

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021524\
 Data File : VX040256.D
 Acq On : 15 Feb 2024 16:45
 Operator : JC/MD
 Sample : P1471-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30985

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\82X020924W.M
 Title : SW846 8260

Signal : TIC: VX040256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.050	152	158	170	rBV	29655	51519	7.48%	1.045%
2	2.380	204	212	216	rBV2	4158	7140	1.04%	0.145%
3	5.007	636	643	651	rBV4	6518	19741	2.87%	0.400%
4	5.385	695	705	721	rBV	44985	129709	18.84%	2.631%
5	5.550	721	732	748	rBV	70325	203336	29.53%	4.124%
6	5.958	790	799	813	rBV	48857	129546	18.82%	2.627%
7	6.757	922	930	950	rBV	116713	280212	40.70%	5.683%
8	8.647	1234	1240	1249	rBV	242975	378572	54.98%	7.677%
9	9.275	1332	1343	1348	rBV4	8851	15291	2.22%	0.310%
10	10.055	1465	1471	1486	rVB	261611	356166	51.73%	7.223%
11	10.195	1488	1494	1501	rVV	102685	139858	20.31%	2.836%
12	10.299	1505	1511	1518	rVV	105719	148833	21.62%	3.018%
13	10.640	1561	1567	1578	rBV	255245	334595	48.60%	6.786%
14	10.774	1583	1589	1595	rBV2	5799	9934	1.44%	0.201%
15	11.079	1634	1639	1651	rVB	226910	295528	42.92%	5.993%
16	11.189	1651	1657	1667	rVB7	3848	8900	1.29%	0.180%
17	11.280	1667	1672	1680	rBV2	24017	48432	7.03%	0.982%
18	11.378	1685	1688	1695	rVV	22413	47934	6.96%	0.972%
19	11.451	1695	1700	1707	rVV2	36498	66646	9.68%	1.352%
20	11.512	1707	1710	1716	rVB4	8602	13692	1.99%	0.278%
21	11.610	1722	1726	1734	rVB	34904	48620	7.06%	0.986%
22	11.701	1734	1741	1746	rVV6	14776	28687	4.17%	0.582%
23	11.756	1746	1750	1759	rVB2	16818	32311	4.69%	0.655%
24	11.884	1766	1771	1778	rBV4	28466	46306	6.73%	0.939%
25	11.969	1778	1785	1788	rVV2	89141	132562	19.25%	2.688%
26	12.018	1788	1793	1800	rVV2	312791	456126	66.25%	9.250%
27	12.091	1800	1805	1812	rVV3	56852	103187	14.99%	2.093%
28	12.146	1812	1814	1822	rVB3	12667	17865	2.59%	0.362%
29	12.238	1822	1829	1837	rBV7	21332	55873	8.12%	1.133%
30	12.317	1837	1842	1846	rVV4	8565	14947	2.17%	0.303%
31	12.353	1846	1848	1854	rVB2	12658	15423	2.24%	0.313%
32	12.421	1855	1859	1863	rBV2	10302	12336	1.79%	0.250%
33	12.579	1882	1885	1888	rBV3	11597	14328	2.08%	0.291%
34	12.762	1910	1915	1920	rBV3	10748	18542	2.69%	0.376%
35	12.817	1920	1924	1928	rBV2	9570	11937	1.73%	0.242%
36	13.237	1985	1993	1995	rBV7	4990	7312	1.06%	0.148%

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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37	13.335	1999	2009	2018	rVV	224762	314220	45.64%	6.372%
38	13.426	2018	2024	2031	rVV5	12834	31293	4.55%	0.635%
39	13.487	2031	2034	2041	rVB7	5645	10081	1.46%	0.204%
40	13.591	2047	2051	2060	rVB9	6588	11860	1.72%	0.241%
41	14.067	2126	2129	2136	rBV2	7451	8964	1.30%	0.182%
42	14.134	2136	2140	2146	rBV	19985	28858	4.19%	0.585%
43	14.201	2147	2151	2157	rBV4	11900	25774	3.74%	0.523%
44	14.530	2201	2205	2207	rBV	9545	10259	1.49%	0.208%
45	14.560	2207	2210	2214	rVB	18206	20429	2.97%	0.414%
46	14.701	2226	2233	2235	rBV	22556	31690	4.60%	0.643%
47	14.737	2235	2239	2244	rVV	618298	688508	100.00%	13.963%
48	14.798	2245	2249	2254	rVB4	21640	28505	4.14%	0.578%
49	14.902	2262	2266	2270	rBV4	5741	7992	1.16%	0.162%
50	16.091	2456	2461	2469	rVB5	5566	10557	1.53%	0.214%

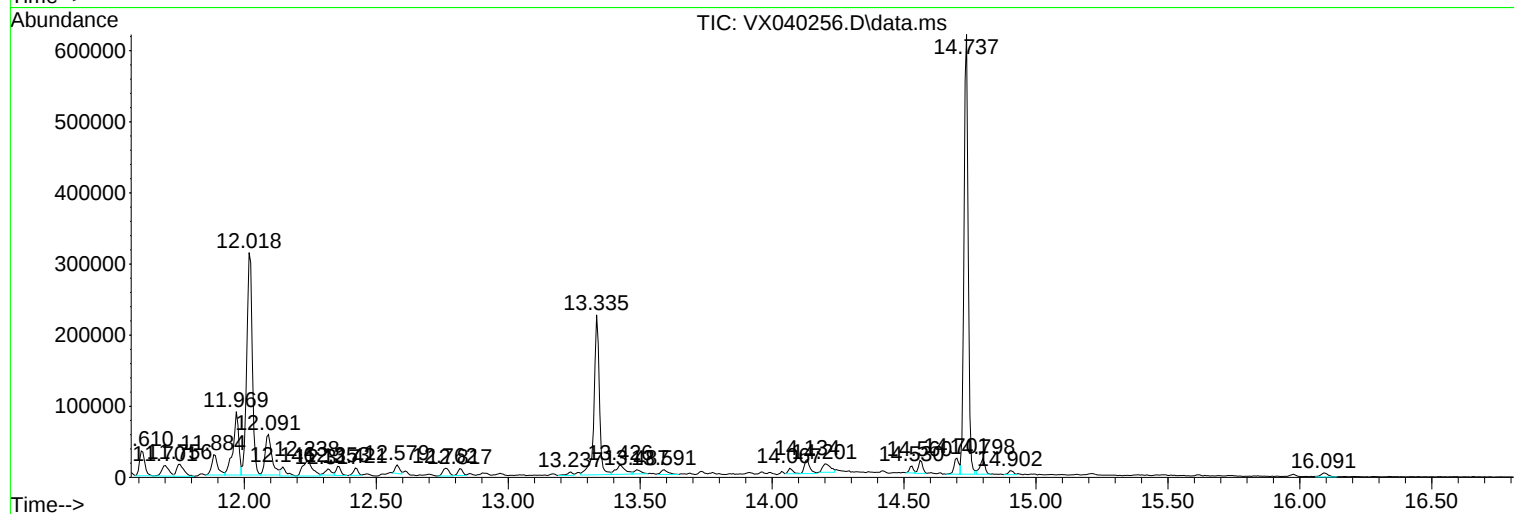
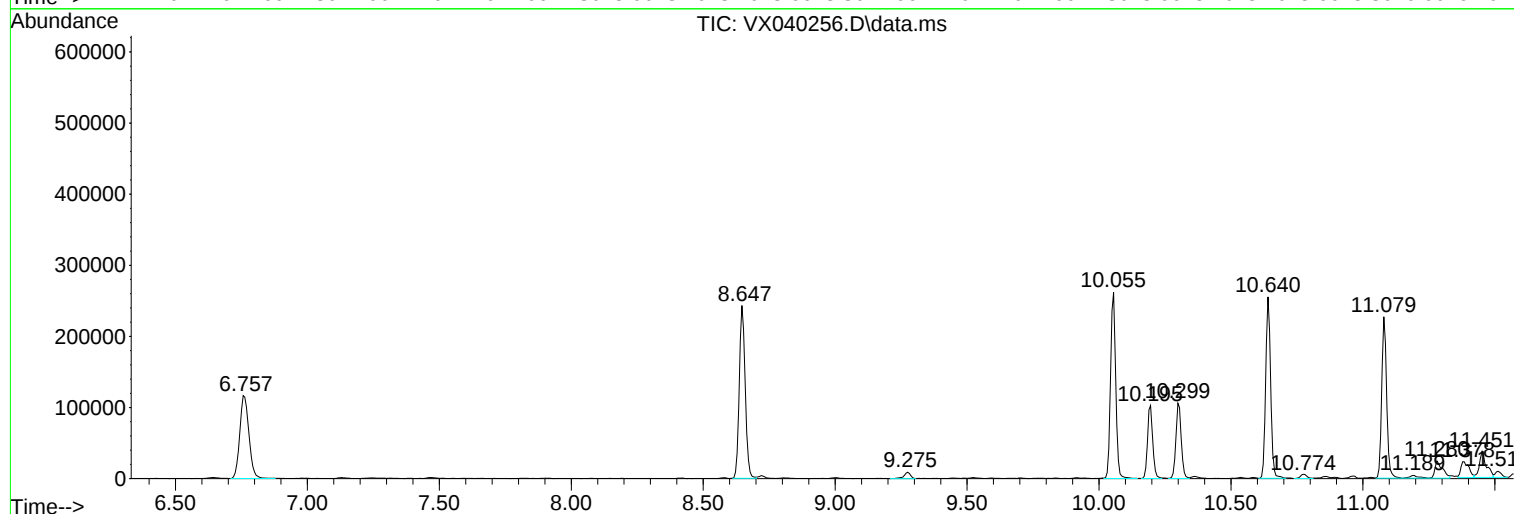
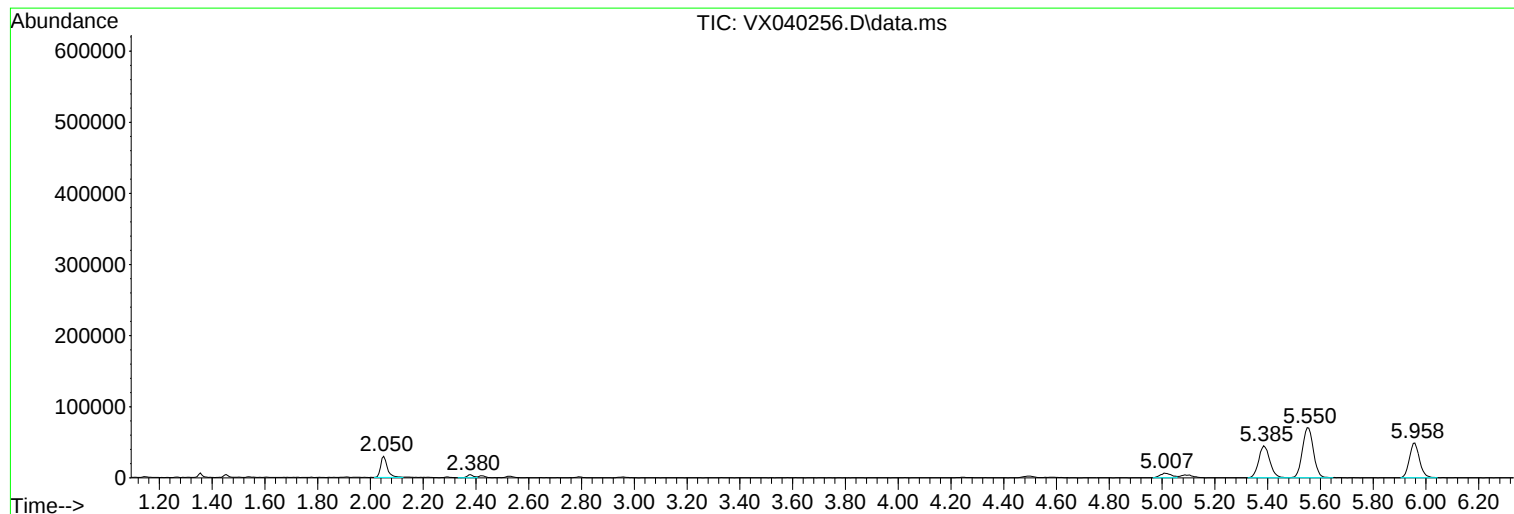
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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



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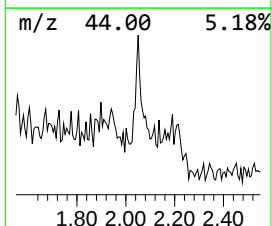
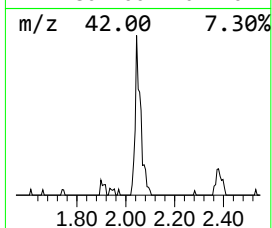
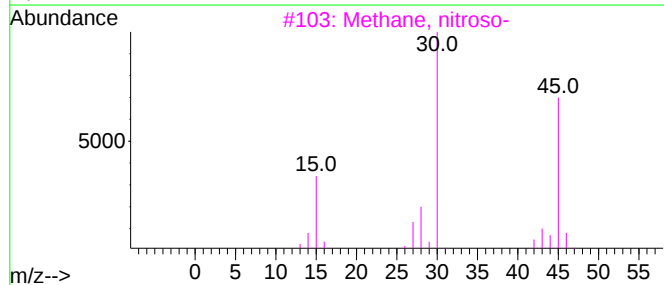
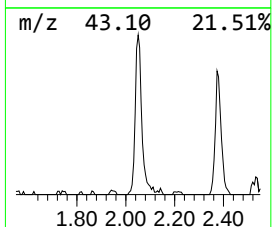
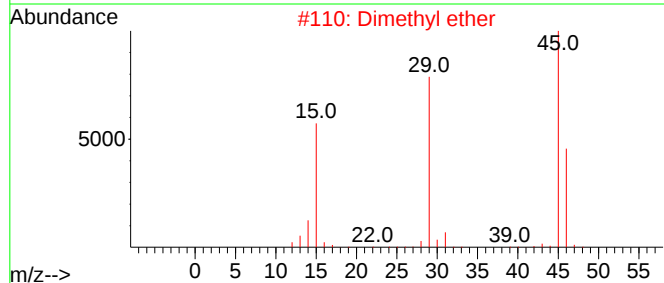
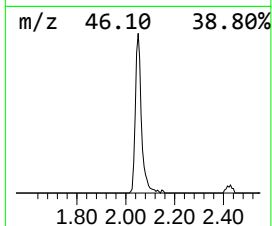
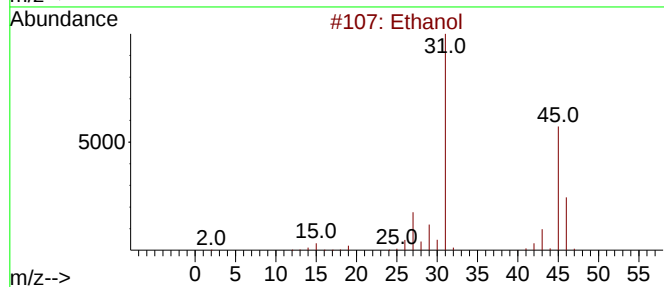
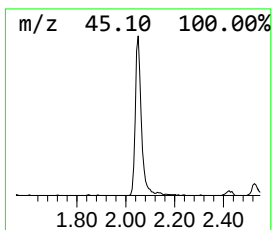
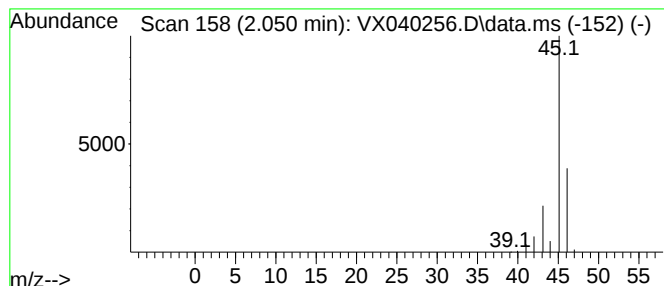
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	12.67 ug/l	51519	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
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			Methyltartronic acid	134	C4H6O5	000595-98-2	2



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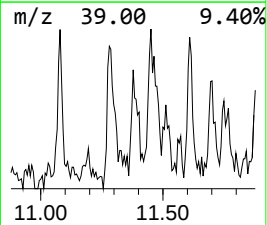
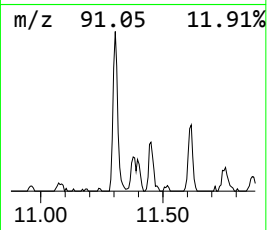
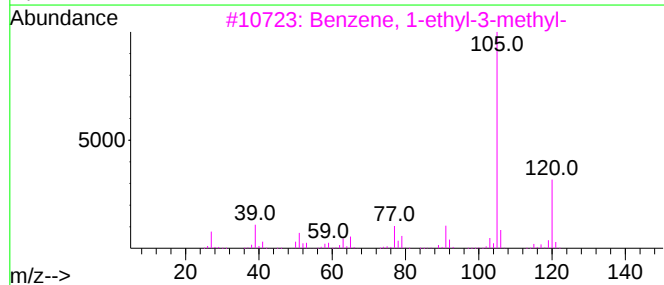
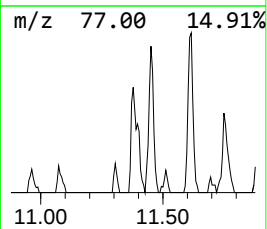
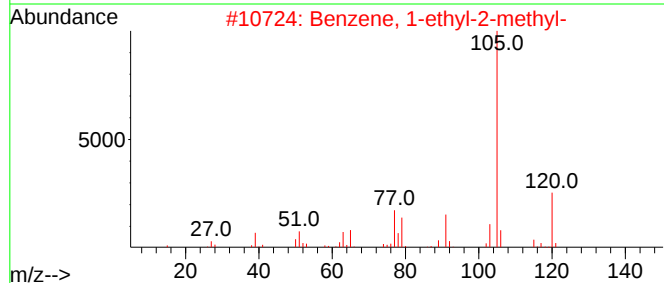
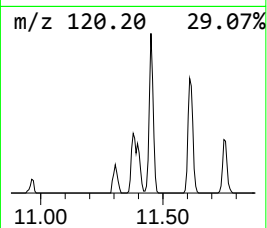
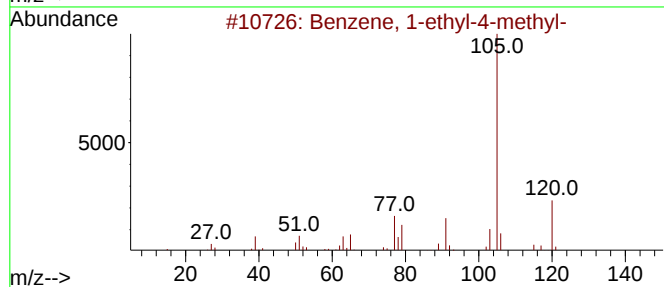
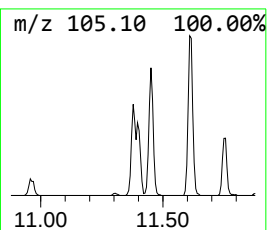
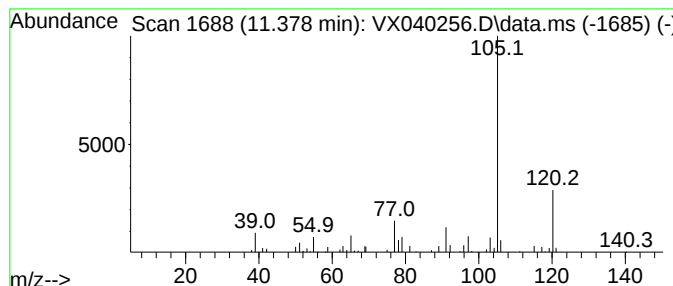
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	5.25 ug/l	47934	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	83
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	81
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	72



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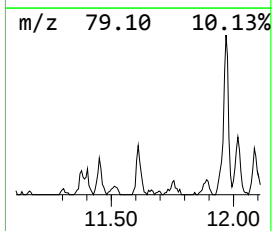
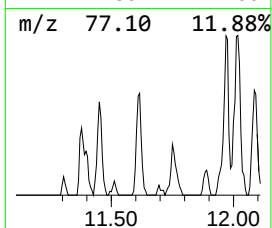
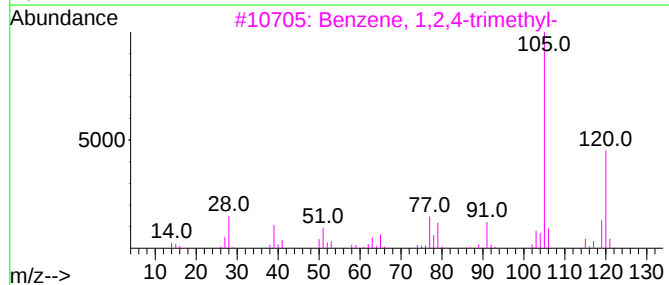
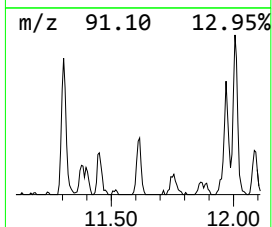
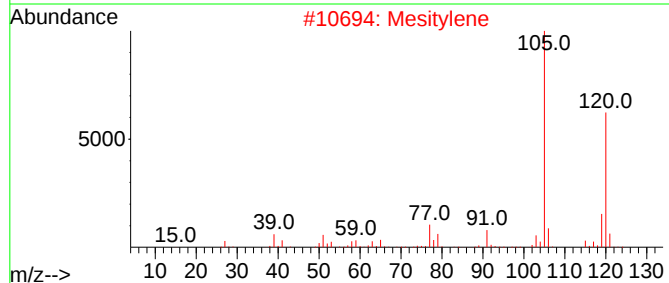
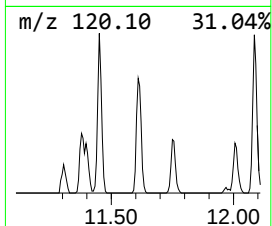
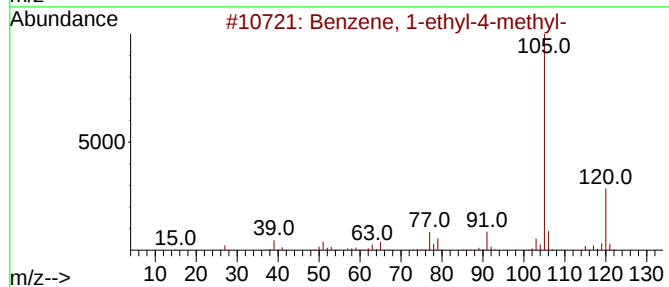
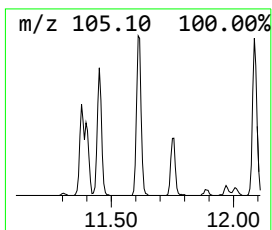
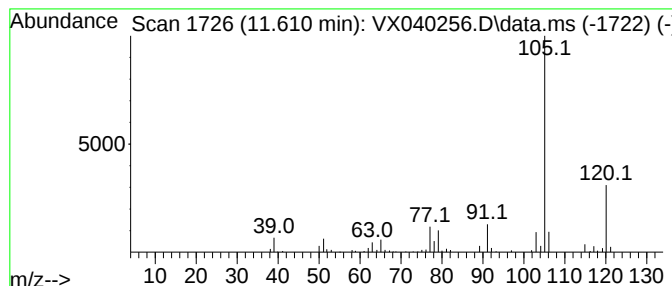
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	5.33 ug/l	48620	1,4-Dichlorobenzene-d4	12.024

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



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Instrument :
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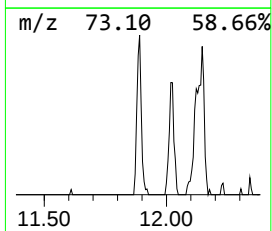
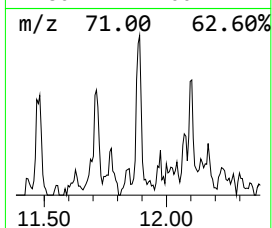
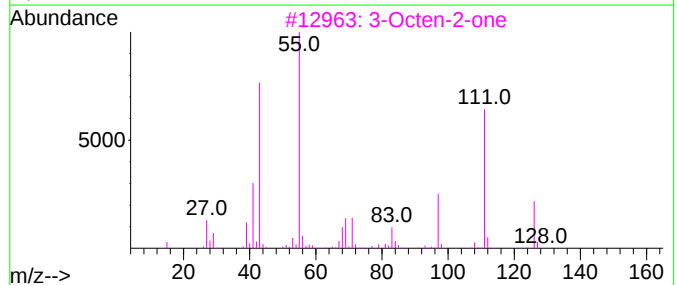
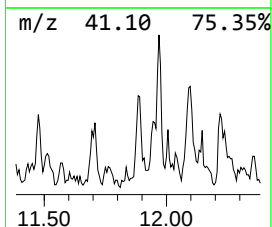
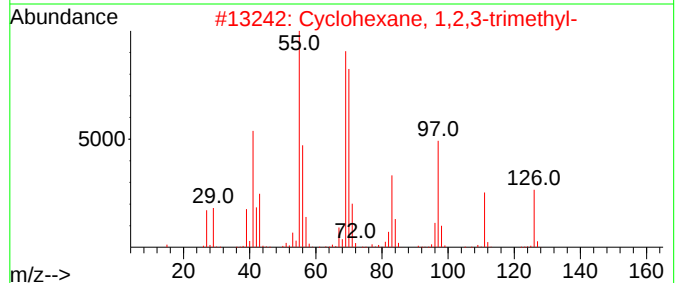
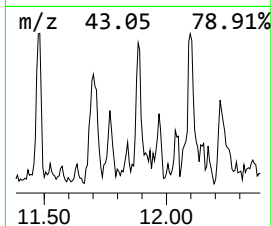
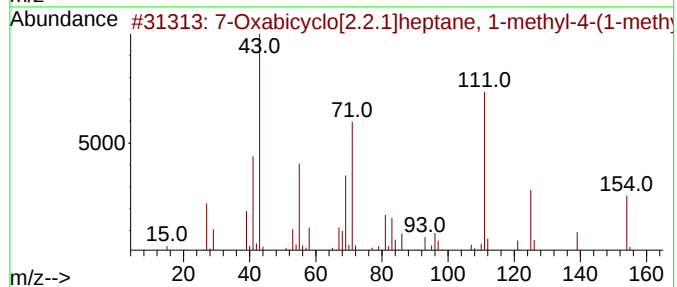
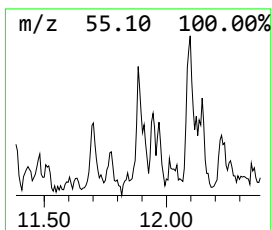
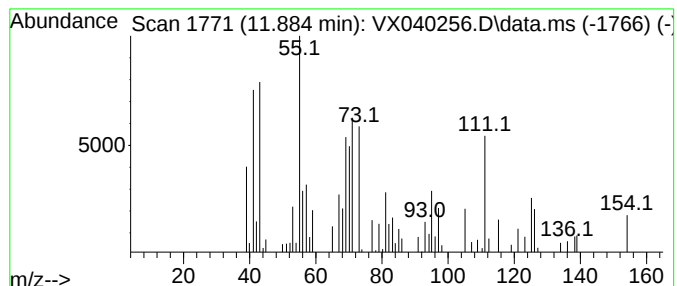
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Quant Title : SW846 8260

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

Peak Number 4 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.884	5.08 ug/l	46306	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	50
2			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	42
3			3-Octen-2-one	126	C8H14O	001669-44-9	25
4			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	18
5			Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001839-88-9	18



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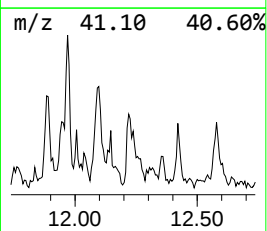
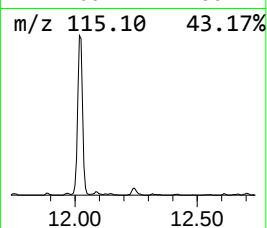
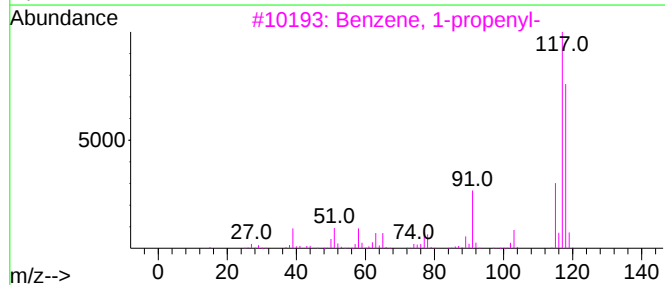
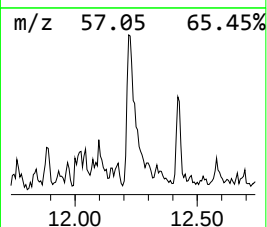
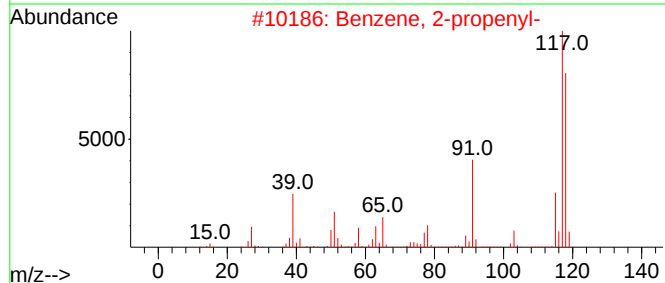
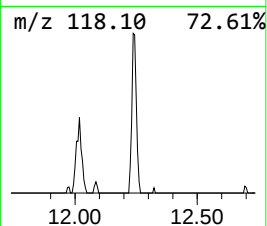
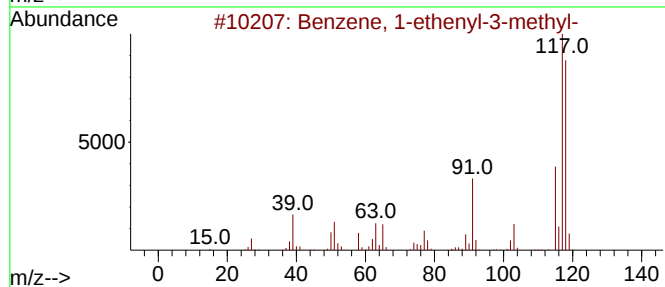
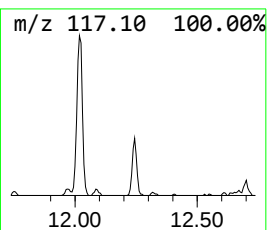
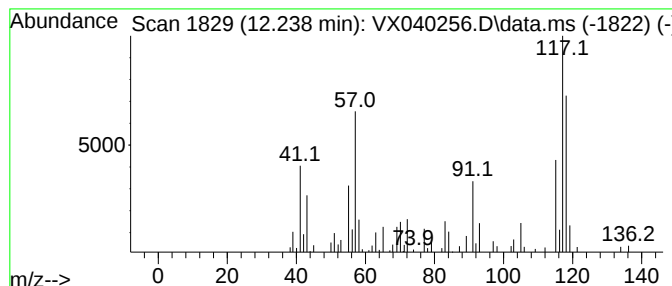
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.238	6.12 ug/l	55873	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	64
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
4			Indane	118	C9H10	000496-11-7	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021524\
Data File : VX040256.D
Acq On : 15 Feb 2024 16:45
Operator : JC/MD
Sample : P1471-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30985

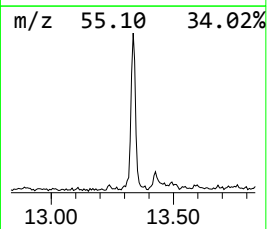
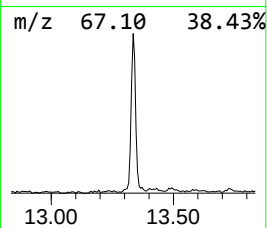
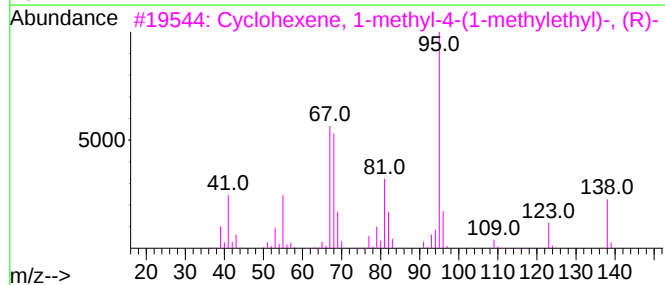
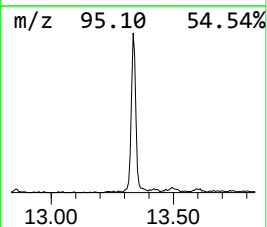
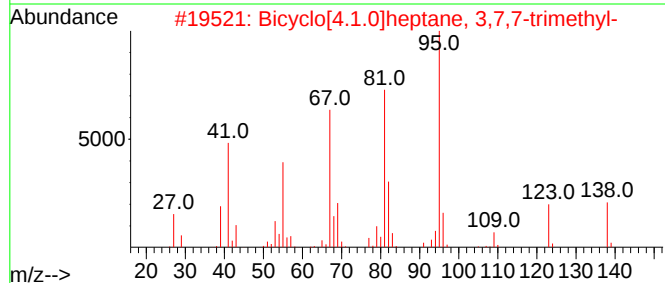
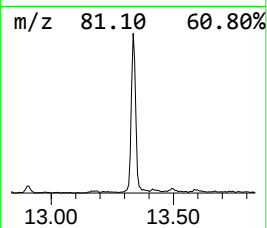
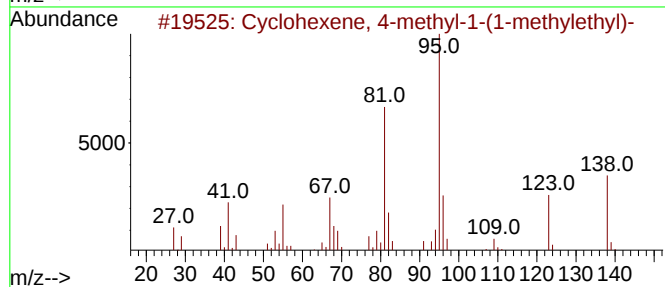
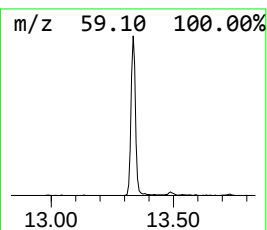
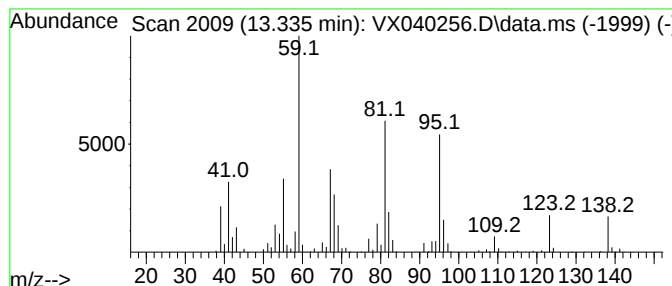
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexene, 4-methyl-1-(1-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	34.44 ug/l	314220	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	89
2			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	55
3			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	001195-31-9	55
4			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	50
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021524\
Data File : VX040256.D
Acq On : 15 Feb 2024 16:45
Operator : JC/MD
Sample : P1471-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30985

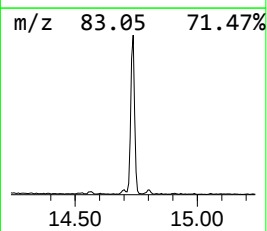
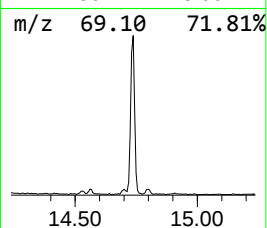
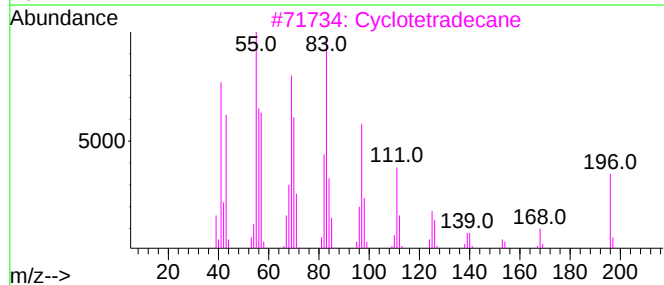
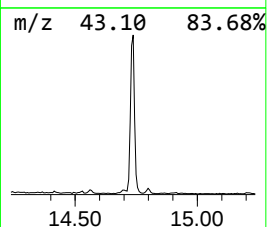
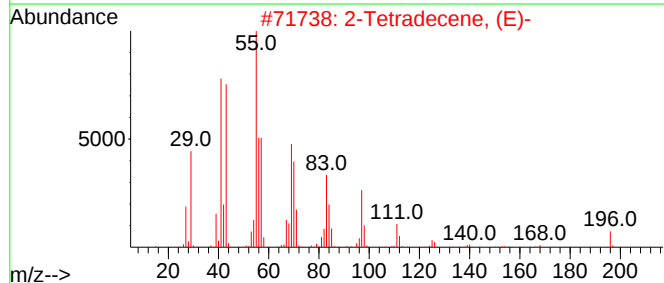
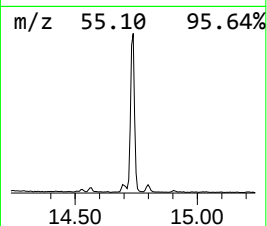
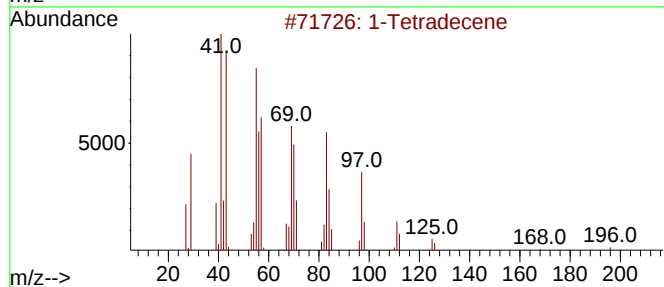
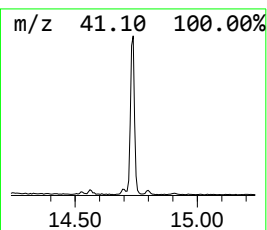
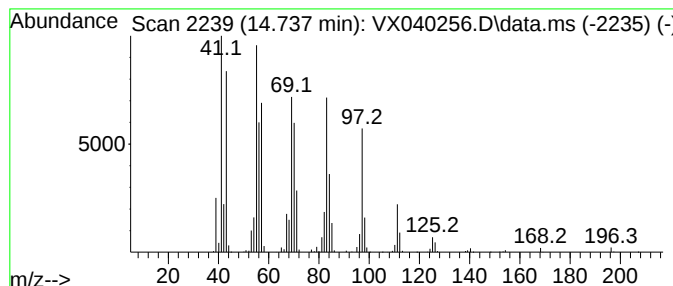
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Tetradecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.737	75.47 ug/l	688508	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetradecene	196	C14H28	001120-36-1	98
2			2-Tetradecene, (E)-	196	C14H28	035953-54-9	96
3			Cyclotetradecane	196	C14H28	000295-17-0	93
4			5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5			Cetene	224	C16H32	000629-73-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021524\
Data File : VX040256.D
Acq On : 15 Feb 2024 16:45
Operator : JC/MD
Sample : P1471-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.050	12.7	ug/l	51519	1	5.550	203336	50.0
Benzene, 1-ethy...	11.378	5.3	ug/l	47934	4	12.024	456126	50.0
Benzene, 1-ethy...	11.610	5.3	ug/l	48620	4	12.024	456126	50.0
7-Oxabicyclo[2....	11.884	5.1	ug/l	46306	4	12.024	456126	50.0
Benzene, 2-prop...	12.238	6.1	ug/l	55873	4	12.024	456126	50.0
Cyclohexene, 4-...	13.335	34.4	ug/l	314220	4	12.024	456126	50.0
1-Tetradecene	14.737	75.5	ug/l	688508	4	12.024	456126	50.0