

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
 Data File : VX020759.D
 Acq On : 26 Jan 2021 17:28
 Operator : JC/SP
 Sample : M1189-09 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 41052

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\82X012521W.M
 Title : SW846 8260

Signal : TIC: VX020759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	59	63	74	rBV	238847	279641	3.85%	0.783%
2	2.099	158	166	199	rBV	4173510	7269761	100.00%	20.354%
3	2.416	212	218	232	rBV	1193372	1952284	26.85%	5.466%
4	5.464	707	718	733	rBV	214234	606147	8.34%	1.697%
5	5.629	733	745	761	rVB	351728	999476	13.75%	2.798%
6	6.031	799	811	820	rBV	230803	606545	8.34%	1.698%
7	6.830	931	942	959	rBV	568252	1327246	18.26%	3.716%
8	8.695	1241	1248	1253	rBV	1162783	1843123	25.35%	5.160%
9	8.762	1253	1259	1270	rVB	2040410	3046867	41.91%	8.531%
10	10.092	1472	1477	1487	rBV	1186432	1623258	22.33%	4.545%
11	10.232	1495	1500	1507	rBV	167592	220203	3.03%	0.617%
12	10.341	1510	1518	1524	rBV	647561	874240	12.03%	2.448%
13	10.683	1568	1574	1584	rVB	383232	514167	7.07%	1.440%
14	11.122	1640	1646	1657	rBV	983948	1287592	17.71%	3.605%
15	11.341	1677	1682	1688	rBV	103936	126705	1.74%	0.355%
16	11.414	1689	1694	1702	rVV	375675	683573	9.40%	1.914%
17	11.488	1702	1706	1716	rVB	194105	264236	3.63%	0.740%
18	11.652	1728	1733	1741	rVB	234781	308955	4.25%	0.865%
19	11.792	1751	1756	1762	rVB	798400	983319	13.53%	2.753%
20	12.006	1783	1791	1795	rBV	66993	94681	1.30%	0.265%
21	12.061	1795	1800	1806	rVV	1335857	1598501	21.99%	4.475%
22	12.128	1806	1811	1816	rVV	334715	430155	5.92%	1.204%
23	12.280	1829	1836	1839	rBV	305744	438043	6.03%	1.226%
24	12.305	1839	1840	1844	rVB	181023	144823	1.99%	0.405%
25	12.353	1844	1848	1856	rVB3	275988	430343	5.92%	1.205%
26	12.457	1856	1865	1868	rBV3	46945	92676	1.27%	0.259%
27	12.500	1868	1872	1878	rVB	123377	152137	2.09%	0.426%
28	12.567	1878	1883	1885	rBV	158718	201337	2.77%	0.564%
29	12.591	1885	1887	1892	rVB	161830	175167	2.41%	0.490%
30	12.652	1892	1897	1900	rBV	229661	270254	3.72%	0.757%
31	12.737	1906	1911	1914	rBV	149093	231125	3.18%	0.647%
32	12.884	1931	1935	1939	rVB2	90801	124596	1.71%	0.349%
33	12.957	1939	1947	1951	rBV	154401	222546	3.06%	0.623%
34	13.000	1951	1954	1961	rVB	253516	305753	4.21%	0.856%
35	13.207	1980	1988	1992	rBV2	228391	334173	4.60%	0.936%
36	13.292	1998	2002	2004	rBV2	74661	114788	1.58%	0.321%

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37	13.329	2004	2008	2013	rVB2	536833	714932	9.83%	2.002%
38	13.463	2025	2030	2038	rVB	437103	575335	7.91%	1.611%
39	13.542	2038	2043	2046	rBV2	54883	77678	1.07%	0.217%
40	13.579	2046	2049	2052	rBV	76429	99398	1.37%	0.278%
41	13.621	2052	2056	2061	rVV3	106438	170590	2.35%	0.478%
42	13.701	2067	2069	2075	rVB2	110023	158458	2.18%	0.444%
43	13.816	2082	2088	2093	rBV	208473	265358	3.65%	0.743%
44	13.890	2094	2100	2106	rVB	191407	284280	3.91%	0.796%
45	13.963	2106	2112	2117	rBV3	185801	287357	3.95%	0.805%
46	14.115	2133	2137	2141	rBV	128471	152232	2.09%	0.426%
47	14.268	2155	2162	2169	rBV	481498	742141	10.21%	2.078%
48	14.414	2182	2186	2190	rVB2	123669	149557	2.06%	0.419%
49	14.518	2199	2203	2209	rBV2	298813	416392	5.73%	1.166%
50	14.652	2221	2225	2227	rBV	187597	241177	3.32%	0.675%
51	14.676	2227	2229	2232	rVV	173307	201537	2.77%	0.564%
52	14.713	2232	2235	2240	rVB2	109237	143304	1.97%	0.401%
53	14.822	2250	2253	2256	rVV2	66162	86968	1.20%	0.243%
54	14.859	2256	2259	2261	rVV	69534	94276	1.30%	0.264%
55	14.883	2261	2263	2269	rVB2	59765	75884	1.04%	0.212%
56	14.944	2269	2273	2280	rBV2	61722	116003	1.60%	0.325%
57	15.225	2314	2319	2327	rBV2	134684	287668	3.96%	0.805%
58	15.530	2364	2369	2373	rBV3	71899	118956	1.64%	0.333%
59	15.664	2386	2391	2395	rBV3	47715	79368	1.09%	0.222%

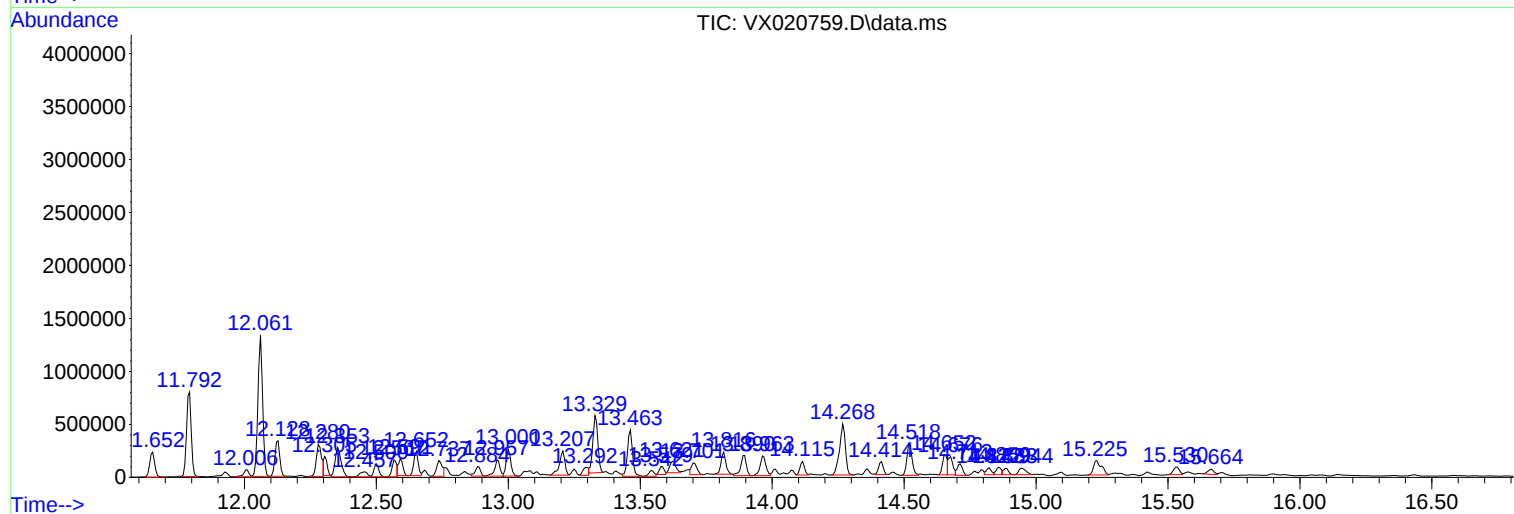
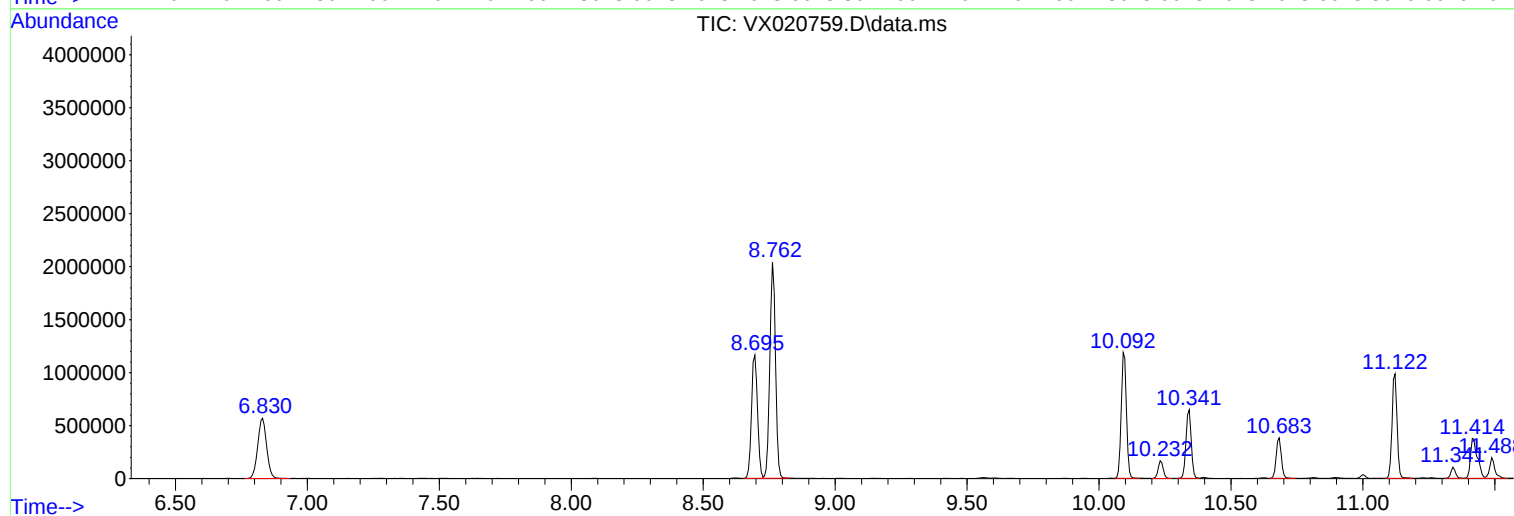
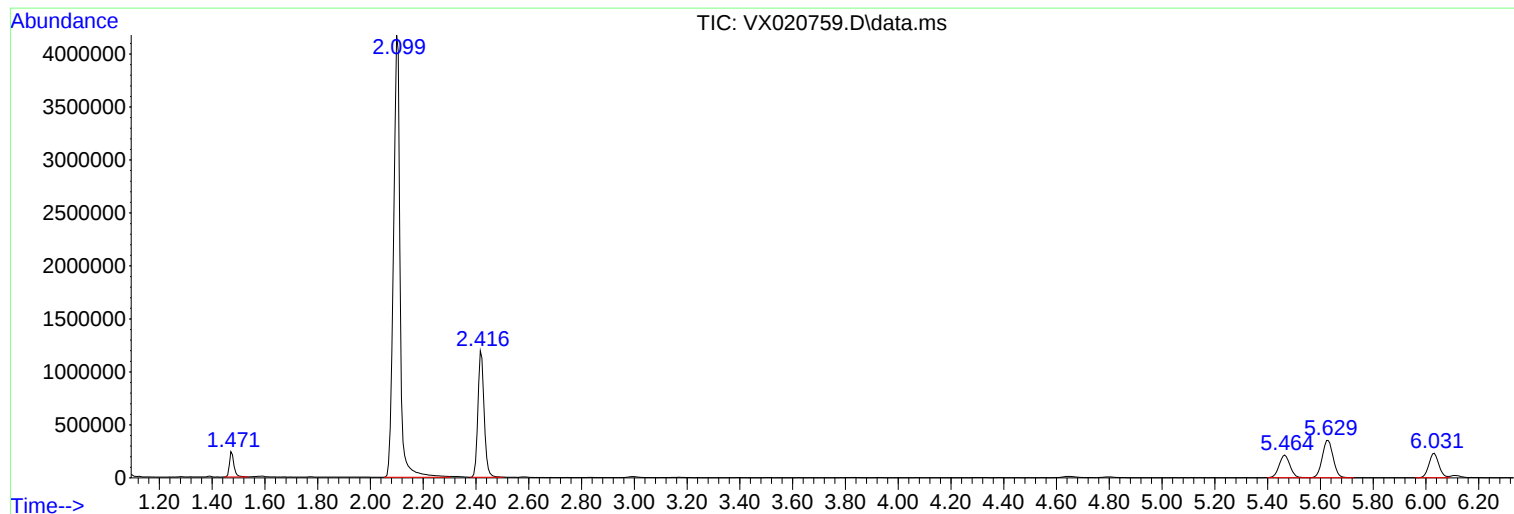
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Quant Title : SW846 8260

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



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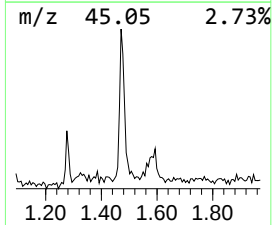
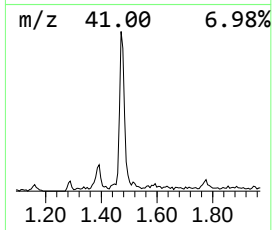
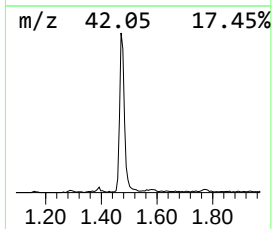
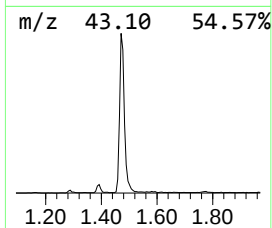
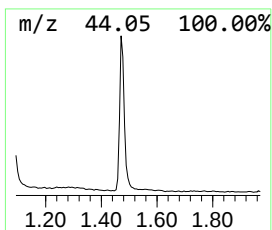
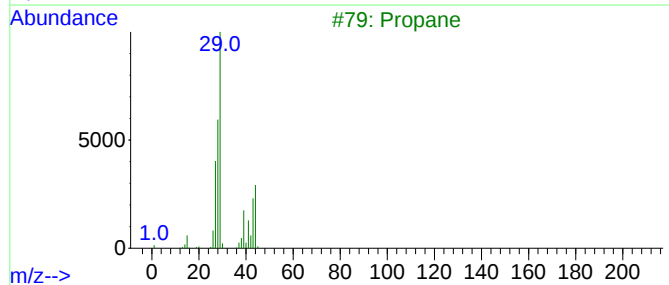
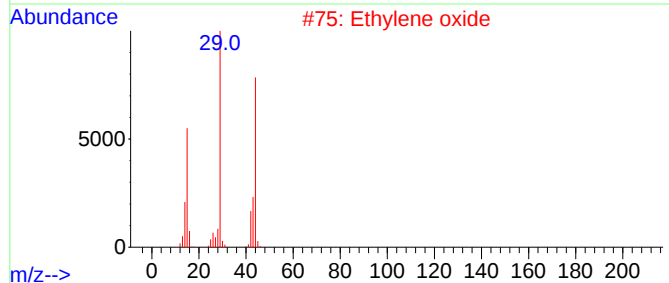
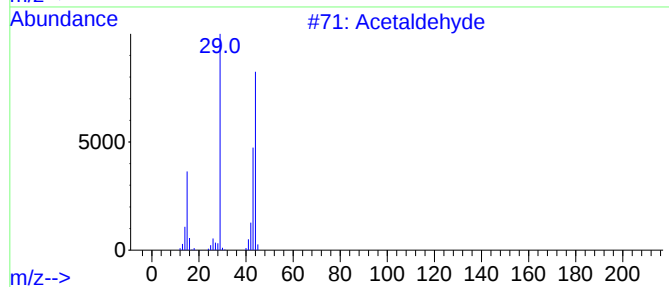
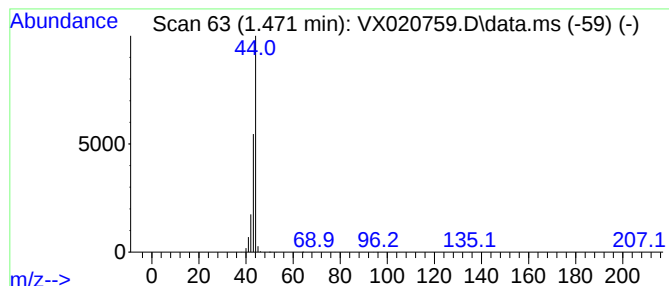
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.471	13.99 ug/l	279641	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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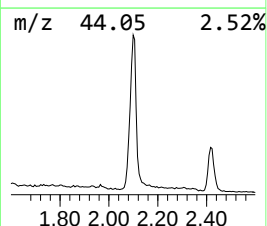
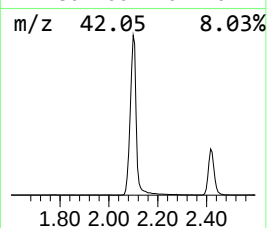
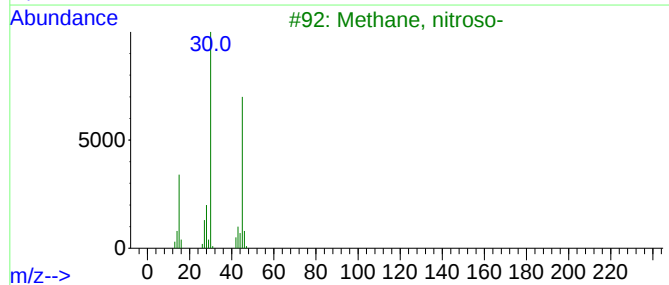
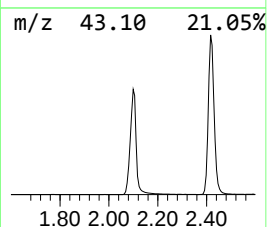
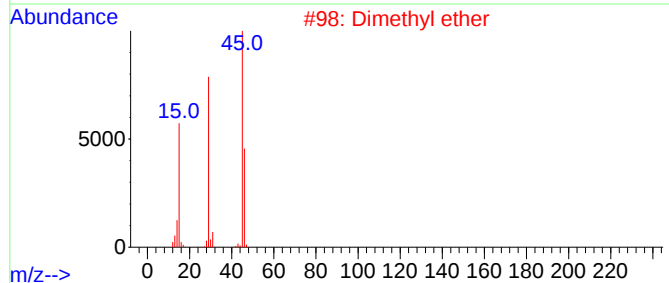
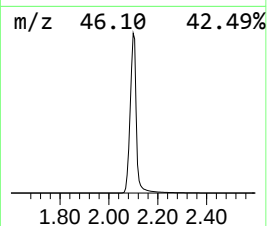
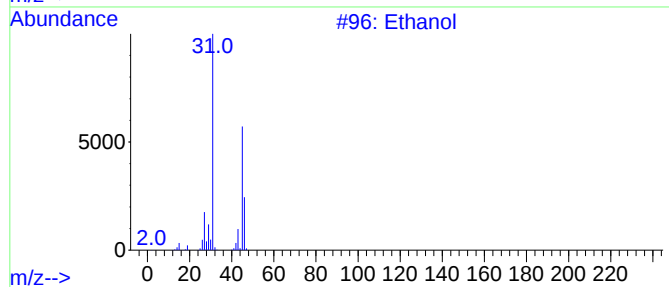
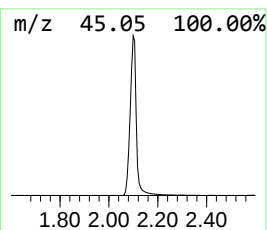
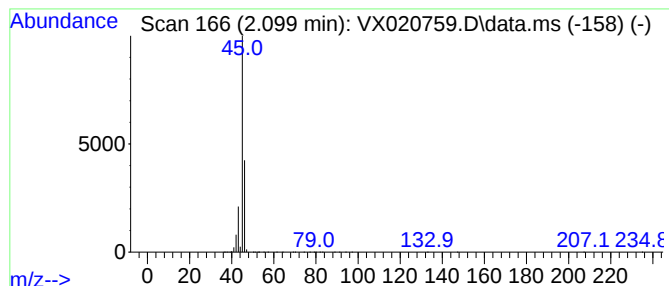
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	363.68 ug/l	7269760	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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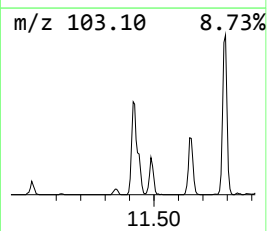
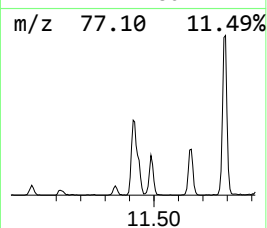
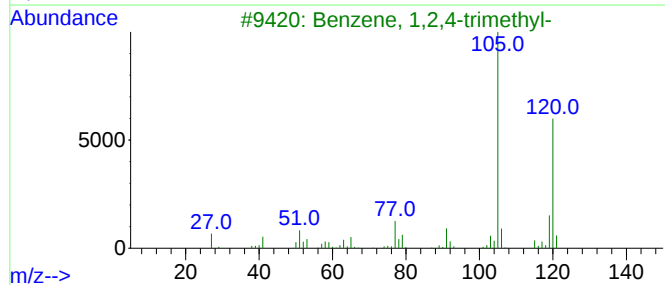
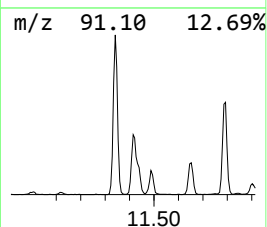
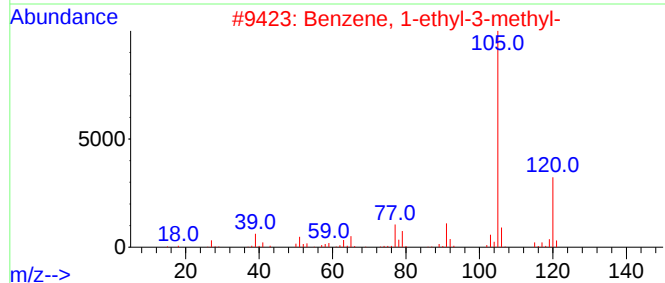
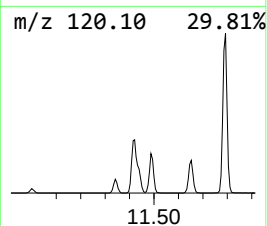
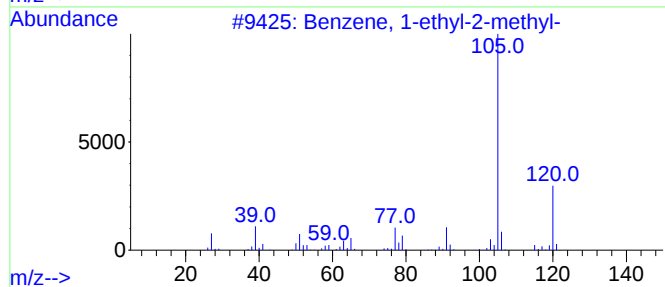
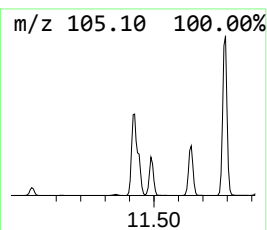
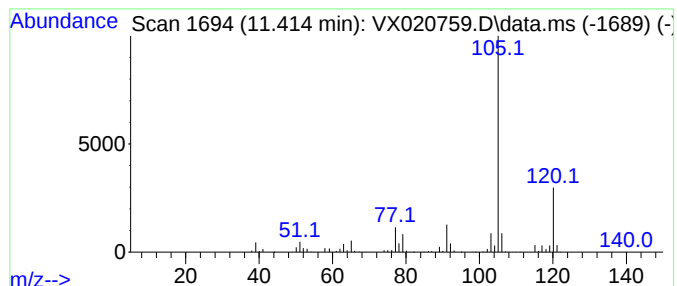
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.414	21.38 ug/l	683573	1,4-Dichlorobenzene-d4	12.061

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	90
5			Mesitylene	120	C9H12	000108-67-8	90



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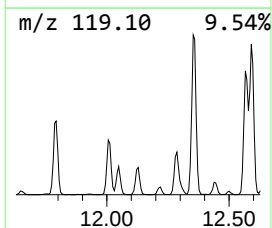
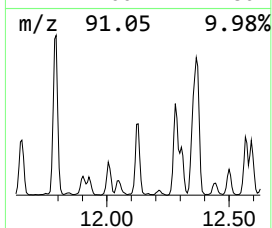
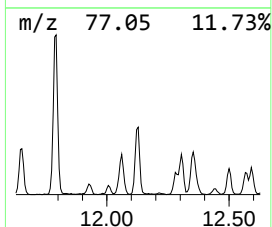
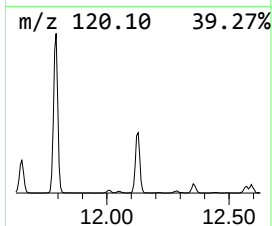
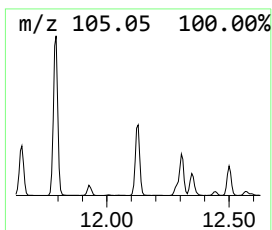
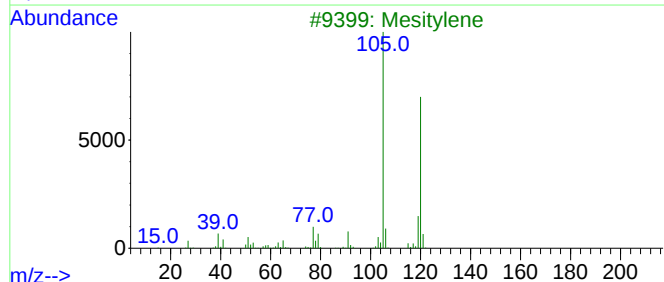
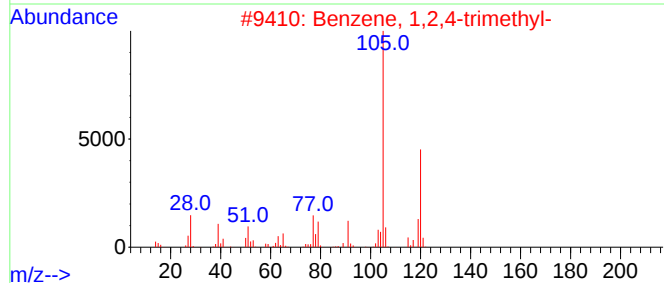
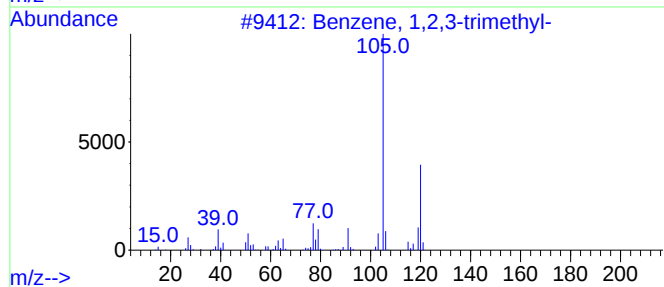
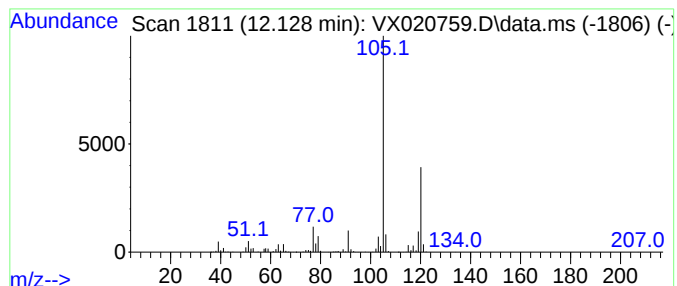
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.128	13.45 ug/l	430155	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3			Mesitylene	120	C9H12	000108-67-8	91
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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41052

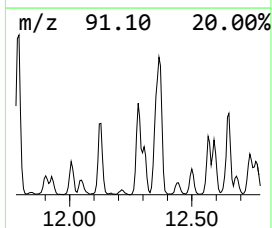
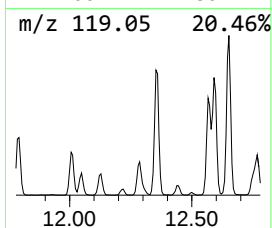
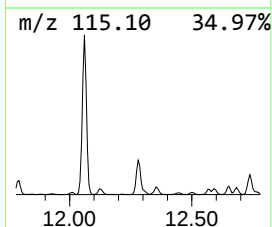
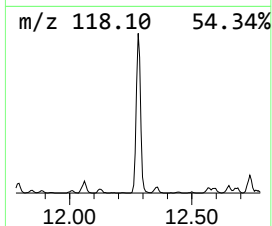
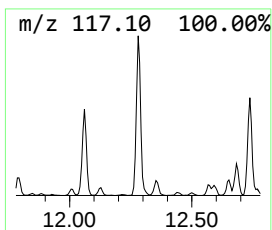
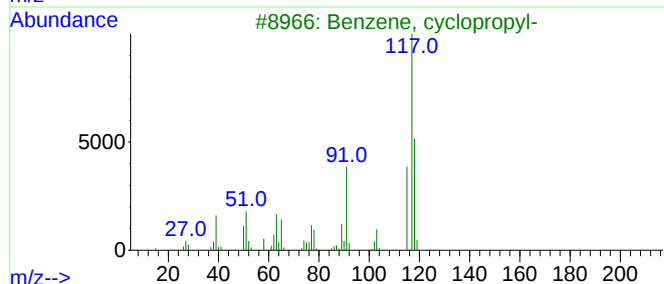
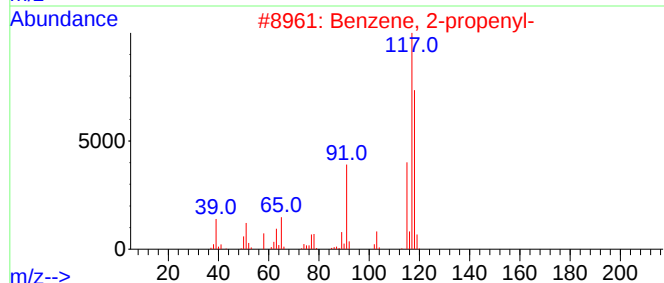
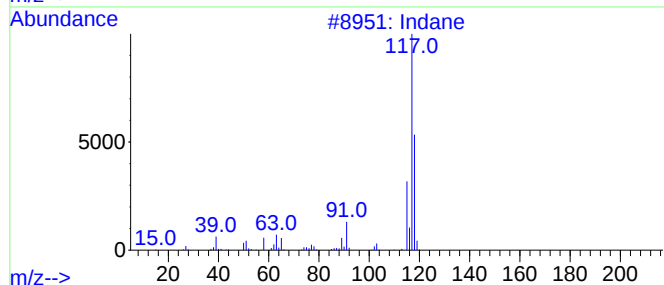
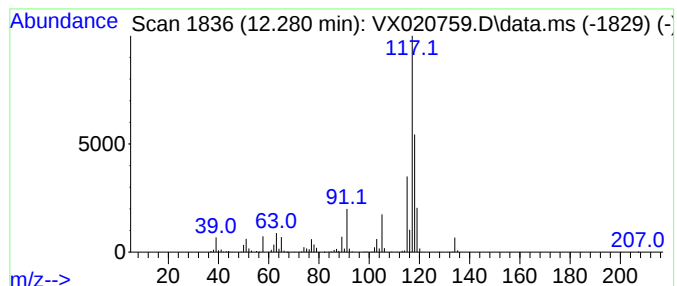
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.280	13.70 ug/l	438043	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	62
5	Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020759.D
Acq On : 26 Jan 2021 17:28
Operator : JC/SP
Sample : M1189-09 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41052

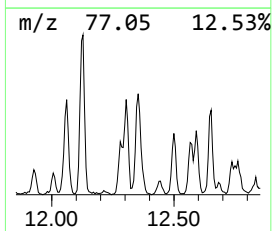
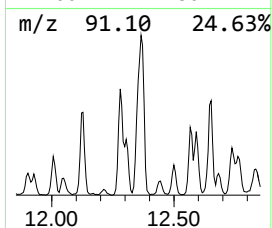
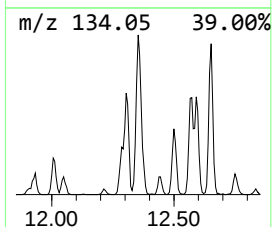
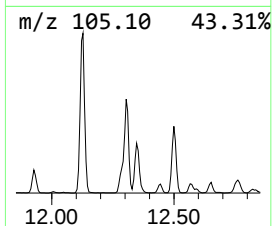
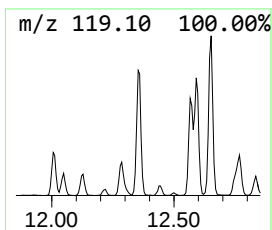
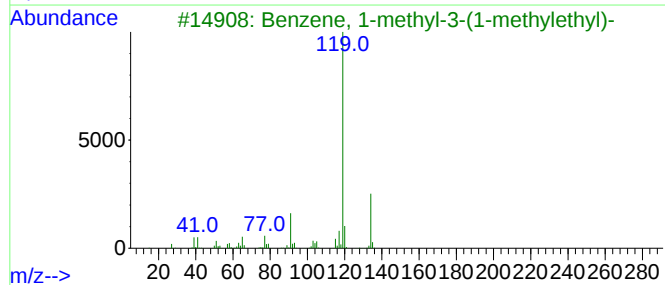
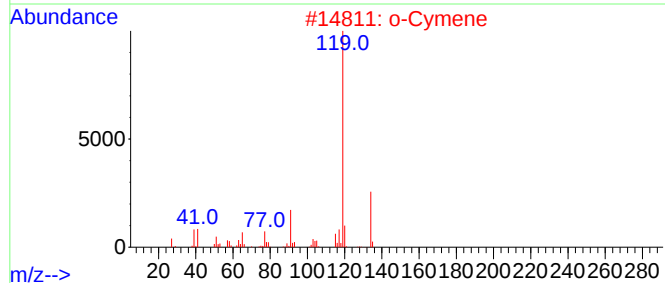
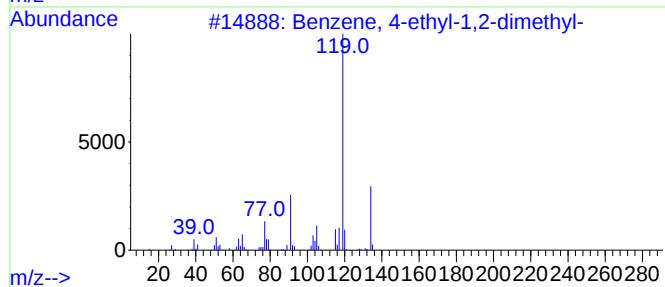
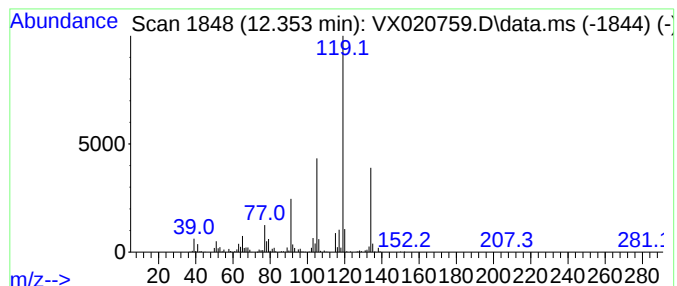
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.353	13.46 ug/l	430343	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020759.D
Acq On : 26 Jan 2021 17:28
Operator : JC/SP
Sample : M1189-09 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41052

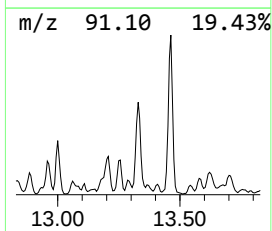
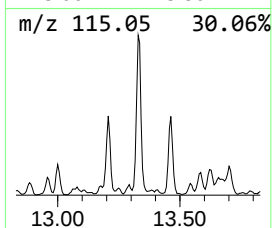
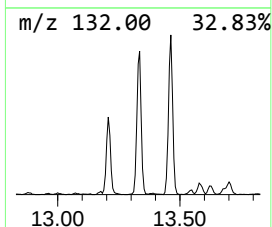
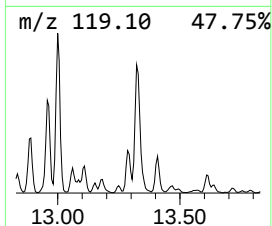
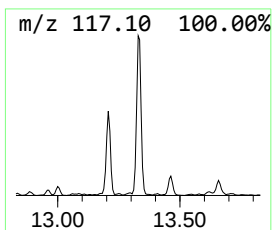
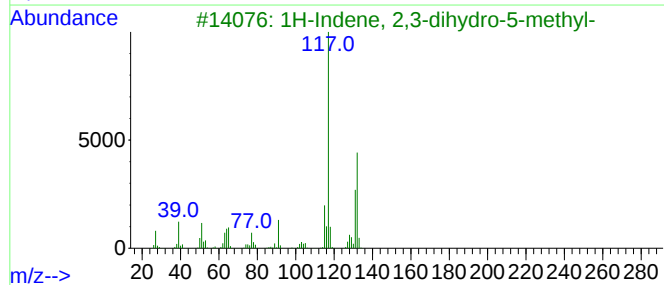
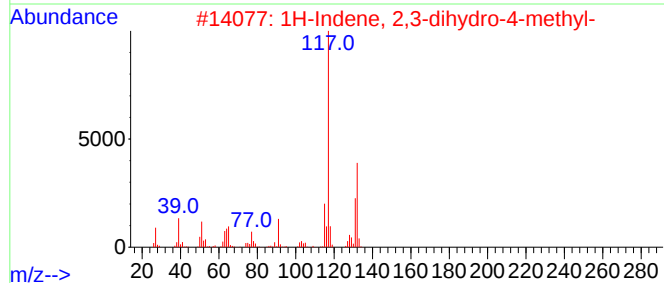
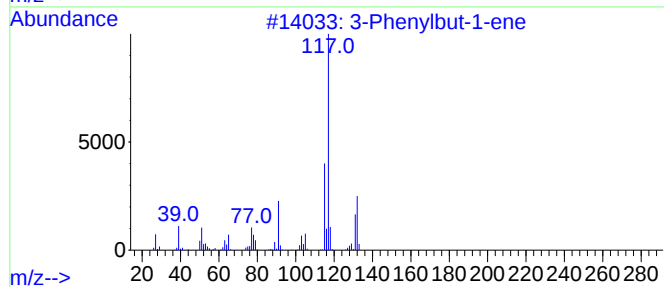
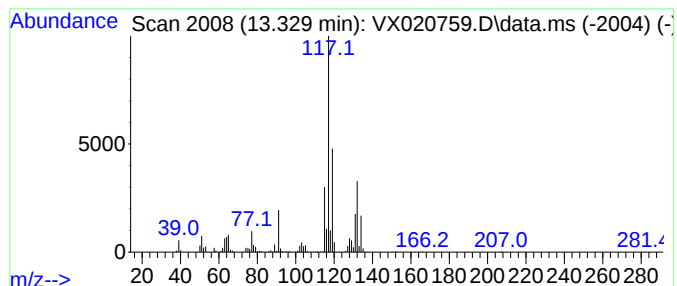
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Quant Title : SW846 8260

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

Peak Number 7 3-Phenylbut-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.329	22.36 ug/l	714932	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
4			Indan, 1-methyl-	132	C10H12	000767-58-8	70
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020759.D
Acq On : 26 Jan 2021 17:28
Operator : JC/SP
Sample : M1189-09 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41052

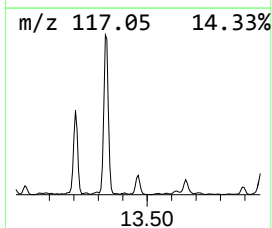
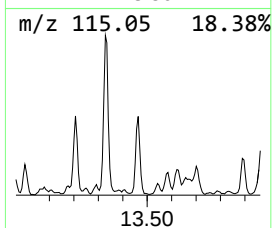
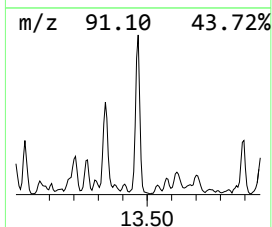
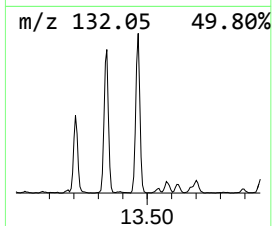
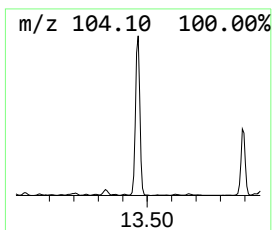
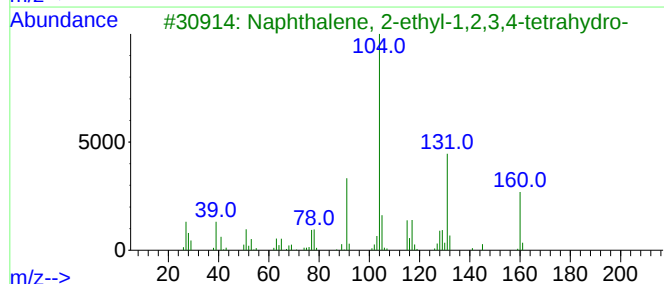
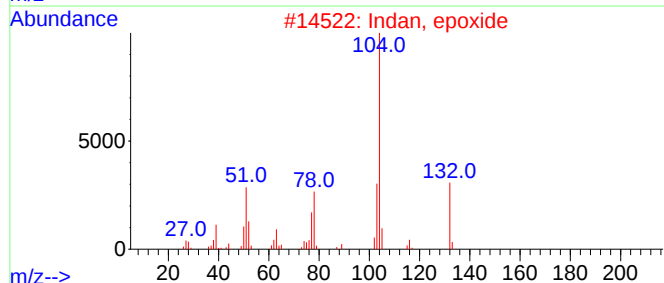
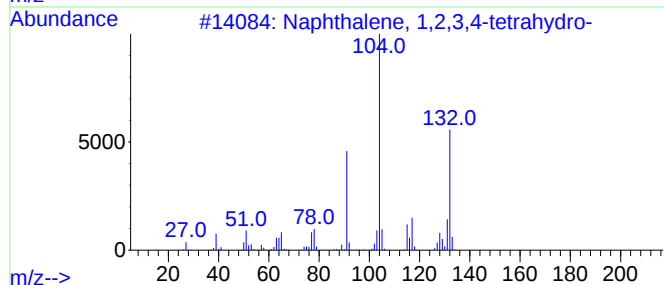
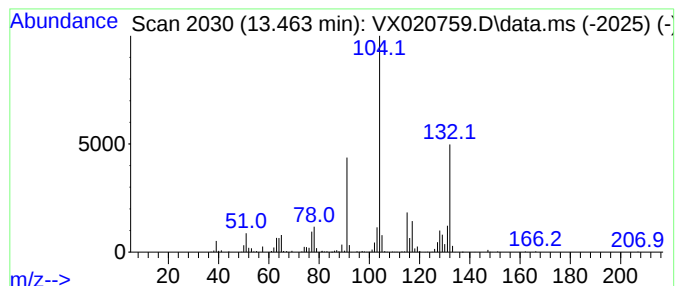
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	18.00 ug/l	575335	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	91
2			Indan, epoxide	132	C9H8O	000768-22-9	58
3			Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	53
4			N-Ethylbenzimidoyl bromide	211	C9H10BrN	041182-87-0	50
5			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020759.D
Acq On : 26 Jan 2021 17:28
Operator : JC/SP
Sample : M1189-09 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41052

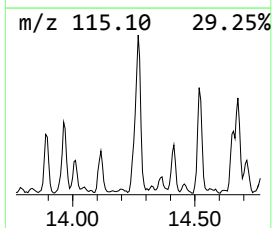
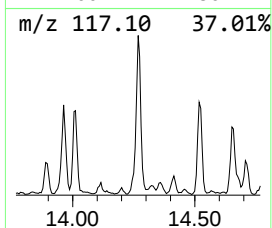
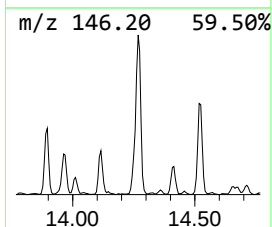
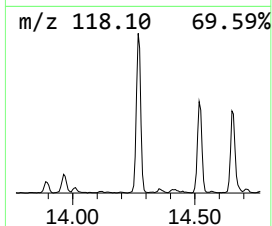
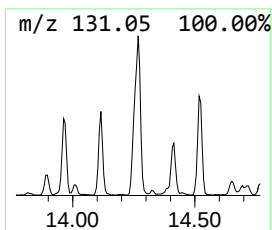
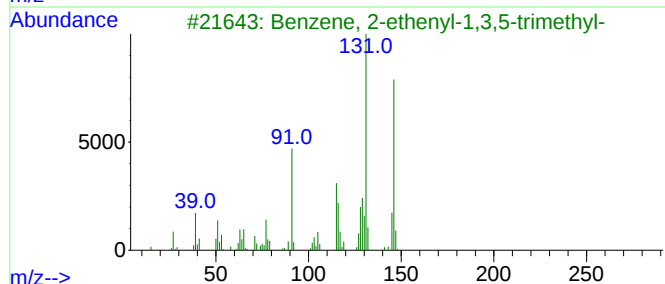
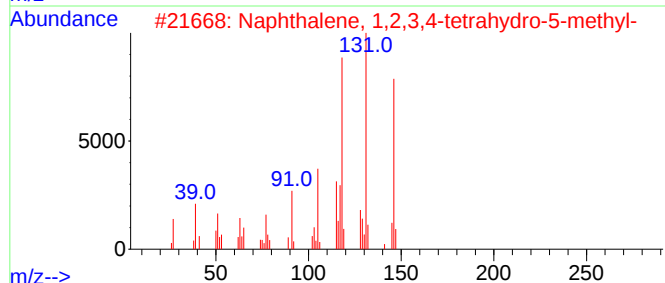
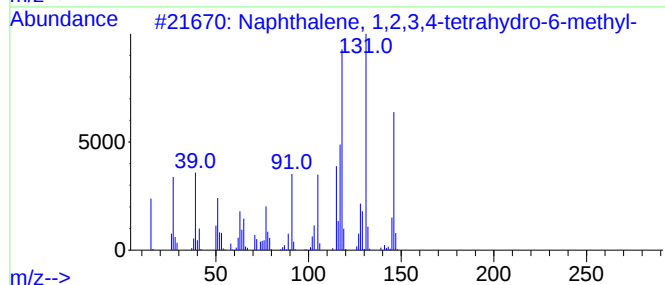
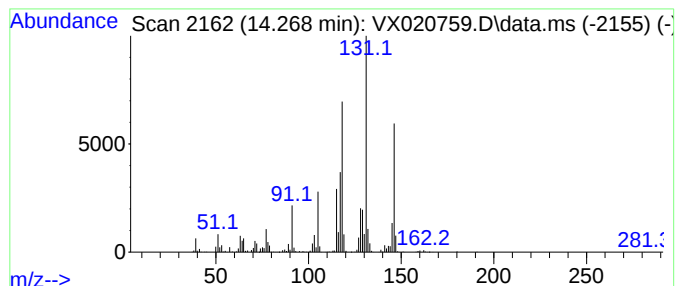
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	23.21 ug/l	742141	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	89
4			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	76
5			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020759.D
Acq On : 26 Jan 2021 17:28
Operator : JC/SP
Sample : M1189-09 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41052

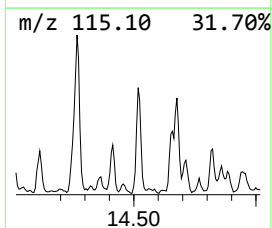
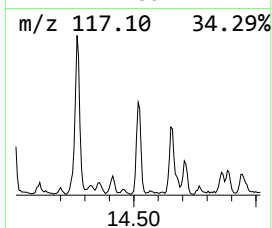
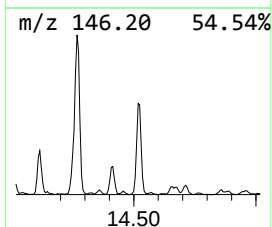
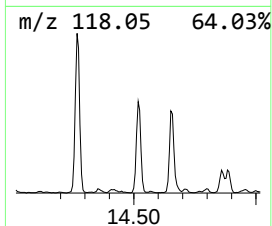
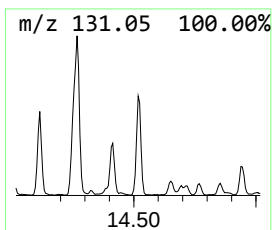
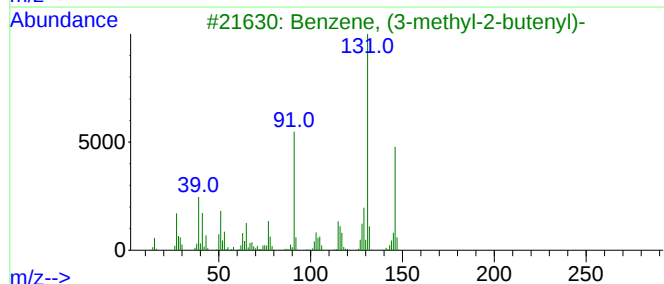
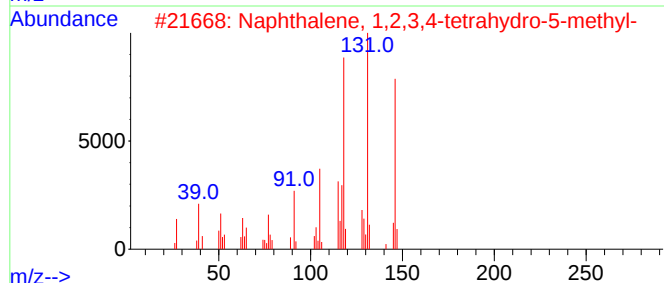
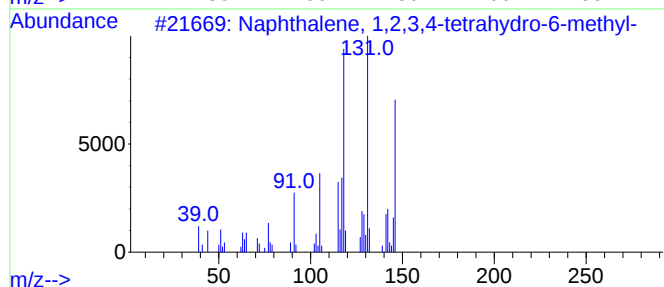
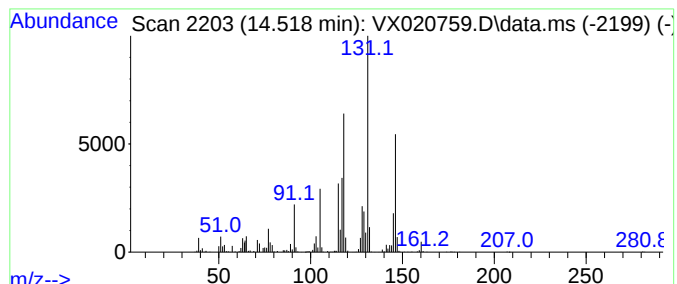
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.518	13.02 ug/l	416392	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	70
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020759.D
Acq On : 26 Jan 2021 17:28
Operator : JC/SP
Sample : M1189-09 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41052

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.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
Acetaldehyde	1.471	14.0	ug/l	279641	1	5.623	999476	50.0
Ethanol	2.099	363.7	ug/l	7269760	1	5.623	999476	50.0
Benzene, 1-ethy...	11.414	21.4	ug/l	683573	4	12.061	1598500	50.0
Benzene, 1,2,3-...	12.128	13.4	ug/l	430155	4	12.061	1598500	50.0
Indane	12.280	13.7	ug/l	438043	4	12.061	1598500	50.0
Benzene, 4-ethy...	12.353	13.5	ug/l	430343	4	12.061	1598500	50.0
3-Phenylbut-1-ene	13.329	22.4	ug/l	714932	4	12.061	1598500	50.0
Naphthalene, 1,...	13.463	18.0	ug/l	575335	4	12.061	1598500	50.0
Naphthalene, 1,...	14.268	23.2	ug/l	742141	4	12.061	1598500	50.0
Naphthalene, 1,...	14.518	13.0	ug/l	416392	4	12.061	1598500	50.0