

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
 Data File : VX029026.D
 Acq On : 27 May 2022 16:00
 Operator : JC/MD
 Sample : N2968-12 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP-051922

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX029026.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	23	27	32	rBV2	20141	39096	2.12%	0.188%
2	1.368	42	46	51	rVB	39939	41263	2.24%	0.198%
3	1.746	103	108	117	rVB	52276	69093	3.75%	0.332%
4	1.959	137	143	153	rVB3	26615	55360	3.01%	0.266%
5	2.069	156	161	168	rVV	31788	48597	2.64%	0.233%
6	2.160	171	176	180	rVV	18903	31420	1.71%	0.151%
7	2.215	180	185	193	rVB	45711	73539	3.99%	0.353%
8	2.752	258	273	281	rBV3	21250	61193	3.32%	0.294%
9	2.867	287	292	299	rVV	27820	50351	2.73%	0.242%
10	2.953	299	306	319	rVB3	43197	108160	5.87%	0.519%
11	3.111	323	332	344	rVB3	18541	48791	2.65%	0.234%
12	3.733	428	434	445	rVB5	12960	32893	1.79%	0.158%
13	3.837	445	451	456	rBV4	7898	18588	1.01%	0.089%
14	4.105	486	495	506	rBV3	9036	24401	1.32%	0.117%
15	4.306	518	528	539	rBV2	37782	107960	5.86%	0.518%
16	5.202	662	675	685	rVB4	7207	24609	1.34%	0.118%
17	5.391	692	706	715	rBV	221917	646828	35.11%	3.106%
18	5.556	724	733	753	rVB	353505	1006897	54.66%	4.834%
19	5.958	789	799	805	rBV	218732	577736	31.36%	2.774%
20	6.044	805	813	827	rVV	519950	1392615	75.60%	6.686%
21	6.202	830	839	858	rVB6	12768	65532	3.56%	0.315%
22	6.763	922	931	944	rBV	568400	1366531	74.19%	6.561%
23	7.379	1023	1032	1043	rVB5	20421	51057	2.77%	0.245%
24	8.147	1153	1158	1163	rVB	16463	28264	1.53%	0.136%
25	8.507	1210	1217	1226	rVB2	15430	28063	1.52%	0.135%
26	8.653	1234	1241	1248	rBV	1175874	1842040	100.00%	8.844%
27	8.720	1248	1252	1263	rVB	72119	114022	6.19%	0.547%
28	10.055	1465	1471	1482	rBV	1288568	1678926	91.14%	8.061%
29	10.195	1489	1494	1501	rBV	947183	1212149	65.80%	5.820%
30	10.305	1505	1512	1523	rVB	946229	1289186	69.99%	6.190%
31	10.640	1562	1567	1579	rVB	500007	677562	36.78%	3.253%
32	10.964	1612	1620	1626	rBV	73871	93924	5.10%	0.451%
33	11.085	1634	1640	1651	rBV	1015003	1350156	73.30%	6.482%
34	11.305	1671	1676	1683	rVB	167169	203275	11.04%	0.976%
35	11.378	1683	1688	1690	rVV	188647	255865	13.89%	1.228%
36	11.403	1690	1692	1696	rVV	201583	214964	11.67%	1.032%

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37	11.451	1696	1700	1710	rVB	151020	188330	10.22%	0.904%
38	11.616	1721	1727	1735	rBV	209297	266221	14.45%	1.278%
39	11.750	1744	1749	1757	rBV	885018	1085961	58.95%	5.214%
40	12.024	1788	1794	1800	rVV	1407934	1726549	93.73%	8.289%
41	12.085	1800	1804	1810	rVB	297377	381362	20.70%	1.831%
42	12.244	1824	1830	1838	rBV	378455	486309	26.40%	2.335%
43	12.317	1838	1842	1852	rVB4	55380	90588	4.92%	0.435%
44	12.415	1852	1858	1862	rBV3	25052	36325	1.97%	0.174%
45	12.463	1862	1866	1872	rVB	26817	32099	1.74%	0.154%
46	12.530	1872	1877	1879	rBV	48104	56893	3.09%	0.273%
47	12.555	1879	1881	1886	rVB	33489	38584	2.09%	0.185%
48	12.616	1886	1891	1894	rBV	93137	113841	6.18%	0.547%
49	12.646	1894	1896	1900	rVB3	23719	25745	1.40%	0.124%
50	12.701	1900	1905	1913	rBV2	76404	108236	5.88%	0.520%
51	12.847	1925	1929	1934	rVB2	25350	31818	1.73%	0.153%
52	12.921	1934	1941	1945	rBV	56952	72901	3.96%	0.350%
53	12.963	1945	1948	1953	rVB	73134	82906	4.50%	0.398%
54	13.140	1972	1977	1979	rBV	29946	40346	2.19%	0.194%
55	13.170	1979	1982	1987	rVB	65621	79937	4.34%	0.384%
56	13.292	1997	2002	2007	rVB2	152979	200171	10.87%	0.961%
57	13.427	2019	2024	2031	rVB2	43084	58074	3.15%	0.279%
58	13.585	2046	2050	2055	rVB4	14767	23013	1.25%	0.110%
59	13.664	2060	2063	2070	rVB4	15760	26172	1.42%	0.126%
60	13.774	2074	2081	2090	rBV	267374	359742	19.53%	1.727%
61	14.219	2149	2154	2155	rBV2	15456	22135	1.20%	0.106%
62	14.640	2210	2223	2232	rBV	93331	134423	7.30%	0.645%
63	14.780	2240	2246	2255	rBV	79604	107239	5.82%	0.515%
64	15.615	2377	2383	2386	rBV3	14049	21451	1.16%	0.103%

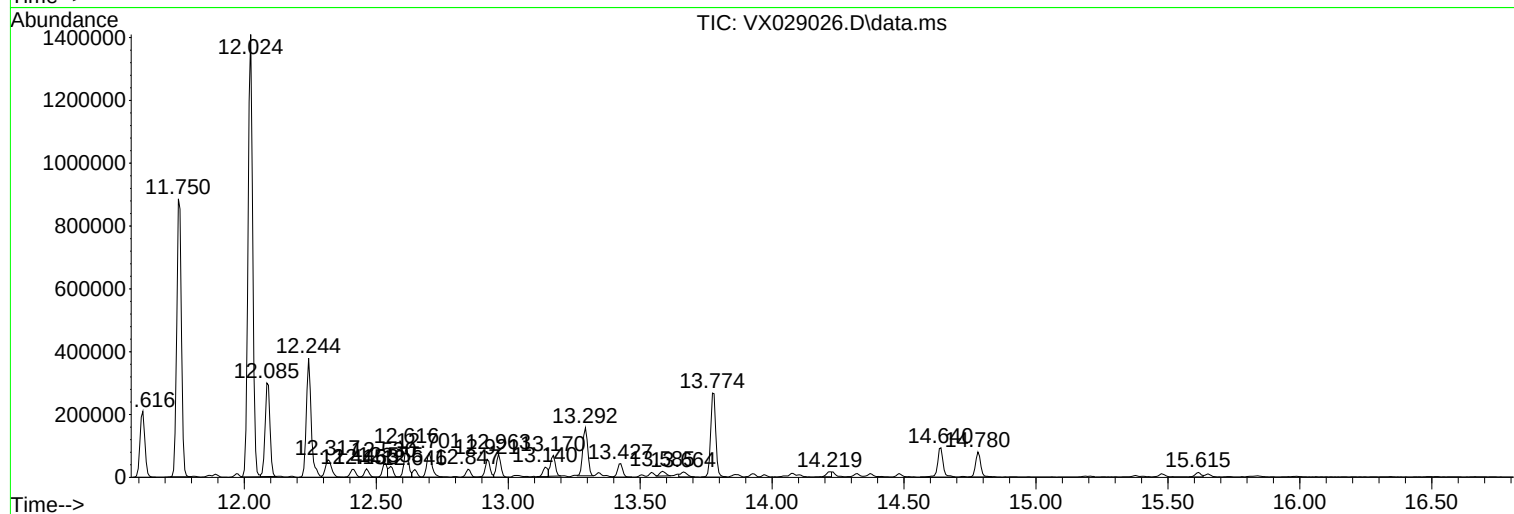
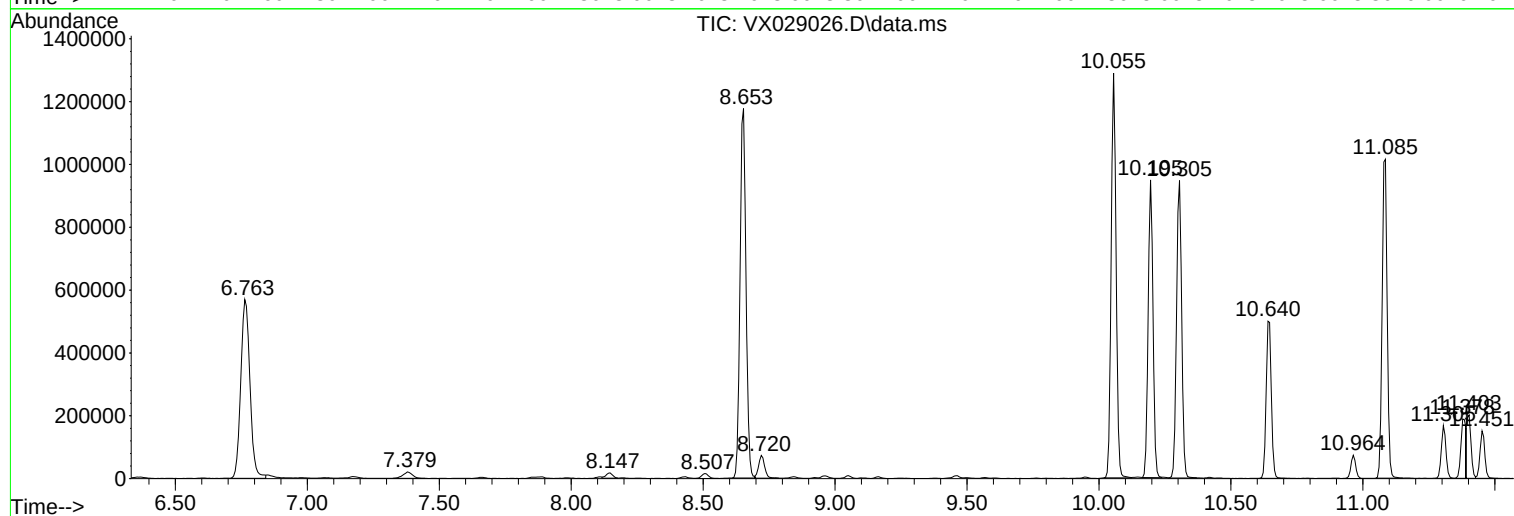
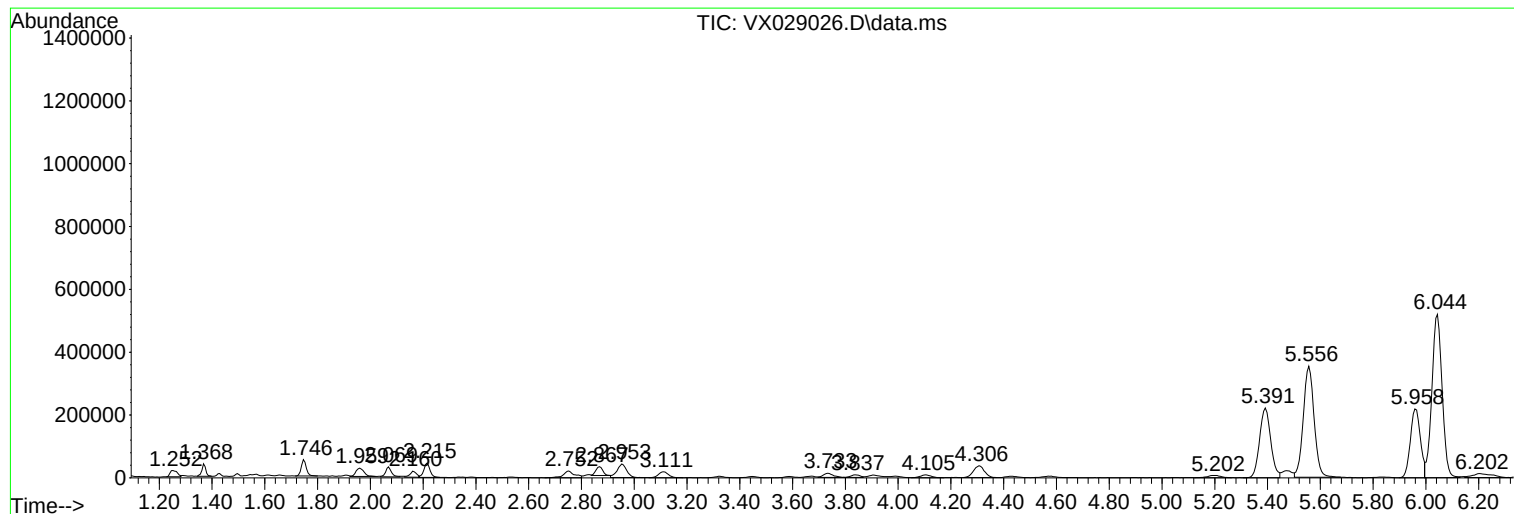
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-051922

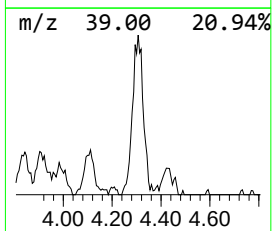
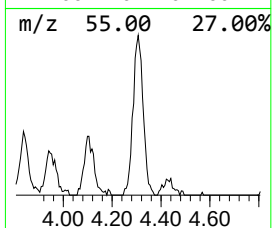
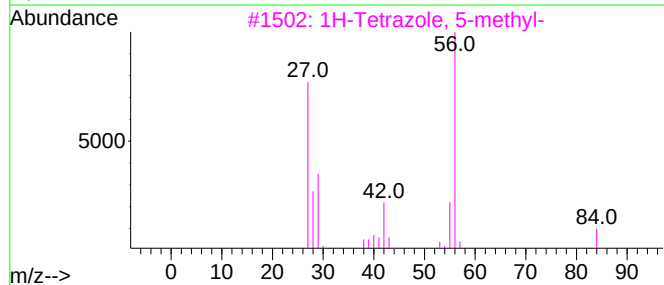
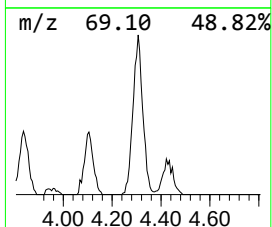
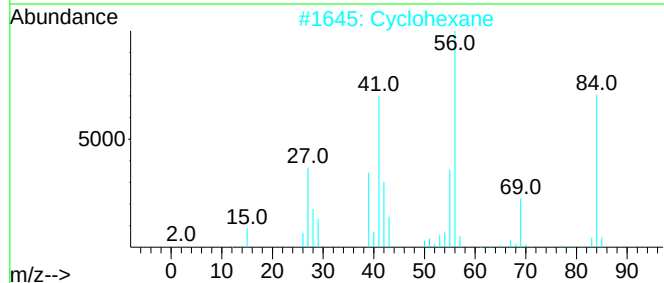
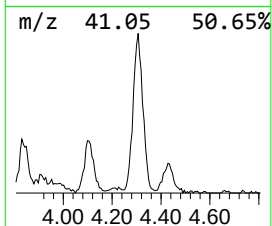
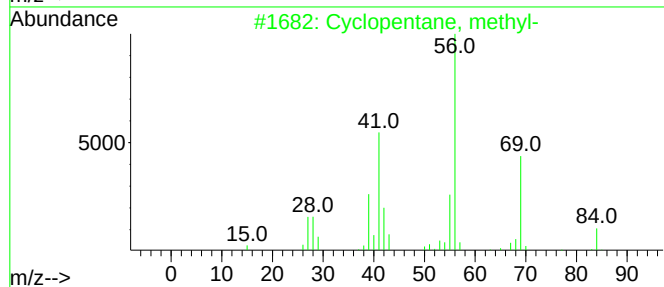
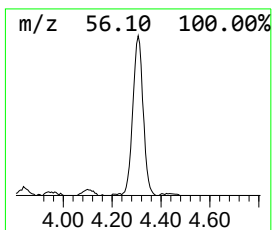
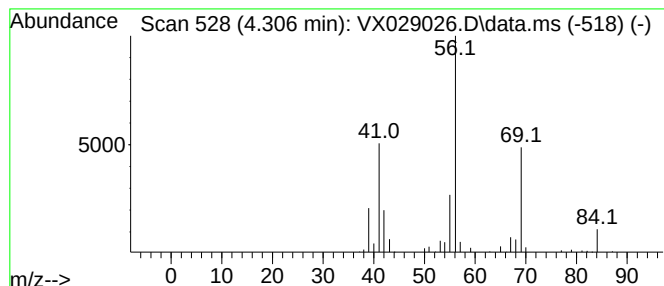
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	5.36 ug/l	107960	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclohexane	84	C6H12	000110-82-7	86
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



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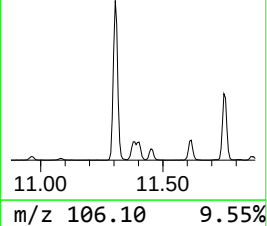
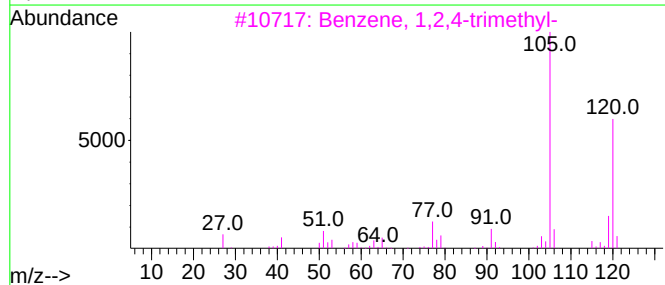
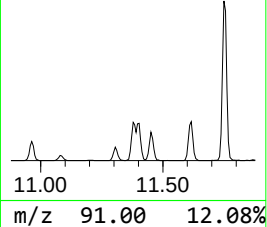
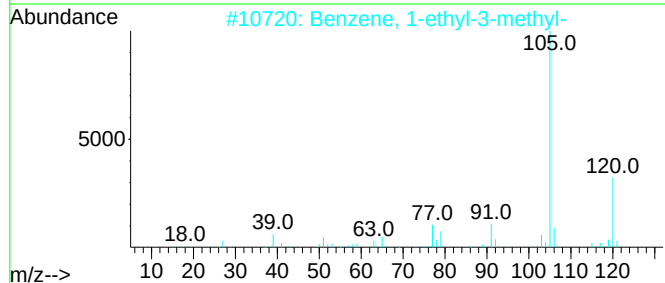
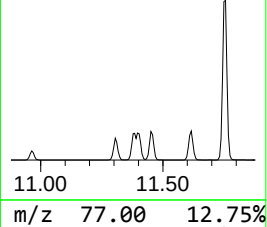
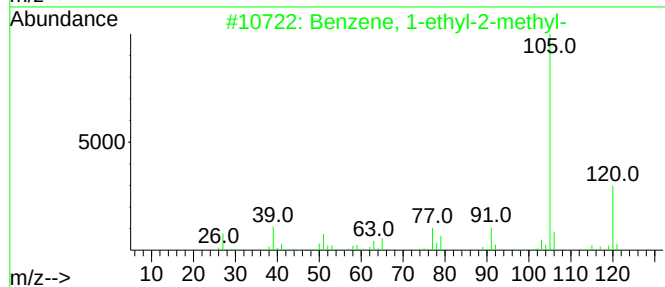
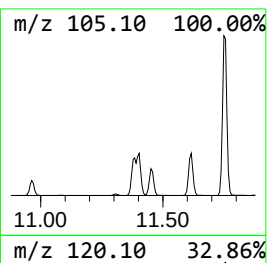
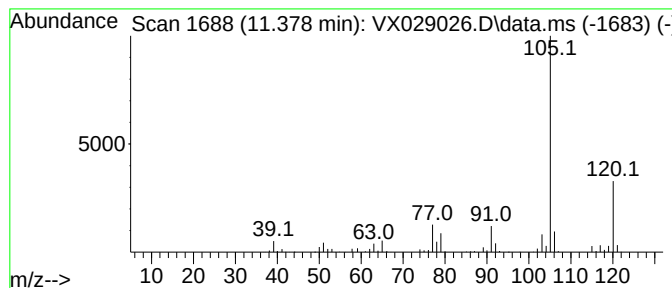
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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.
11.378	7.41 ug/l	255865	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	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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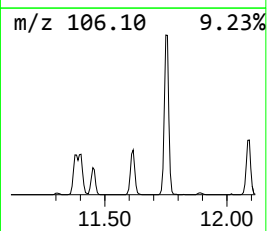
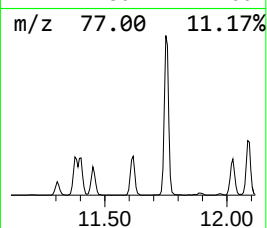
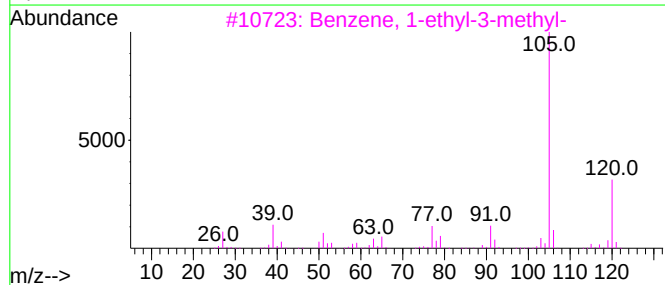
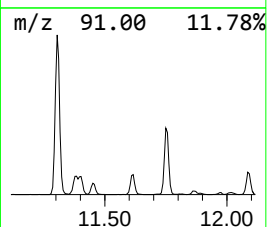
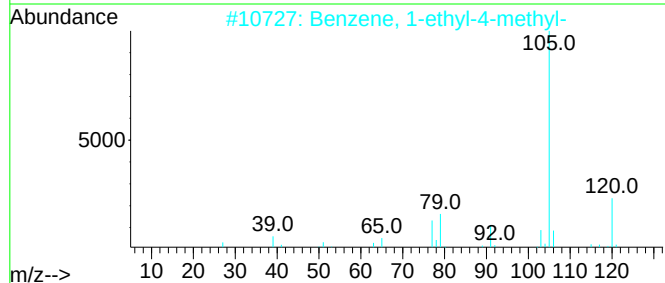
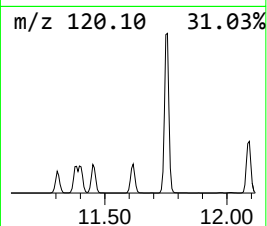
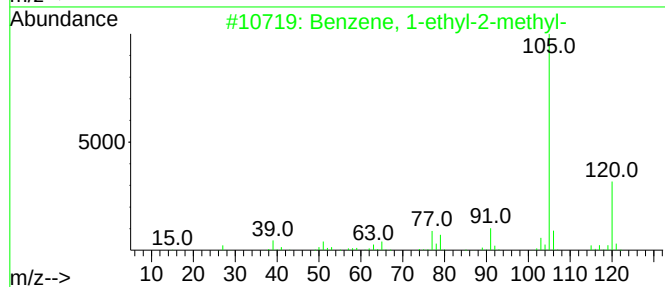
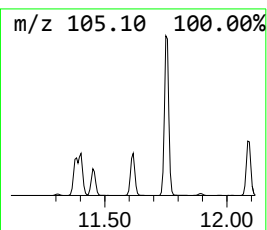
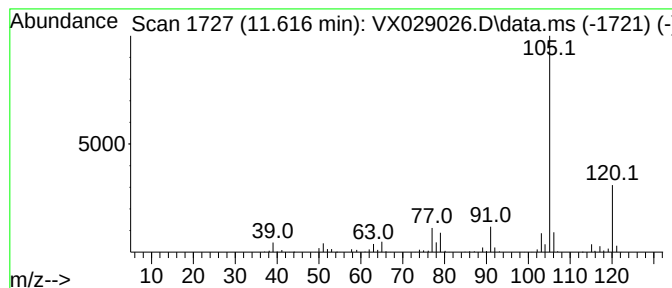
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	7.71 ug/l	266221	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	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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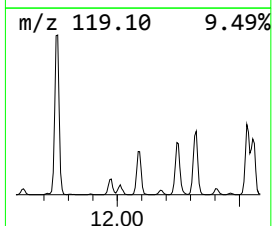
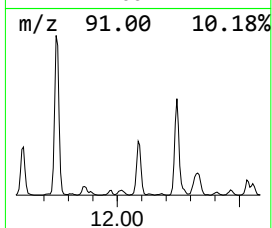
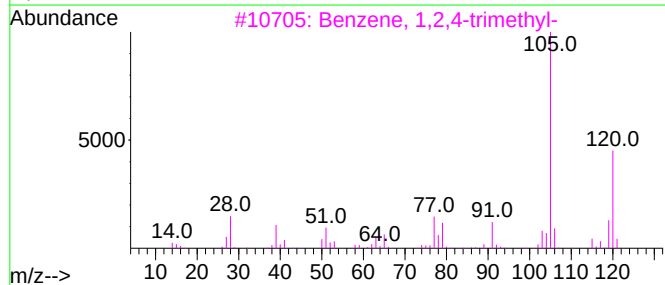
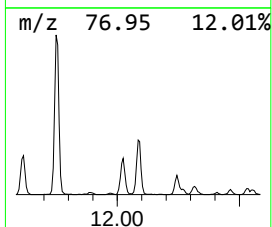
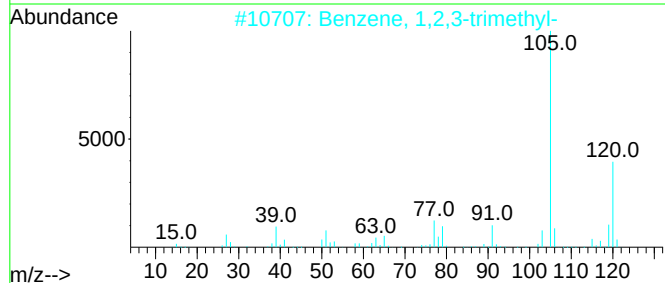
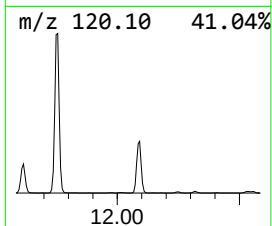
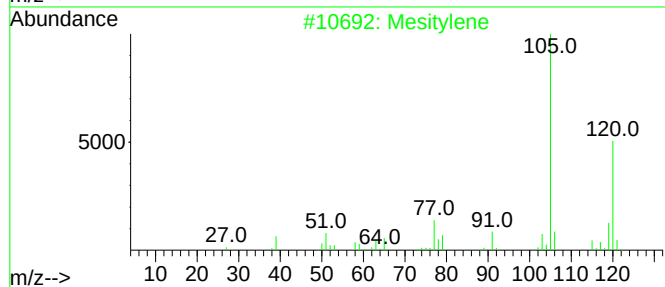
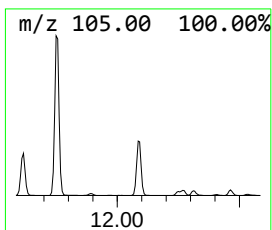
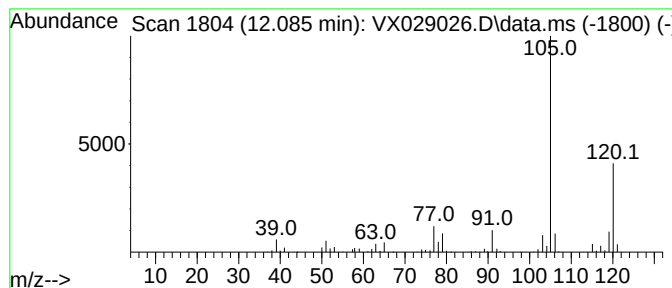
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	11.04 ug/l	381362	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87



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ClientSampleId :
DUP-051922

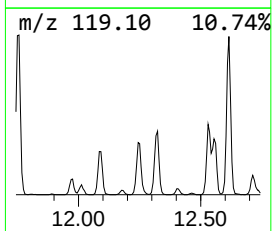
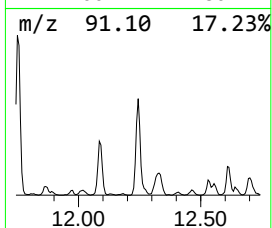
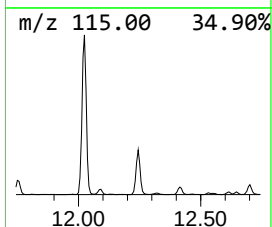
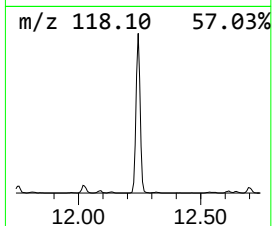
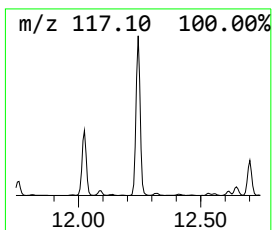
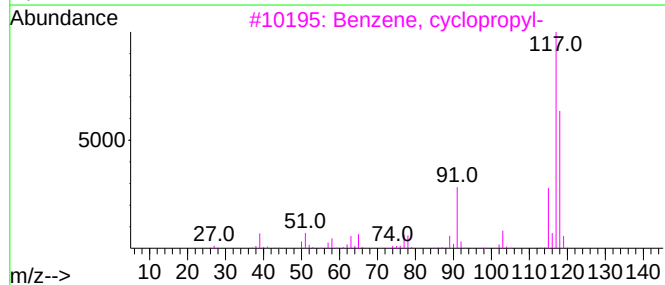
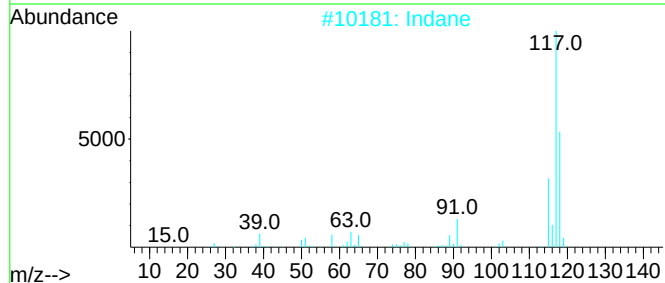
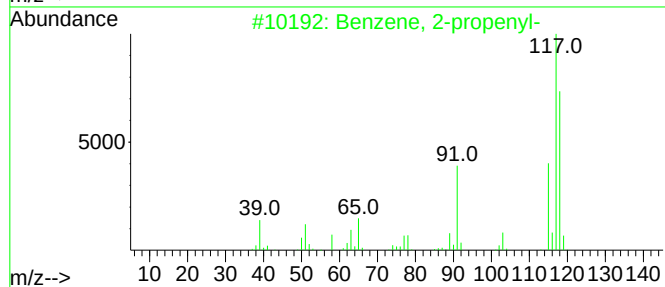
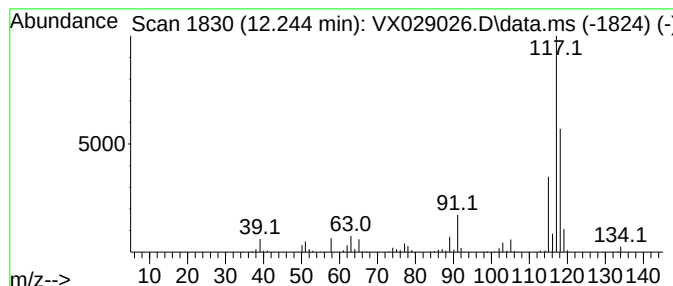
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	14.08 ug/l	486309	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029026.D
Acq On : 27 May 2022 16:00
Operator : JC/MD
Sample : N2968-12 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-051922

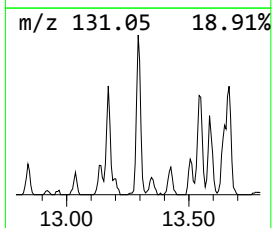
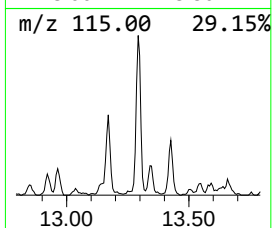
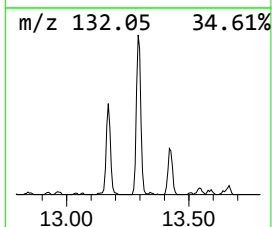
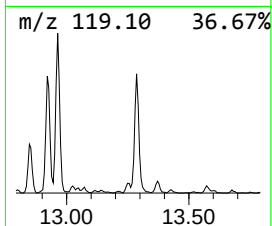
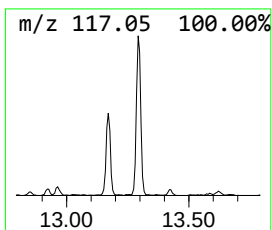
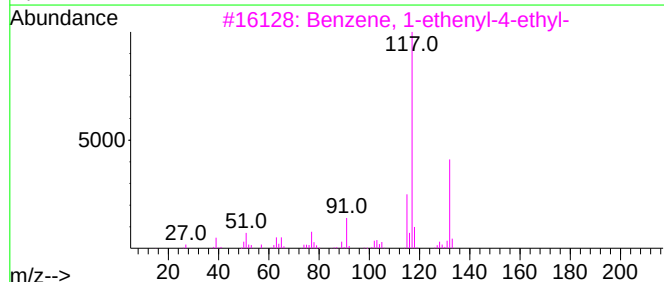
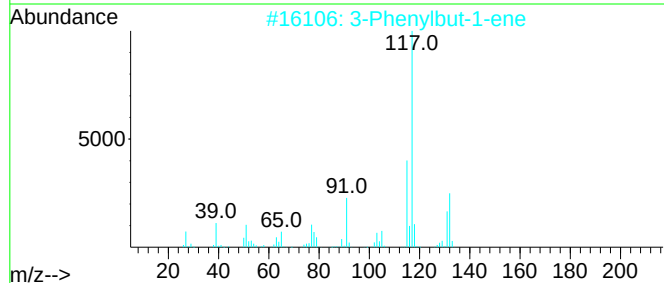
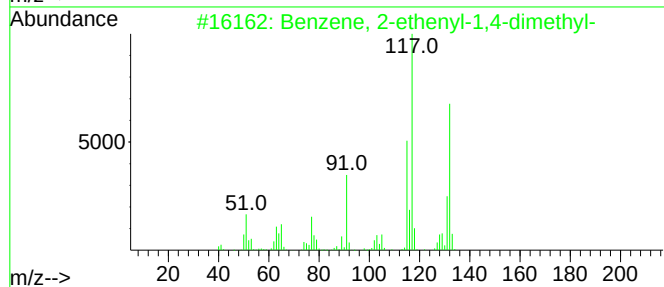
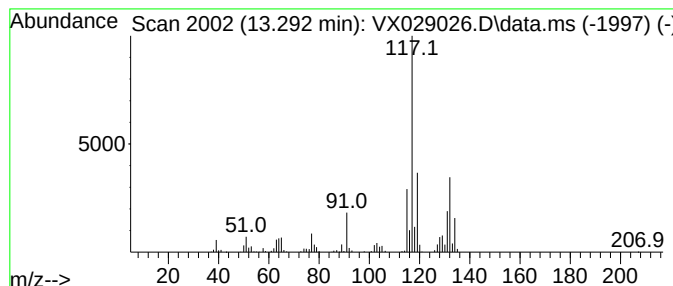
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.80 ug/l	200171	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052722\
Data File : VX029026.D
Acq On : 27 May 2022 16:00
Operator : JC/MD
Sample : N2968-12 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP-051922

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
Cyclopentane, m...	4.306	5.4	ug/l	107960	1	5.556	1006900	50.0
Benzene, 1-ethy...	11.378	7.4	ug/l	255865	4	12.024	1726550	50.0
Benzene, 1-ethy...	11.616	7.7	ug/l	266221	4	12.024	1726550	50.0
Benzene, 1,2,3-...	12.085	11.0	ug/l	381362	4	12.024	1726550	50.0
Benzene, 2-prop...	12.244	14.1	ug/l	486309	4	12.024	1726550	50.0
Benzene, 2-ethe...	13.292	5.8	ug/l	200171	4	12.024	1726550	50.0