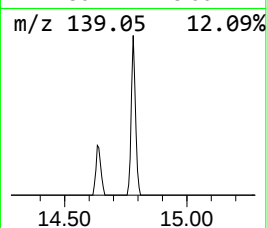
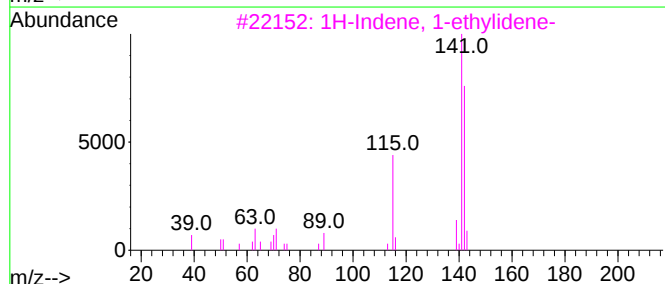
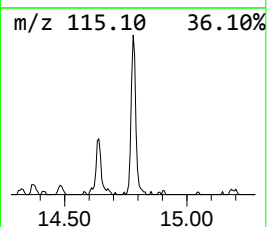
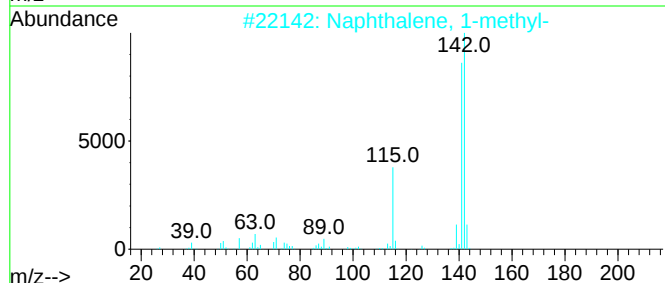
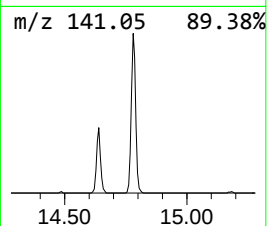
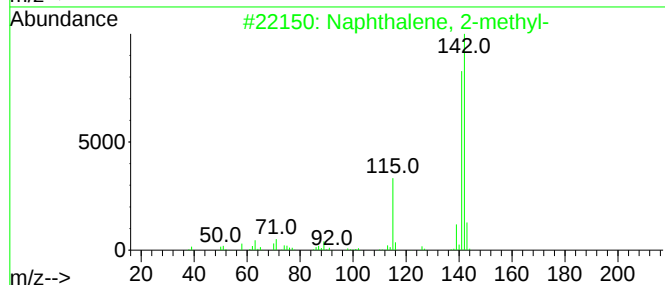
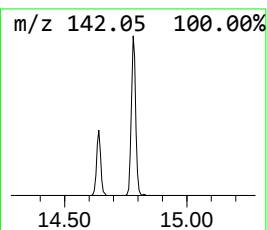
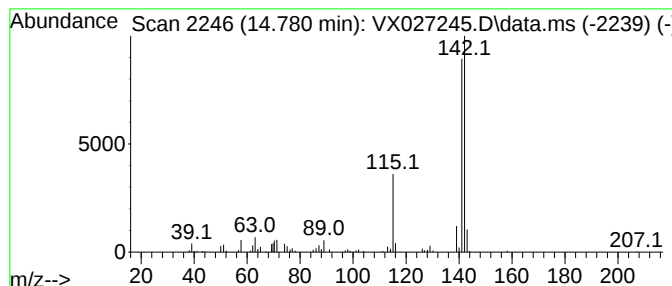
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1H-Indene, 1-ethylidene- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	6.59 ug/l	48734	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027245.D
Acq On : 01 Mar 2022 13:56
Operator : JC/MD
Sample : N1688-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	8.8	ug/l	43816	1	5.562	248229	50.0
Benzene, 1-ethy...	11.616	8.3	ug/l	61780	4	12.024	369894	50.0
Benzene, 1,2,3-...	12.085	9.4	ug/l	69367	4	12.024	369894	50.0
Indane	12.244	10.4	ug/l	76949	4	12.024	369894	50.0
1H-Indene, 2,3-...	13.292	6.3	ug/l	46950	4	12.024	369894	50.0
1H-Indene, 1-et...	14.780	6.6	ug/l	48734	4	12.024	369894	50.0