

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
 Data File : VX040069.D
 Acq On : 01 Feb 2024 14:24
 Operator : JC/MD
 Sample : P1312-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NWB-1999

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\82X013024W.M
 Title : SW846 8260

Signal : TIC: VX040069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	70	rVB	29772	35391	7.03%	0.537%
2	1.557	70	77	85	rVB	5353	9348	1.86%	0.142%
3	2.050	153	158	171	rBV	158785	258929	51.46%	3.931%
4	2.380	206	212	218	rBV2	3502	6491	1.29%	0.099%
5	5.385	692	705	719	rBV	60360	178658	35.51%	2.712%
6	5.550	723	732	750	rVB2	97920	280388	55.72%	4.257%
7	5.958	789	799	807	rBV	70019	188375	37.44%	2.860%
8	6.038	807	812	827	rVB3	10999	30189	6.00%	0.458%
9	6.757	918	930	943	rBV	158915	384594	76.43%	5.839%
10	8.647	1233	1240	1246	rBV	323244	503168	100.00%	7.639%
11	8.720	1246	1252	1271	rVB	126821	207876	41.31%	3.156%
12	9.531	1375	1385	1388	rBV4	2921	5749	1.14%	0.087%
13	10.055	1465	1471	1481	rBV	350443	492686	97.92%	7.480%
14	10.195	1488	1494	1502	rBV	59273	79246	15.75%	1.203%
15	10.299	1505	1511	1519	rBV	236900	320361	63.67%	4.864%
16	10.640	1562	1567	1576	rBV	121983	158059	31.41%	2.400%
17	10.964	1615	1620	1623	rBV	7069	9469	1.88%	0.144%
18	10.994	1623	1625	1634	rVV	5422	9264	1.84%	0.141%
19	11.079	1634	1639	1650	rVB	305576	388628	77.24%	5.900%
20	11.305	1671	1676	1683	rBV	39026	51456	10.23%	0.781%
21	11.378	1683	1688	1696	rVV	180646	322833	64.16%	4.901%
22	11.451	1696	1700	1711	rVB	94713	118590	23.57%	1.800%
23	11.610	1721	1726	1734	rVB	80615	103807	20.63%	1.576%
24	11.750	1744	1749	1757	rVB	367623	440853	87.62%	6.693%
25	11.890	1769	1772	1776	rVB	7199	7525	1.50%	0.114%
26	11.969	1781	1785	1788	rVV	13459	15860	3.15%	0.241%
27	12.018	1788	1793	1800	rVV	388251	502472	99.86%	7.628%
28	12.085	1800	1804	1811	rVB	111983	138790	27.58%	2.107%
29	12.244	1822	1830	1832	rBV	82100	114272	22.71%	1.735%
30	12.268	1832	1834	1838	rVV	53380	60081	11.94%	0.912%
31	12.317	1838	1842	1849	rVV4	76429	118228	23.50%	1.795%
32	12.402	1853	1856	1862	rVV4	6707	12008	2.39%	0.182%
33	12.463	1862	1866	1872	rVV	23752	28282	5.62%	0.429%
34	12.530	1872	1877	1879	rVV	46594	57432	11.41%	0.872%
35	12.555	1879	1881	1886	rVV	41050	44481	8.84%	0.675%
36	12.610	1886	1890	1894	rVV	69642	87063	17.30%	1.322%

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Instrument :
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ClientSampleId :
NWB-1999

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

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Title : SW846 8260

37	12.640	1894	1895	1900	rVV2	5090	5544	1.10%	0.084%
38	12.701	1900	1905	1914	rVB4	14933	33309	6.62%	0.506%
39	12.847	1925	1929	1935	rBV	21181	28385	5.64%	0.431%
40	12.920	1935	1941	1944	rVV	46348	55182	10.97%	0.838%
41	12.963	1944	1948	1954	rVB	74734	89452	17.78%	1.358%
42	13.024	1954	1958	1960	rBV2	4847	7219	1.43%	0.110%
43	13.164	1974	1981	1986	rVV2	33362	47044	9.35%	0.714%
44	13.292	1997	2002	2007	rVV2	78316	117417	23.34%	1.783%
45	13.341	2007	2010	2012	rVV4	7083	9570	1.90%	0.145%
46	13.372	2012	2015	2019	rVV	7115	8953	1.78%	0.136%
47	13.420	2019	2023	2032	rVB	28711	38861	7.72%	0.590%
48	13.506	2032	2037	2040	rBV3	3996	6617	1.32%	0.100%
49	13.542	2040	2043	2046	rVV	5801	8053	1.60%	0.122%
50	13.579	2046	2049	2056	rVV3	15702	30308	6.02%	0.460%
51	13.670	2060	2064	2069	rVB4	8499	15501	3.08%	0.235%
52	13.774	2076	2081	2088	rVB	86666	113101	22.48%	1.717%
53	13.853	2088	2094	2099	rVB5	10108	15961	3.17%	0.242%
54	13.926	2099	2106	2110	rBV3	12160	19014	3.78%	0.289%
55	13.969	2110	2113	2117	rVB3	4023	5083	1.01%	0.077%
56	14.073	2127	2130	2134	rVB	10893	12531	2.49%	0.190%
57	14.225	2147	2155	2162	rVB	26653	45004	8.94%	0.683%
58	14.323	2167	2171	2174	rBV3	5005	6140	1.22%	0.093%
59	14.371	2175	2179	2183	rBV2	8363	10065	2.00%	0.153%
60	14.481	2191	2197	2203	rBV3	16586	24174	4.80%	0.367%
61	14.615	2214	2219	2220	rBV2	9052	11434	2.27%	0.174%
62	14.640	2220	2223	2226	rVV2	17313	23049	4.58%	0.350%
63	14.780	2243	2246	2249	rVB	6617	7006	1.39%	0.106%
64	15.182	2307	2312	2315	rBV3	6218	10383	2.06%	0.158%
65	15.487	2354	2362	2366	rBV5	7116	11592	2.30%	0.176%

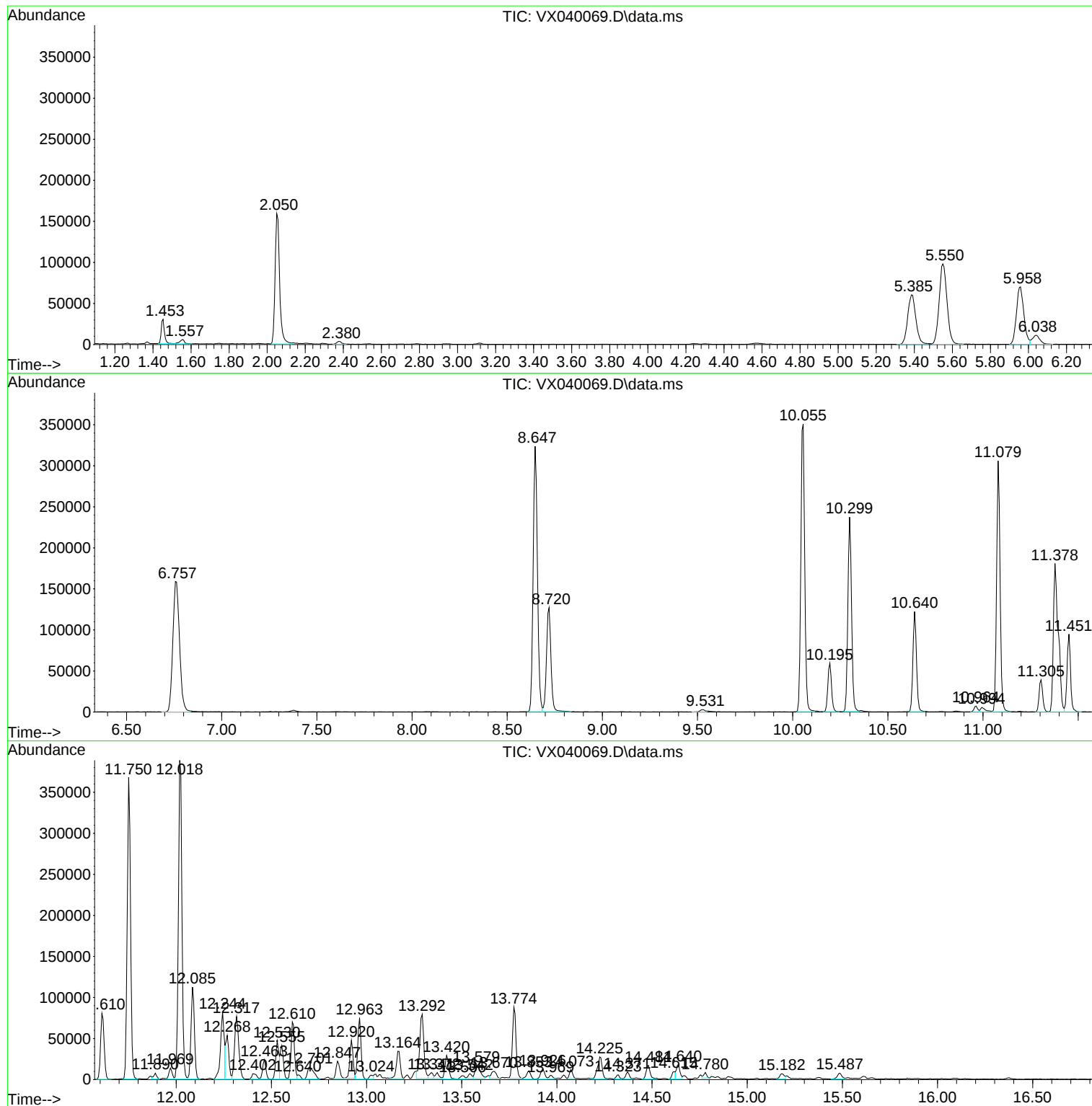
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ClientSampleId :
NWB-1999

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX000124\
Data File : VX040069.D
Acq On : 01 Feb 2024 14:24
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

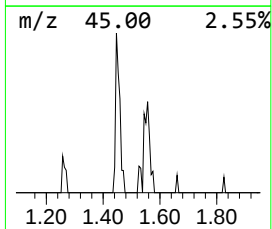
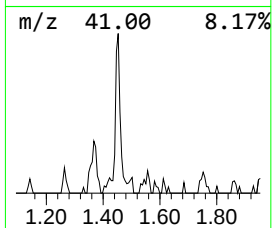
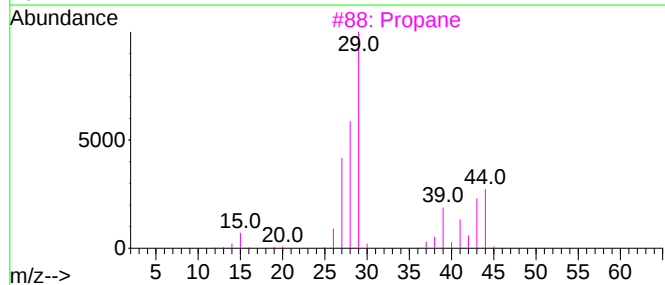
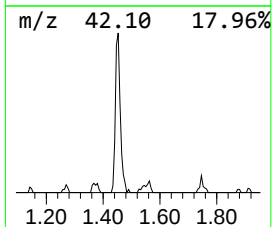
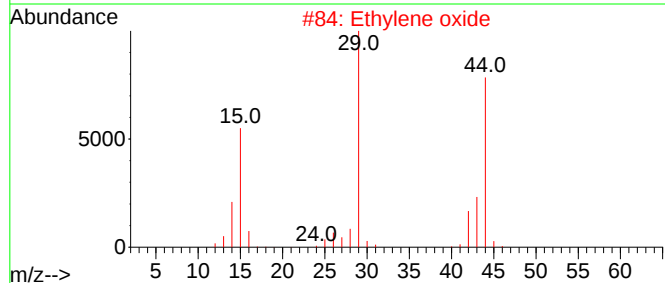
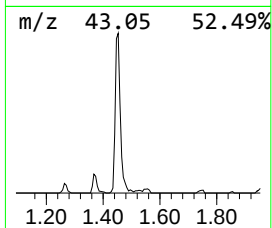
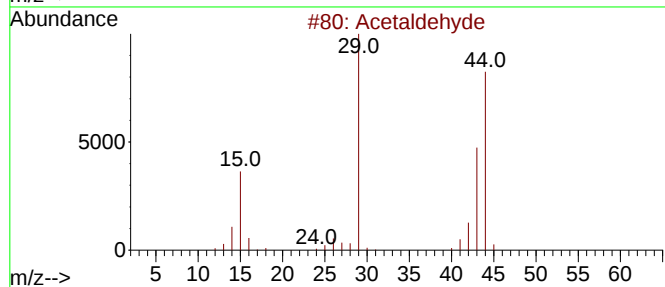
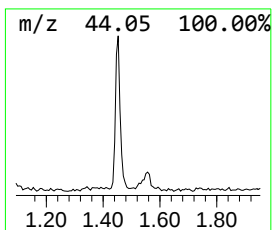
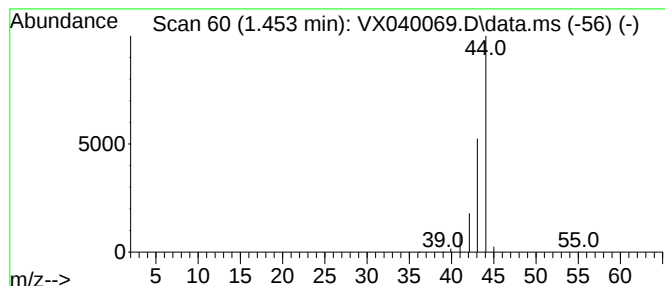
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	6.31 ug/l	35391	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
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			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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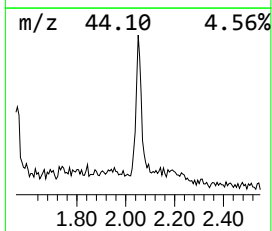
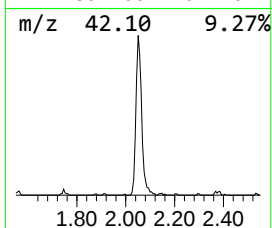
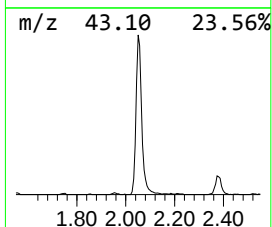
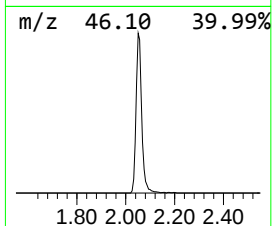
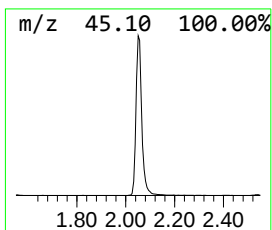
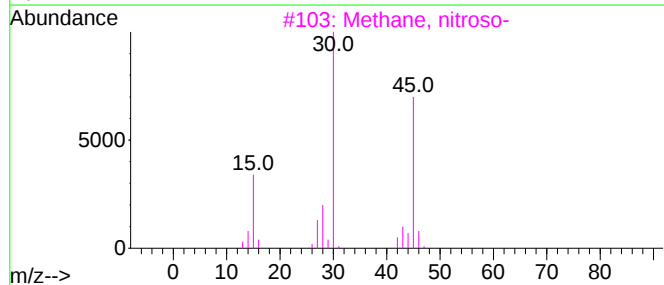
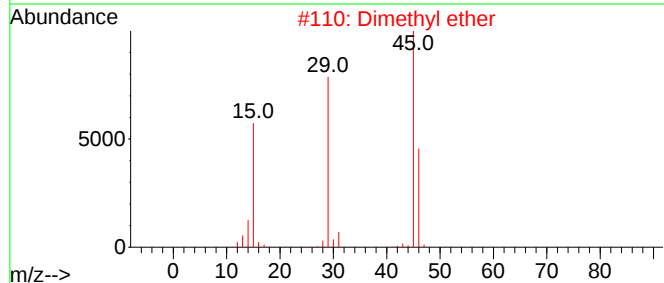
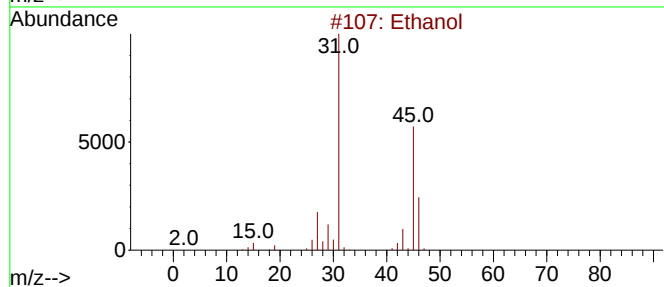
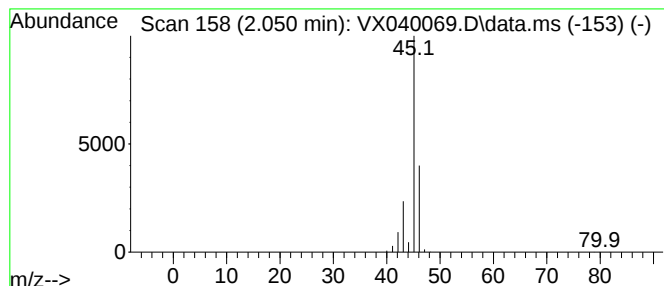
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	46.17 ug/l	258929	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
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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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

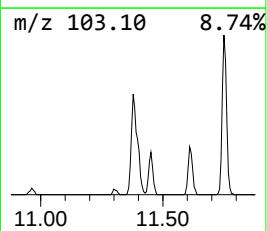
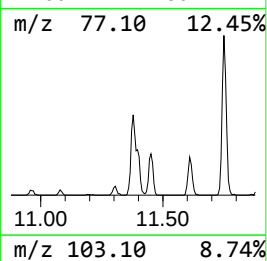
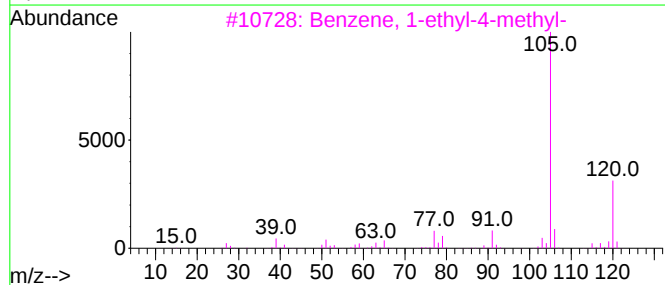
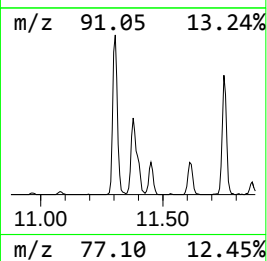
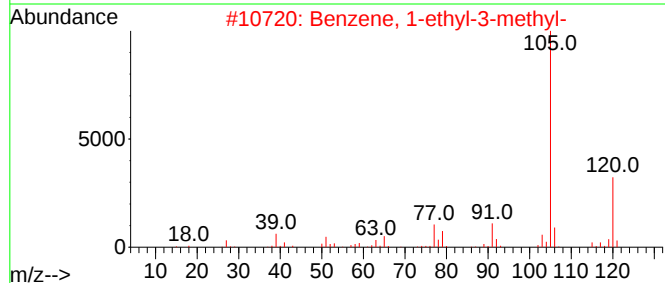
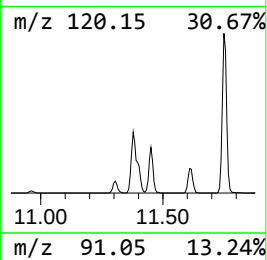
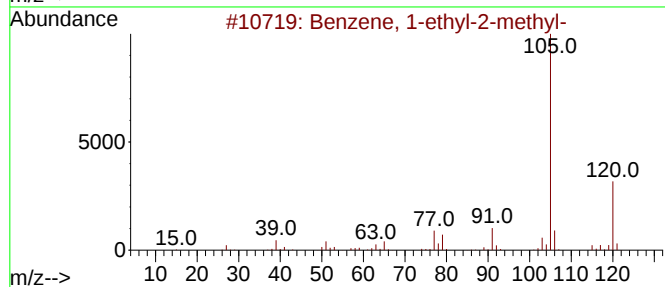
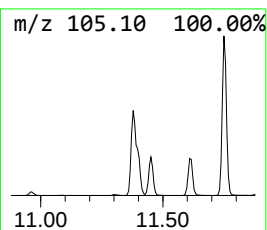
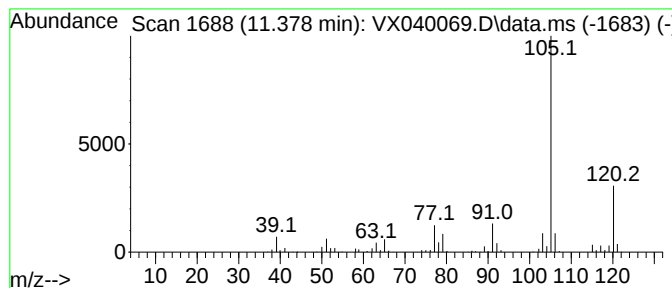
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	32.12 ug/l	322833	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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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Instrument :
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ClientSampleId :
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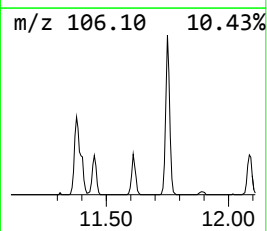
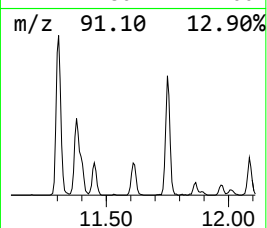
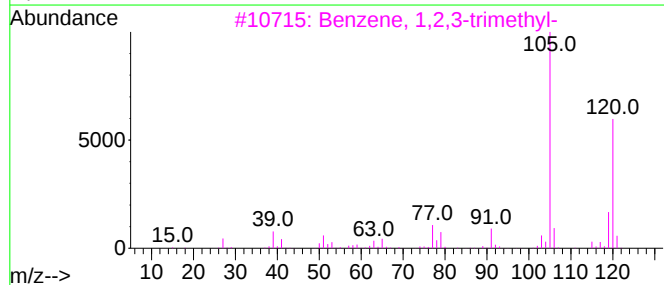
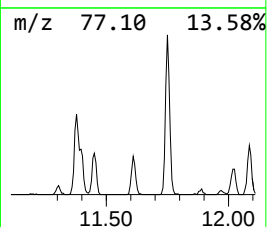
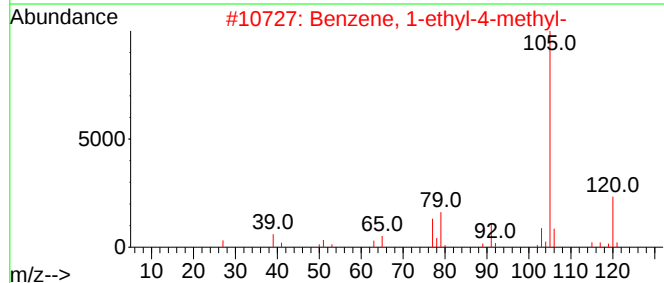
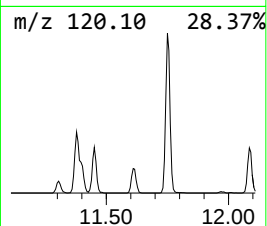
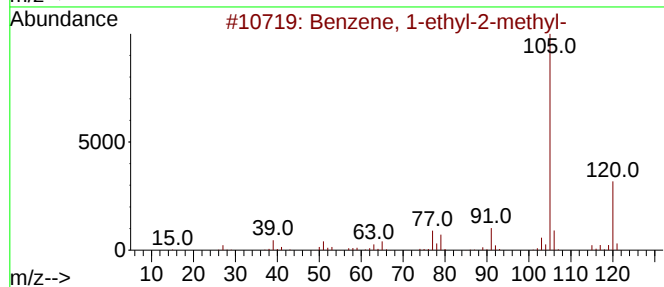
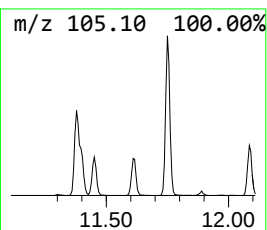
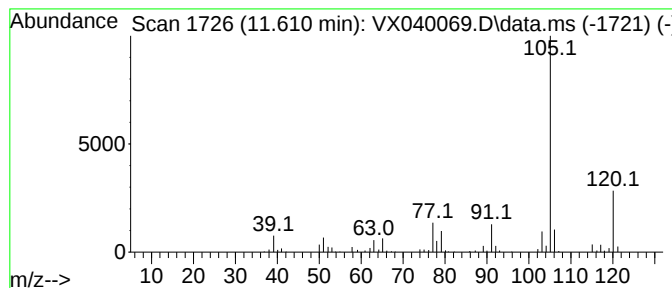
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	10.33 ug/l	103807	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



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NWB-1999

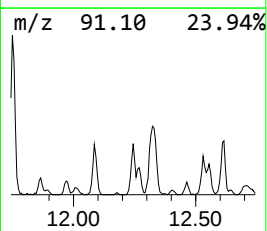
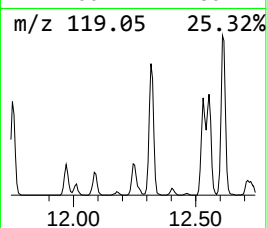
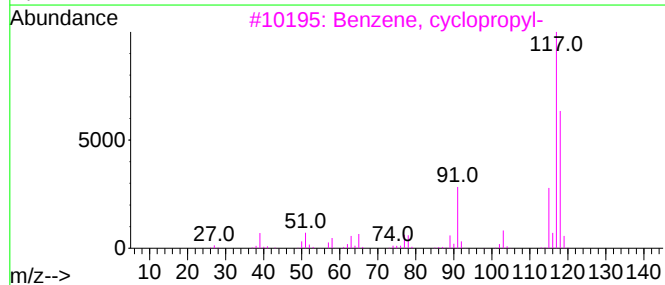
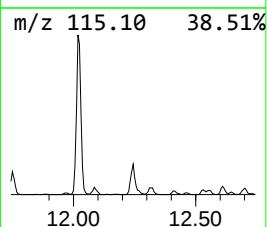
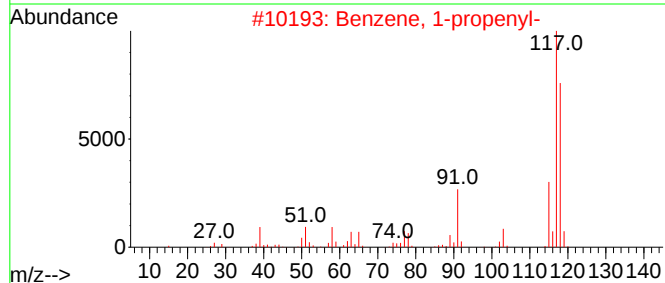
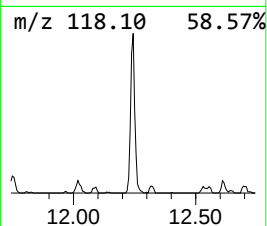
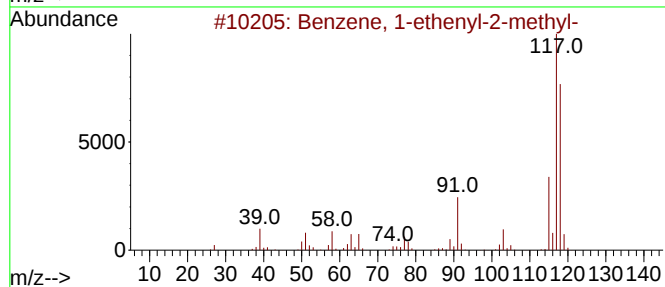
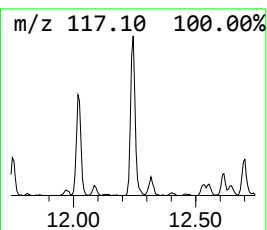
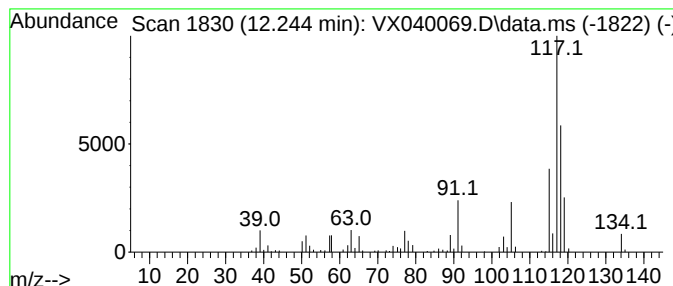
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	11.37 ug/l	114272	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	92
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	92
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	91
4			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	72
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
Data File : VX040069.D
Acq On : 01 Feb 2024 14:24
Operator : JC/MD
Sample : P1312-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

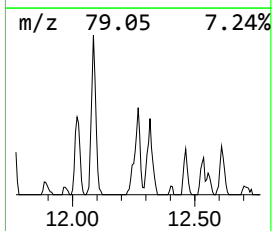
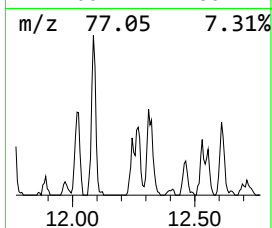
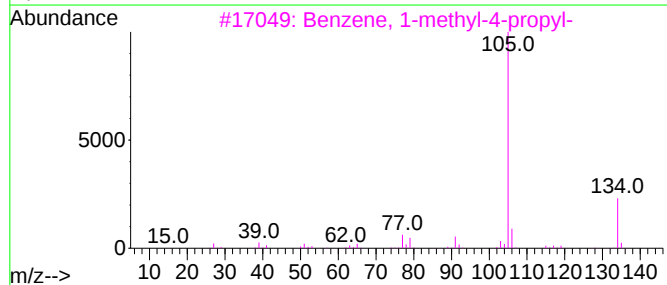
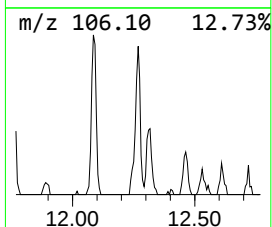
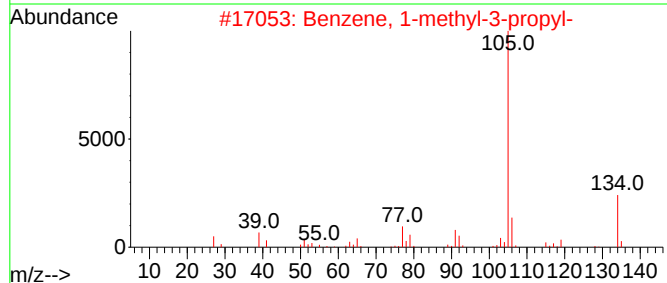
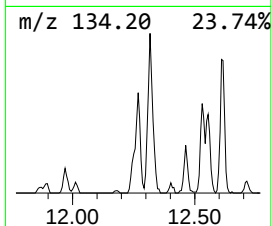
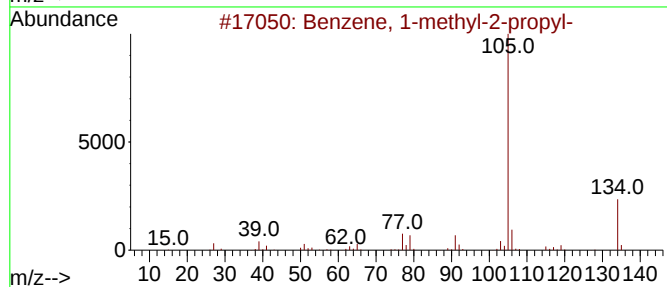
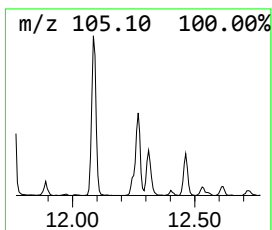
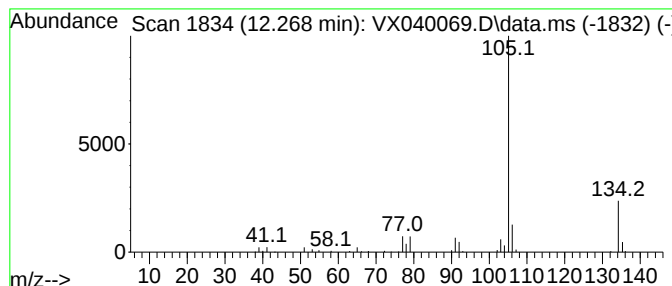
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methyl-2-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.268	5.98 ug/l	60081	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	91
2			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	90
3			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	87
4			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	72
5			Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
Data File : VX040069.D
Acq On : 01 Feb 2024 14:24
Operator : JC/MD
Sample : P1312-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

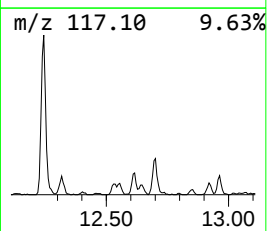
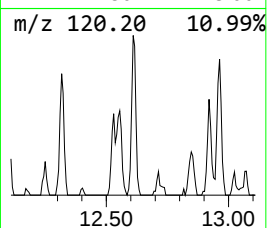
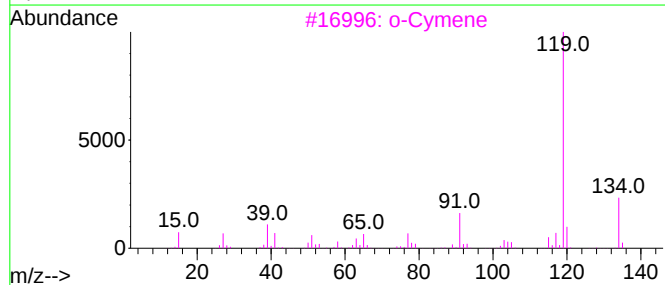
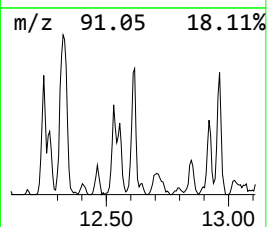
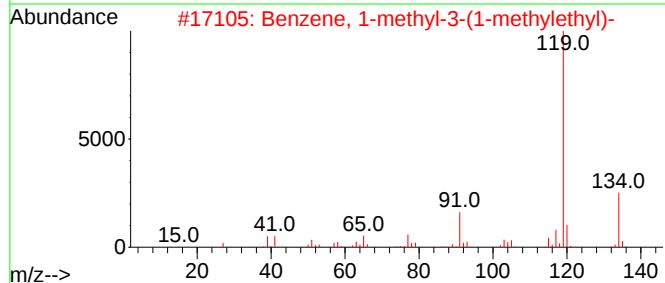
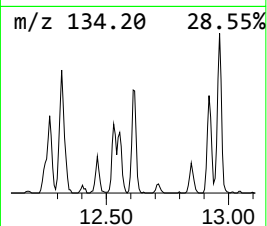
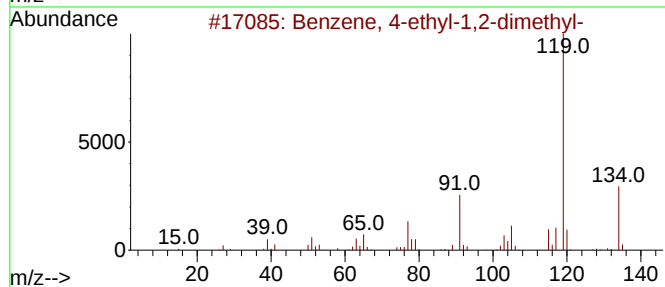
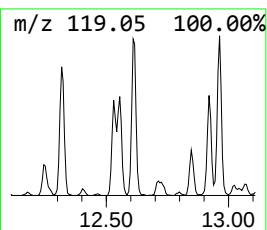
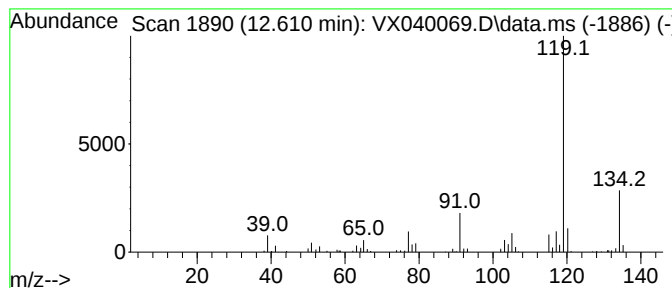
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	8.66 ug/l	87063	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
Data File : VX040069.D
Acq On : 01 Feb 2024 14:24
Operator : JC/MD
Sample : P1312-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

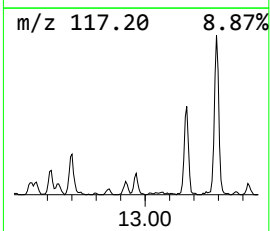
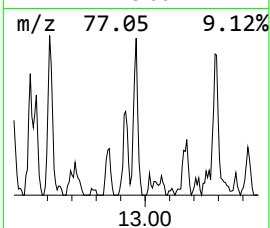
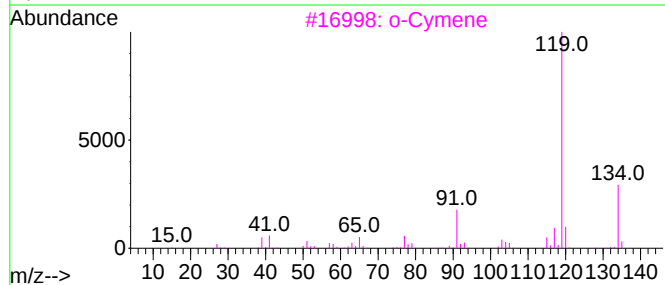
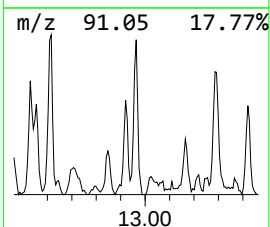
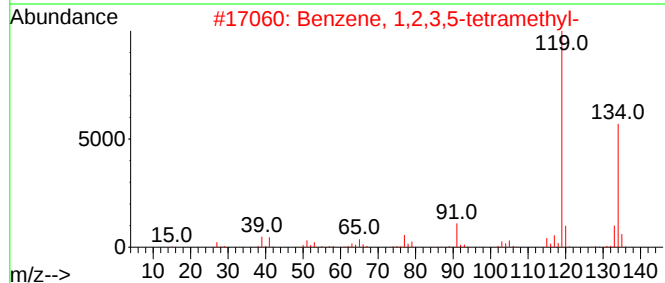
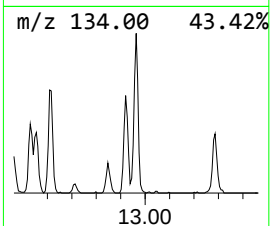
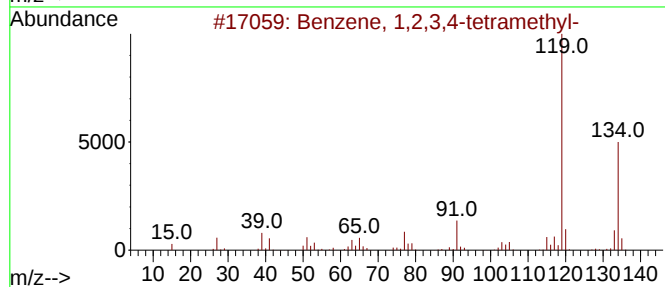
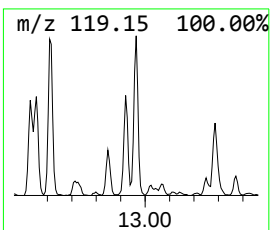
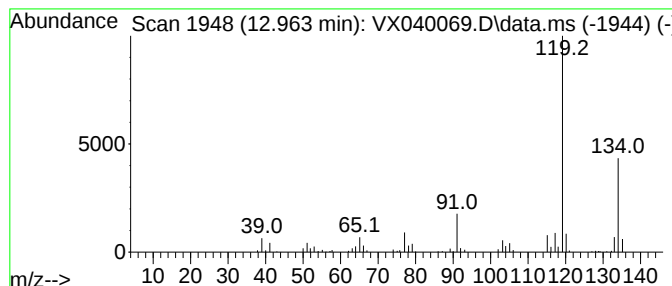
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	8.90 ug/l	89452	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			o-Cymene	134	C10H14	000527-84-4	94
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
Data File : VX040069.D
Acq On : 01 Feb 2024 14:24
Operator : JC/MD
Sample : P1312-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

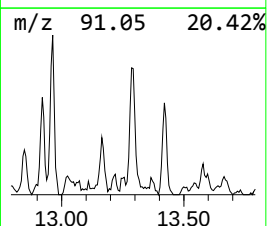
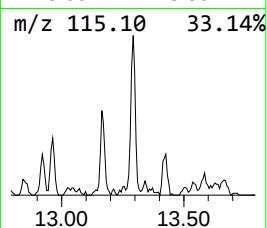
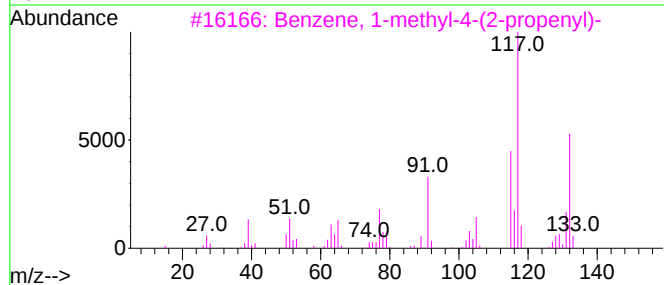
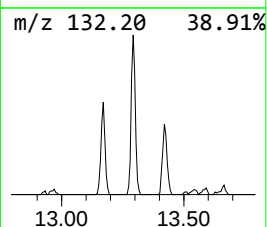
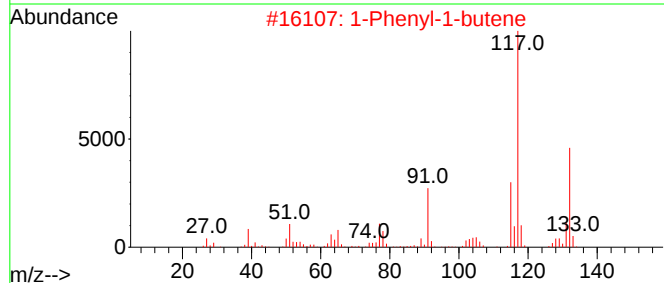
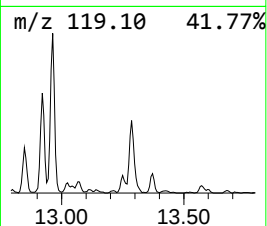
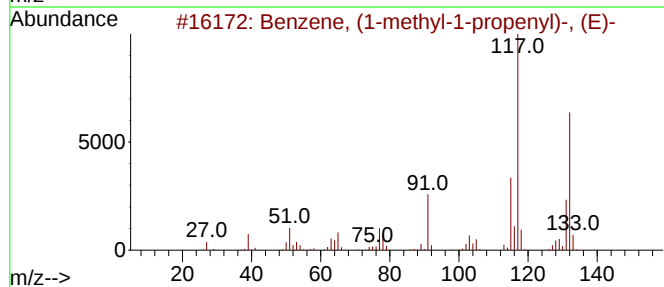
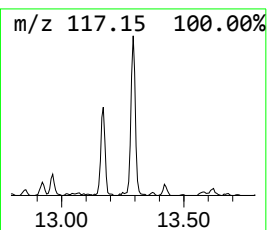
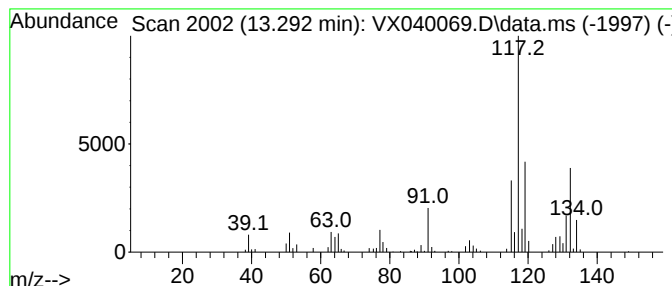
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, (1-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	11.68 ug/l	117417	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	76
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
4			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	70
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
Data File : VX040069.D
Acq On : 01 Feb 2024 14:24
Operator : JC/MD
Sample : P1312-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1999

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.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
Acetaldehyde	1.453	6.3	ug/l	35391	1	5.550	280388	50.0
Ethanol	2.050	46.2	ug/l	258929	1	5.550	280388	50.0
Benzene, 1-ethy...	11.378	32.1	ug/l	322833	4	12.024	502472	50.0
Benzene, 1-ethy...	11.610	10.3	ug/l	103807	4	12.024	502472	50.0
Benzene, 1-ethe...	12.244	11.4	ug/l	114272	4	12.024	502472	50.0
Benzene, 1-meth...	12.268	6.0	ug/l	60081	4	12.024	502472	50.0
Benzene, 4-ethy...	12.610	8.7	ug/l	87063	4	12.024	502472	50.0
Benzene, 1,2,3,...	12.963	8.9	ug/l	89452	4	12.024	502472	50.0
Benzene, (1-met...	13.292	11.7	ug/l	117417	4	12.024	502472	50.0