

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
 Data File : VX027224.D
 Acq On : 28 Feb 2022 16:49
 Operator : JC/MD
 Sample : N1688-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 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: VX027224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.221	181	186	193	rVB	4587	7315	1.20%	0.152%
2	2.386	207	213	218	rBV	7444	12764	2.09%	0.265%
3	2.751	268	273	279	rVB3	5009	9103	1.49%	0.189%
4	2.867	284	292	301	rBV3	2965	6113	1.00%	0.127%
5	2.965	301	308	317	rVB2	4746	10643	1.74%	0.221%
6	3.117	325	333	343	rVB2	8022	18359	3.01%	0.381%
7	5.391	695	706	718	rBV	52470	153036	25.05%	3.176%
8	5.556	723	733	747	rVB	93467	260734	42.69%	5.411%
9	5.964	790	800	805	rBV	56131	144205	23.61%	2.993%
10	6.043	805	813	830	rVB	230909	610815	100.00%	12.677%
11	6.769	920	932	945	rBV	142683	339454	55.57%	7.045%
12	8.580	1222	1229	1234	rBV	5070	8119	1.33%	0.169%
13	8.653	1234	1241	1248	rVV	293350	454411	74.39%	9.431%
14	8.720	1248	1252	1263	rVB	24873	38470	6.30%	0.798%
15	10.055	1465	1471	1482	rBV	301887	399396	65.39%	8.289%
16	10.195	1488	1494	1506	rBV	228855	294632	48.24%	6.115%
17	10.305	1506	1512	1518	rBV	153394	193405	31.66%	4.014%
18	10.640	1562	1567	1578	rBV	126674	166003	27.18%	3.445%
19	10.963	1615	1620	1625	rVB	16645	19776	3.24%	0.410%
20	11.079	1634	1639	1650	rBV	243428	313677	51.35%	6.510%
21	11.305	1671	1676	1682	rBV	29709	35202	5.76%	0.731%
22	11.402	1685	1692	1697	rBV	28451	43706	7.16%	0.907%
23	11.616	1722	1727	1735	rVB	57049	72484	11.87%	1.504%
24	11.750	1745	1749	1760	rVB	133252	165629	27.12%	3.438%
25	12.024	1789	1794	1800	rBV	321626	385471	63.11%	8.000%
26	12.091	1800	1805	1810	rVB	64172	80044	13.10%	1.661%
27	12.244	1823	1830	1838	rBV	69119	88676	14.52%	1.840%
28	12.311	1838	1841	1849	rVB3	5171	8377	1.37%	0.174%
29	12.463	1862	1866	1871	rVB	6977	7842	1.28%	0.163%
30	12.530	1873	1877	1880	rBV2	8902	12487	2.04%	0.259%
31	12.615	1886	1891	1894	rVV	19805	24209	3.96%	0.502%
32	12.701	1900	1905	1913	rVB2	19083	28355	4.64%	0.588%
33	12.847	1924	1929	1935	rVB2	8278	10844	1.78%	0.225%
34	12.920	1935	1941	1945	rBV	15609	20142	3.30%	0.418%
35	12.963	1945	1948	1954	rVB	21638	25916	4.24%	0.538%
36	13.170	1978	1982	1988	rVB	11514	13220	2.16%	0.274%

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 Title : SW846 8260

37	13.292	1992	2002	2008	rBV2	39202	60616	9.92%	1.258%
38	13.426	2020	2024	2028	rVB	10531	13680	2.24%	0.284%
39	13.585	2046	2050	2056	rVV3	8046	15239	2.49%	0.316%
40	13.664	2060	2063	2072	rVB2	6285	10914	1.79%	0.227%
41	13.774	2072	2081	2089	rBV	40022	58106	9.51%	1.206%
42	13.926	2100	2106	2110	rBV3	4503	7497	1.23%	0.156%
43	14.219	2147	2154	2160	rBV4	6674	13658	2.24%	0.283%
44	14.481	2193	2197	2202	rBV3	5462	7918	1.30%	0.164%
45	14.640	2215	2223	2227	rBV	16143	23446	3.84%	0.487%
46	14.780	2239	2246	2254	rBV	41935	56949	9.32%	1.182%
47	15.115	2296	2301	2306	rBV3	6467	9387	1.54%	0.195%
48	15.481	2355	2361	2366	rBV2	10662	17208	2.82%	0.357%
49	15.615	2377	2383	2387	rBV	14988	24236	3.97%	0.503%
50	15.652	2387	2389	2394	rVB2	6033	7496	1.23%	0.156%
51	15.841	2411	2420	2427	rVB4	3529	8883	1.45%	0.184%

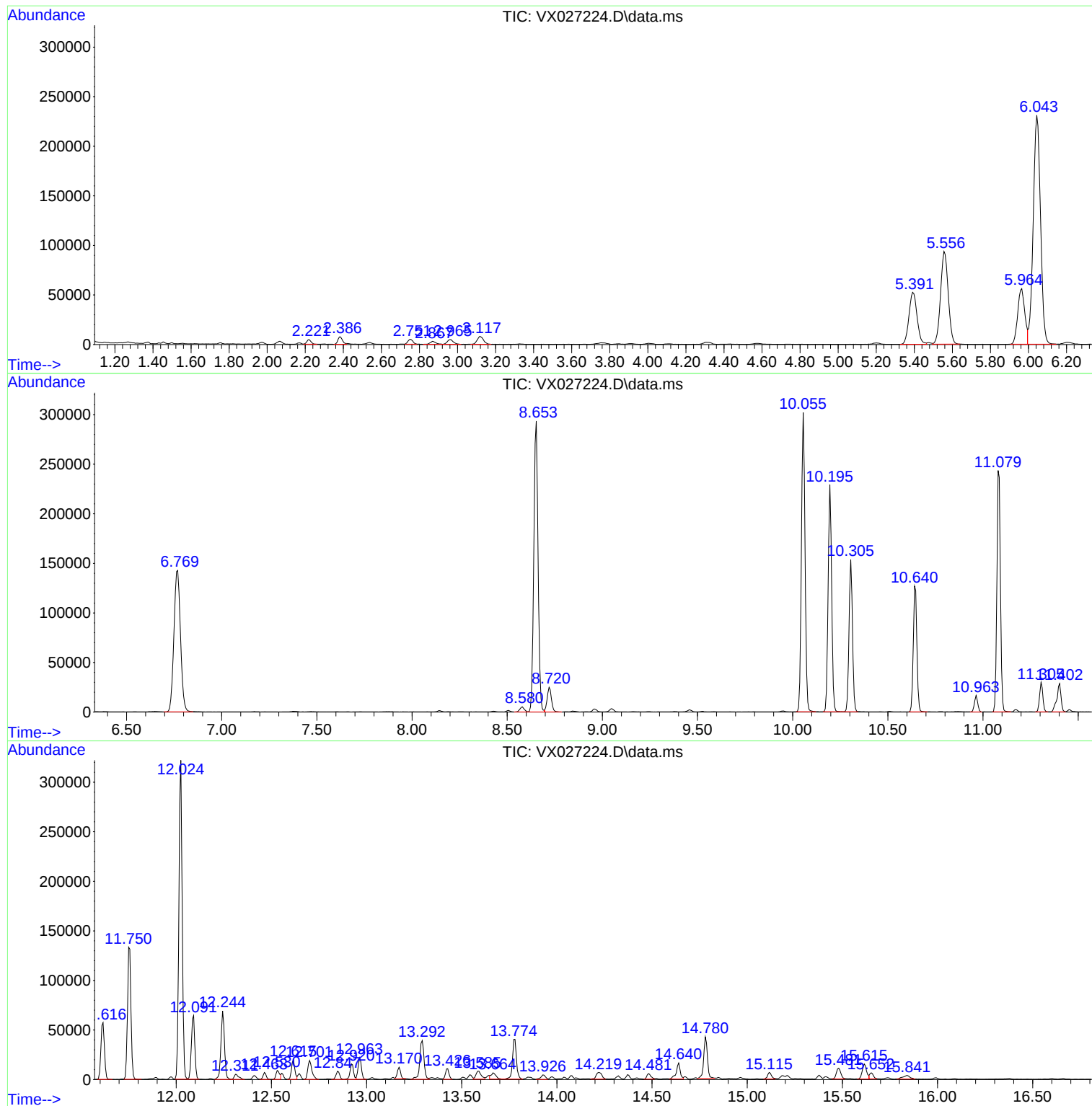
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



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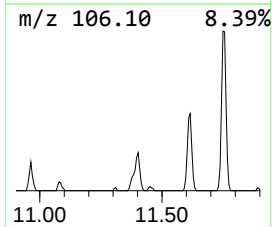
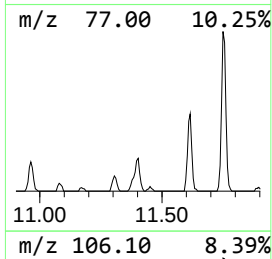
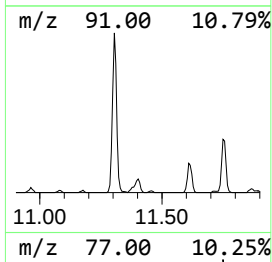
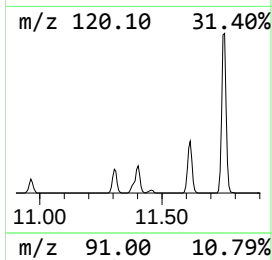
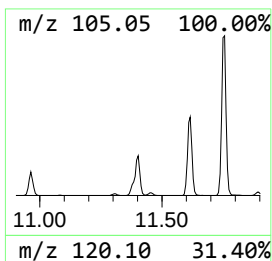
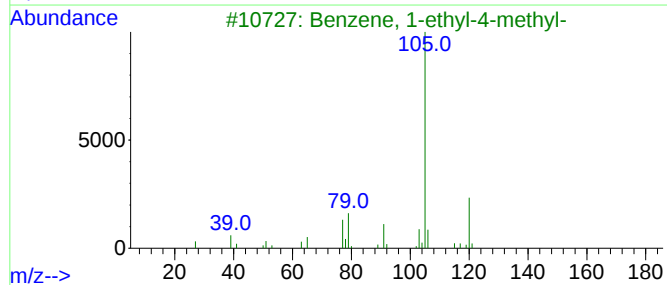
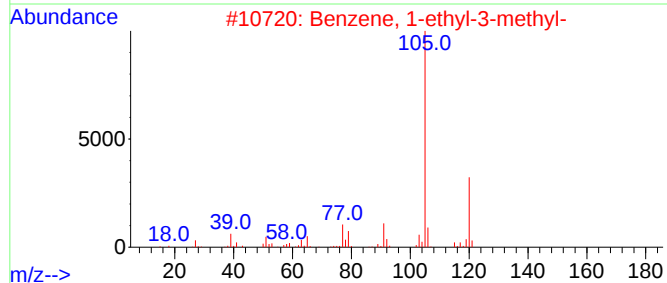
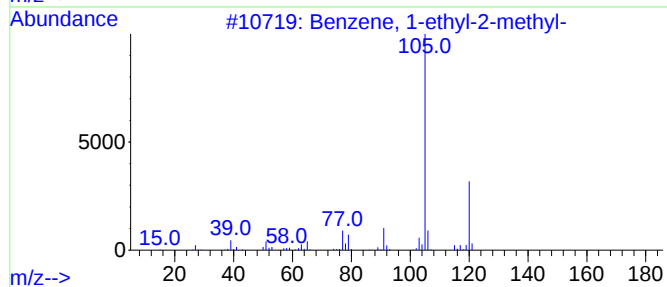
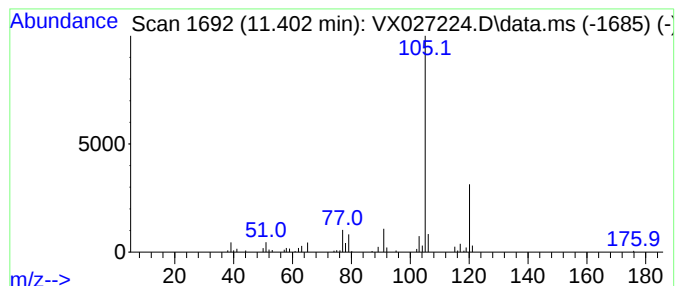
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.402	5.67 ug/l	43706	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	91
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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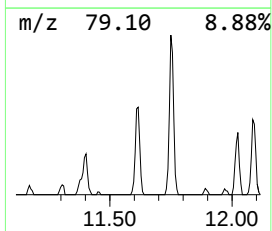
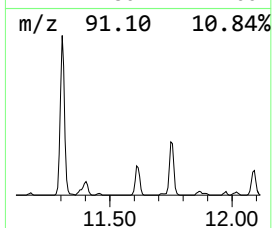
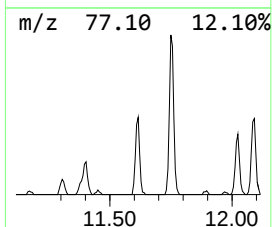
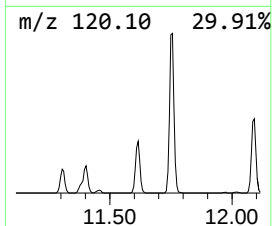
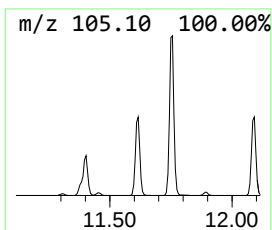
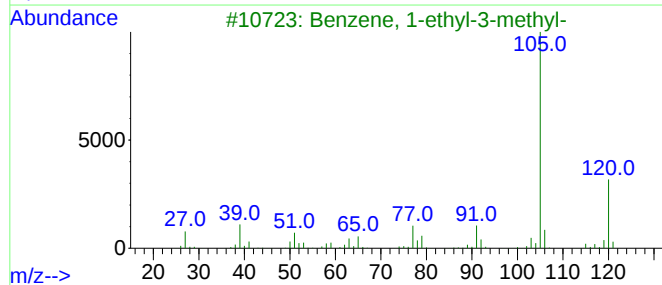
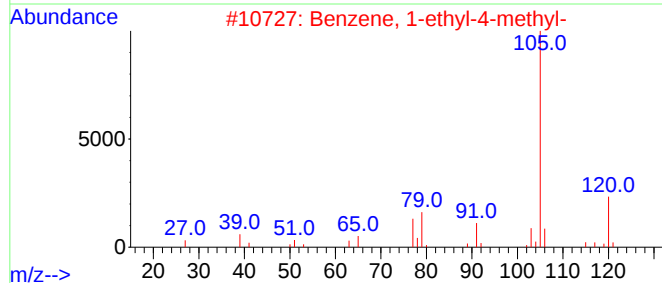
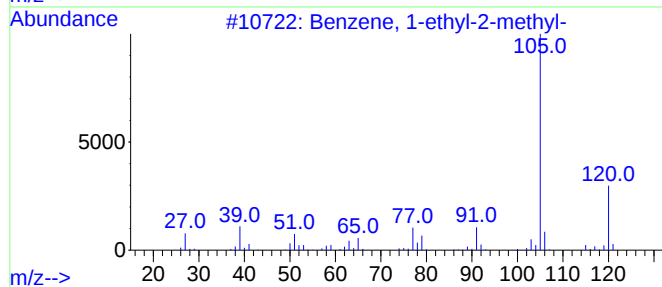
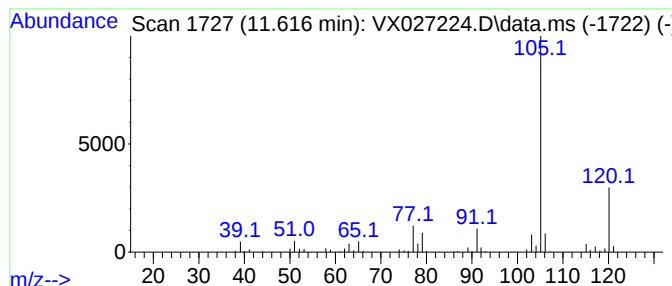
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	9.40 ug/l	72484	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			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
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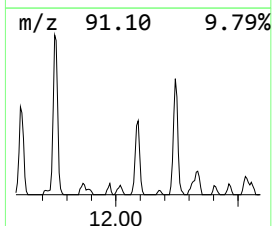
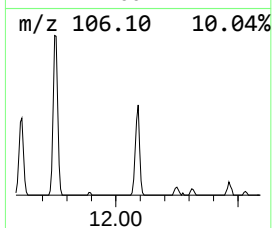
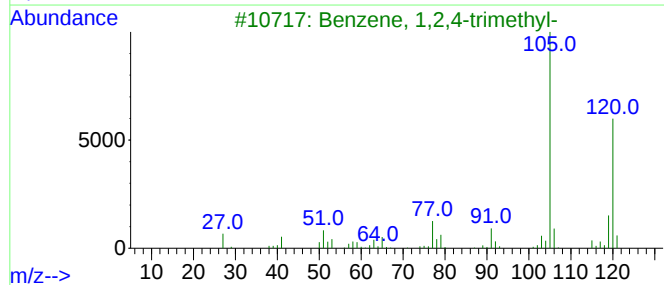
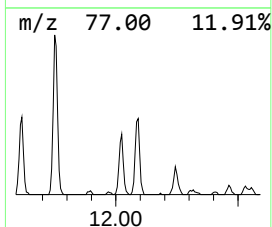
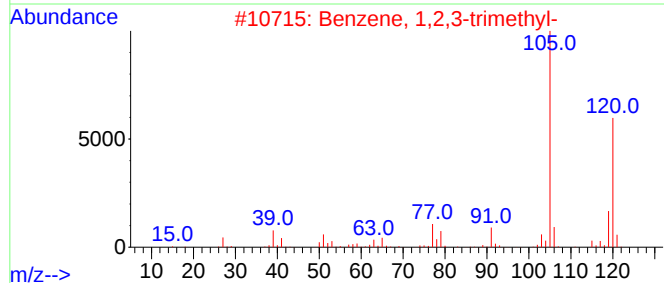
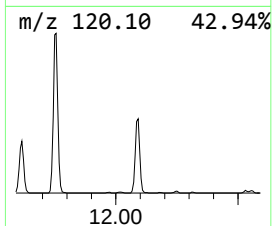
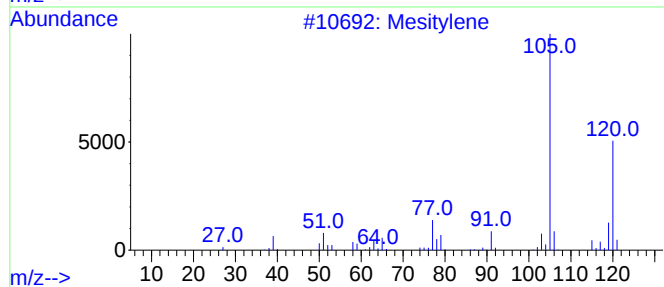
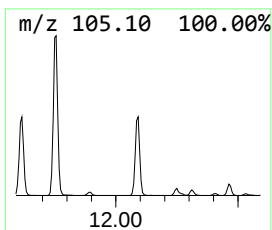
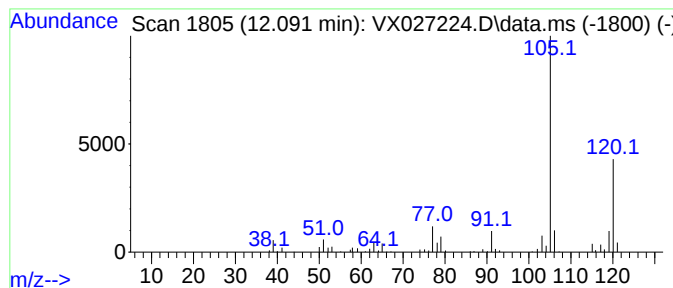
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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.
12.091	10.38 ug/l	80044	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	93
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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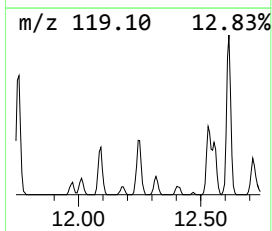
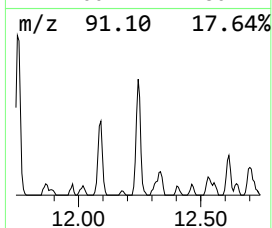
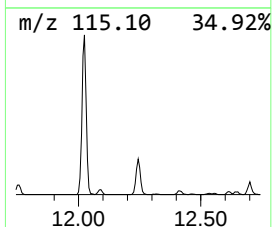
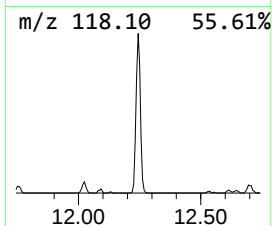
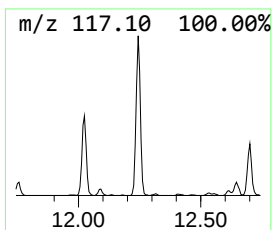
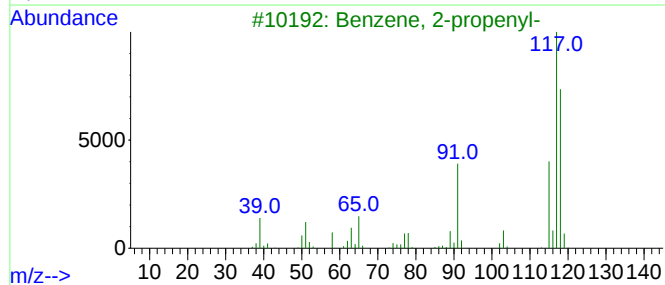
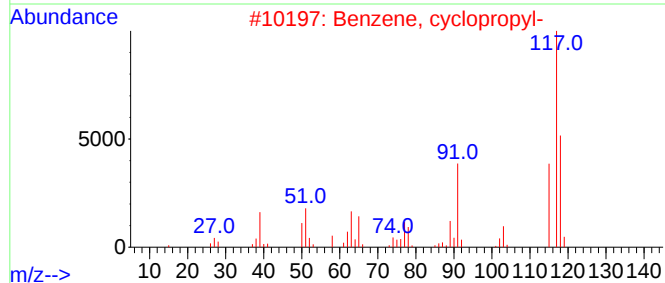
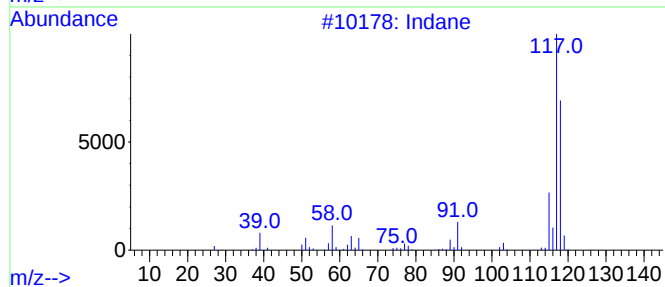
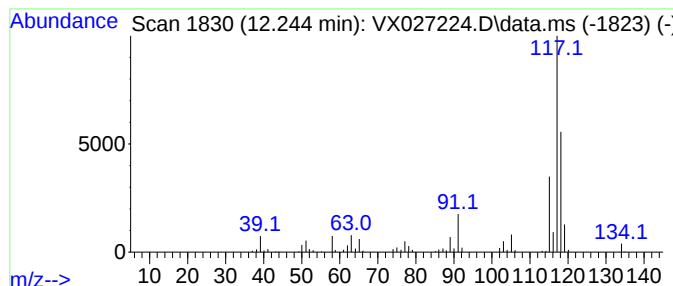
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	11.50 ug/l	88676	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Delatacyclene	118	C9H10	007785-10-6	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53



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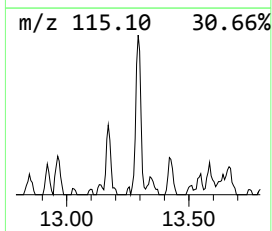
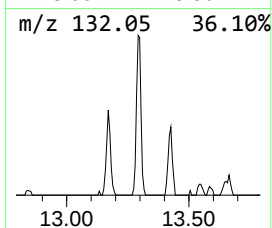
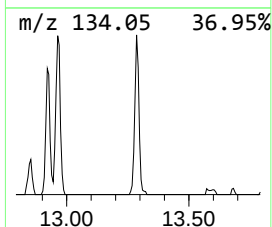
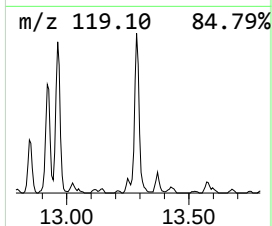
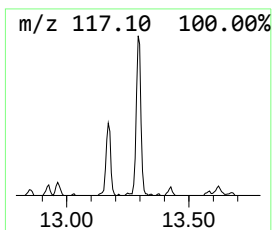
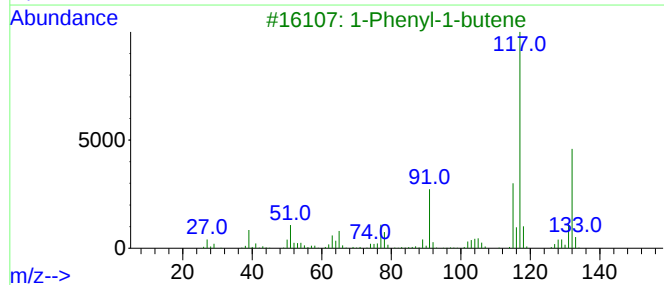
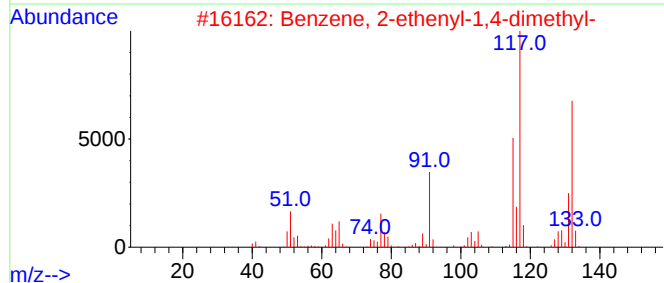
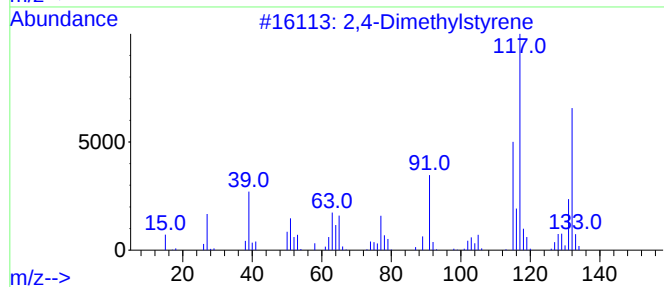
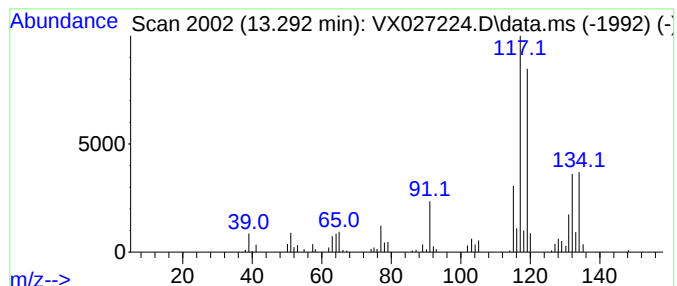
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Quant Title : SW846 8260

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

Peak Number 5 2,4-Dimethylstyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	7.86 ug/l	60616	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	86
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	55
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	55
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027224.D
Acq On : 28 Feb 2022 16:49
Operator : JC/MD
Sample : N1688-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-27

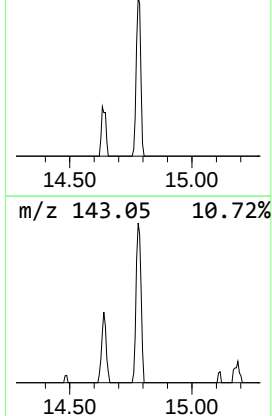
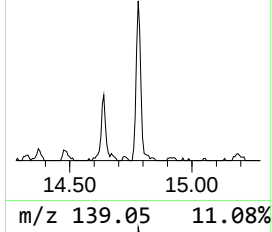
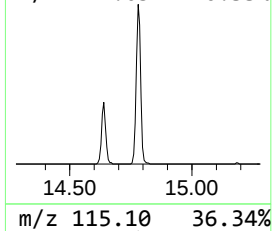
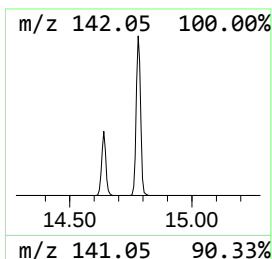
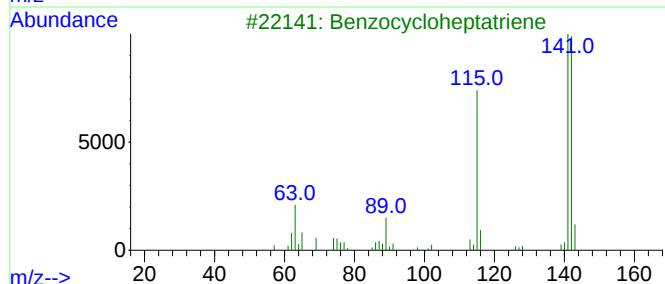
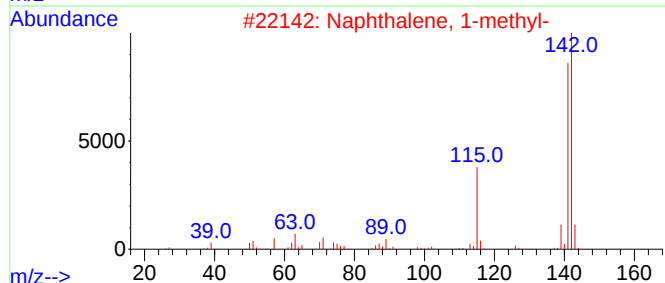
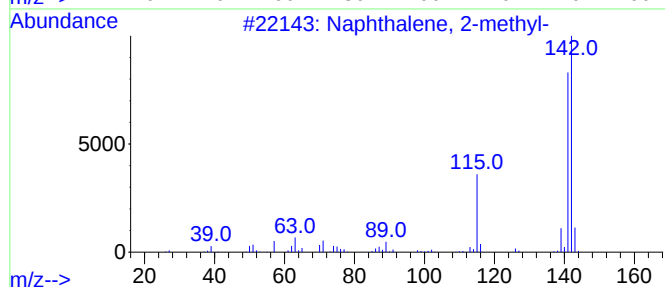
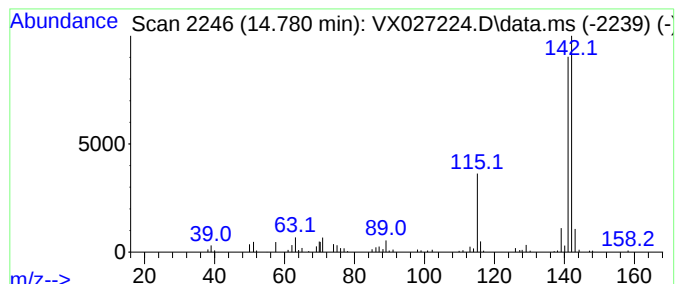
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	7.39 ug/l	56949	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			Benzocycloheptatriene	142	C11H10	000264-09-5	93
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027224.D
Acq On : 28 Feb 2022 16:49
Operator : JC/MD
Sample : N1688-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 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
Benzene, 1-ethy...	11.402	5.7	ug/l	43706	4	12.024	385471	50.0
Benzene, 1-ethy...	11.616	9.4	ug/l	72484	4	12.024	385471	50.0
Benzene, 1,2,3-...	12.091	10.4	ug/l	80044	4	12.024	385471	50.0
Indane	12.244	11.5	ug/l	88676	4	12.024	385471	50.0
2,4-Dimethylsty...	13.292	7.9	ug/l	60616	4	12.024	385471	50.0
Benzocyclohepta...	14.780	7.4	ug/l	56949	4	12.024	385471	50.0