

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021125\
 Data File : VX044906.D
 Acq On : 11 Feb 2025 15:15
 Operator : JC/MD
 Sample : Q1293-01 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NWB-2123

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\82X021025W.M
 Title : SW846 8260

Signal : TIC: VX044906.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	65	rBV	184113	219044	4.84%	1.877%
2	1.508	65	69	84	rVB	17398	48440	1.07%	0.415%
3	2.099	155	166	193	rBV	1840255	4528436	100.00%	38.802%
4	2.380	206	212	225	rVB	38265	68832	1.52%	0.590%
5	3.111	324	332	347	rVB2	24620	58398	1.29%	0.500%
6	5.379	694	704	720	rBV	67253	199240	4.40%	1.707%
7	5.544	722	731	747	rVV2	93881	270235	5.97%	2.315%
8	5.946	788	797	804	rBV	75885	201378	4.45%	1.725%
9	6.031	804	811	822	rVB	73302	202641	4.47%	1.736%
10	6.757	921	930	951	rBV	173170	429103	9.48%	3.677%
11	8.647	1234	1240	1246	rBV	365206	600515	13.26%	5.145%
12	8.714	1246	1251	1273	rVB	419408	702507	15.51%	6.019%
13	9.525	1379	1384	1395	rBV	23513	45395	1.00%	0.389%
14	10.049	1465	1470	1486	rBV	376731	537239	11.86%	4.603%
15	10.189	1489	1493	1505	rBV	65287	95066	2.10%	0.815%
16	10.299	1505	1511	1520	rBV	214118	302753	6.69%	2.594%
17	10.640	1562	1567	1581	rVB	153542	207531	4.58%	1.778%
18	11.079	1634	1639	1651	rBV	307566	398309	8.80%	3.413%
19	11.378	1682	1688	1695	rBV	82491	138199	3.05%	1.184%
20	11.451	1695	1700	1704	rBV	38527	46933	1.04%	0.402%
21	11.610	1721	1726	1731	rBV	53079	67228	1.48%	0.576%
22	11.750	1741	1749	1757	rVB	196872	255366	5.64%	2.188%
23	12.018	1788	1793	1799	rBV	410496	495122	10.93%	4.242%
24	12.085	1799	1804	1813	rVB	93510	114975	2.54%	0.985%
25	12.238	1821	1829	1832	rBV2	82716	142841	3.15%	1.224%
26	12.317	1837	1842	1849	rVB3	39243	63555	1.40%	0.545%
27	12.609	1883	1890	1893	rVV	36078	48417	1.07%	0.415%
28	12.695	1900	1904	1913	rBV2	36211	62887	1.39%	0.539%
29	12.853	1924	1930	1936	rBV4	29737	55535	1.23%	0.476%
30	12.963	1944	1948	1954	rVB	48263	62730	1.39%	0.537%
31	13.164	1977	1981	1985	rVB	57972	68391	1.51%	0.586%
32	13.286	1997	2001	2006	rVB2	131637	177504	3.92%	1.521%
33	13.420	2017	2023	2032	rBV	147282	188982	4.17%	1.619%
34	13.774	2076	2081	2087	rVB	57622	76669	1.69%	0.657%
35	13.853	2087	2094	2099	rVB	35397	52939	1.17%	0.454%
36	13.920	2099	2105	2110	rBV2	40090	59994	1.32%	0.514%

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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\82X021025W.M
Title : SW846 8260

37	14.225	2148	2155	2159	rBV	101698	158644	3.50%	1.359%
38	14.371	2175	2179	2183	rVB	38057	46424	1.03%	0.398%
39	14.475	2192	2196	2202	rBV2	72640	95999	2.12%	0.823%
40	14.633	2220	2222	2226	rVV	61694	76356	1.69%	0.654%

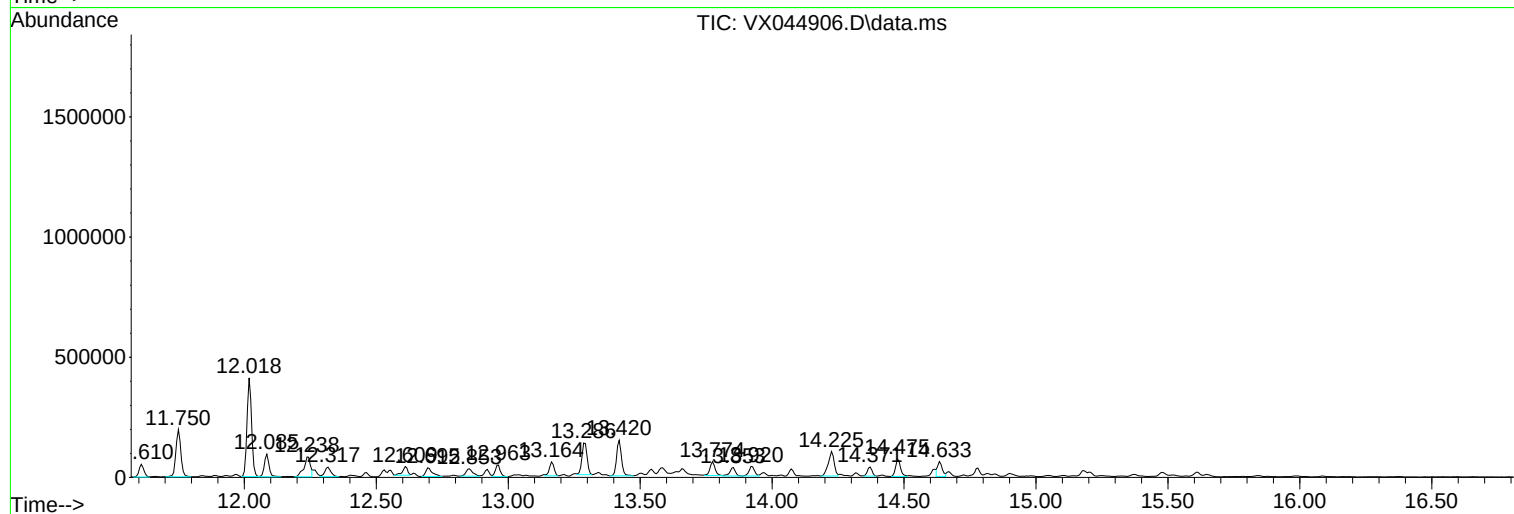
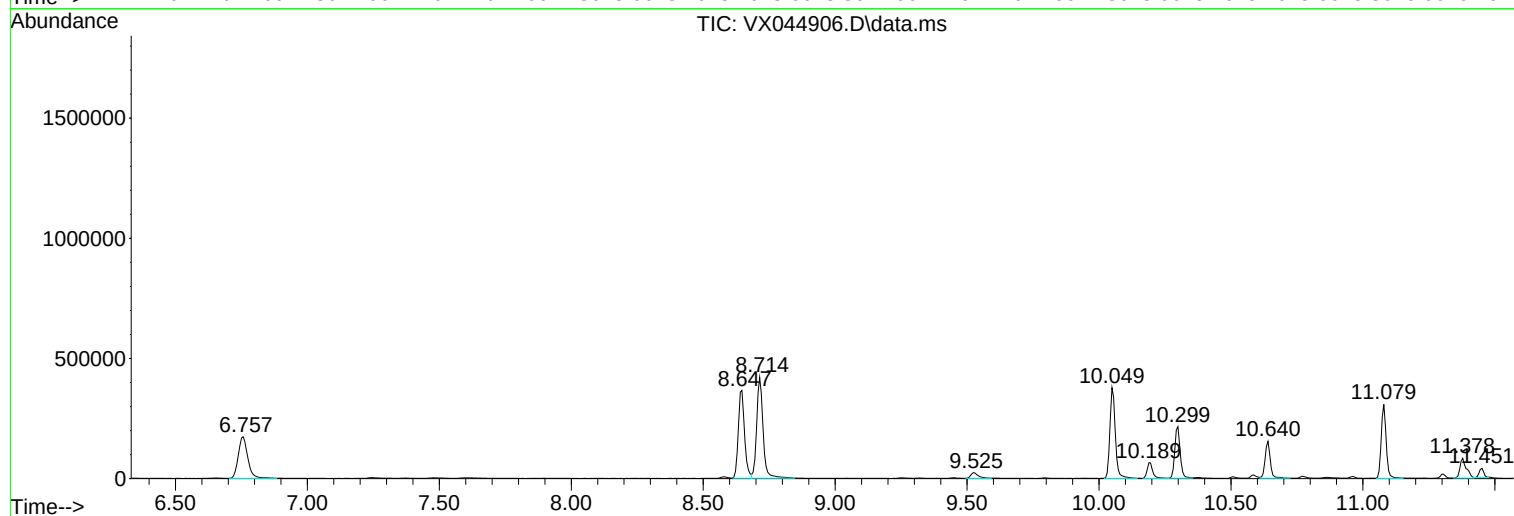
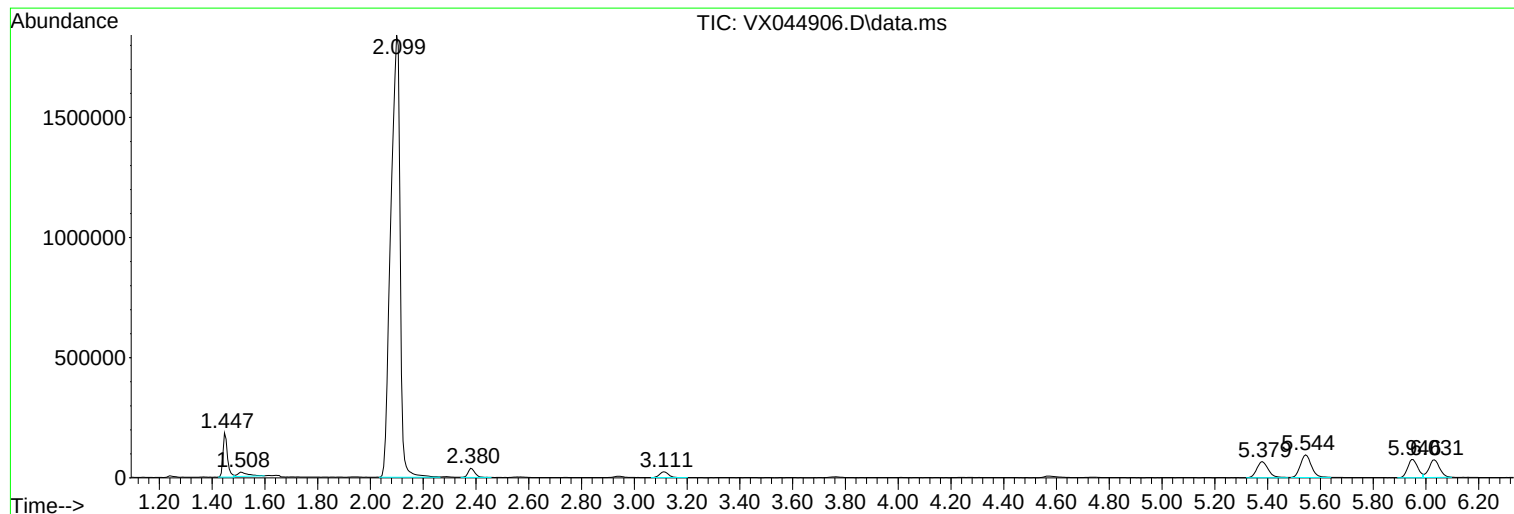
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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



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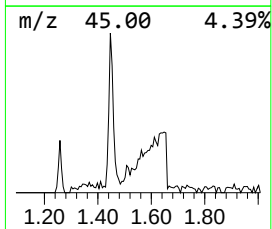
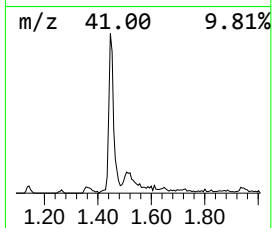
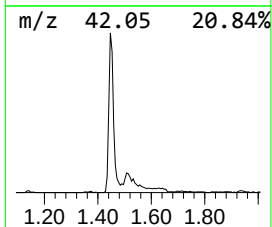
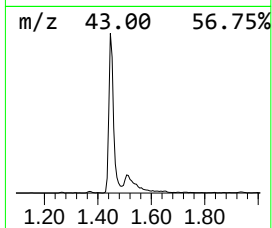
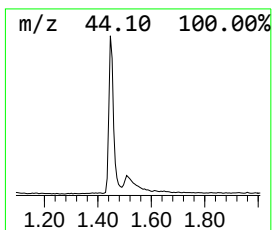
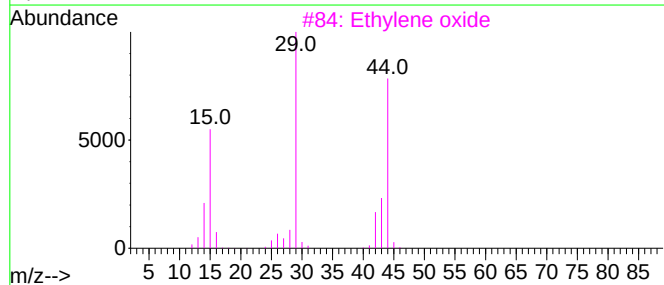
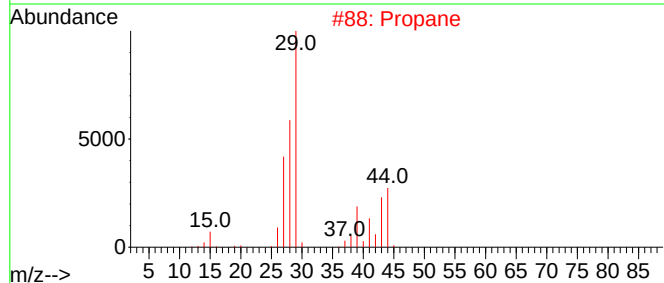
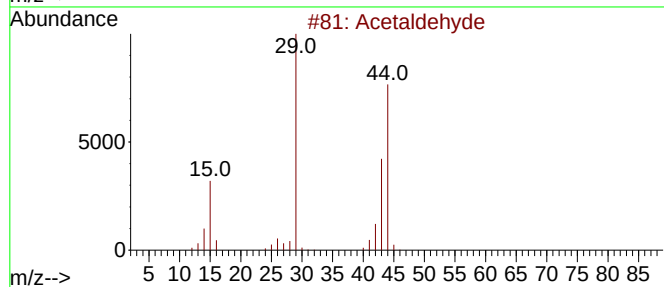
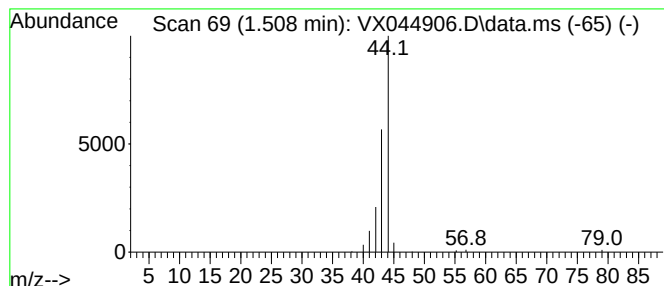
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.508	8.96 ug/l	48440	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			1-Propanol, 2-amino-, (./-.)-	75	C3H9NO	006168-72-5	4
5			1-(Methylamino)propan-2-ol	89	C4H11NO	1000486-79-1	4



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Instrument :
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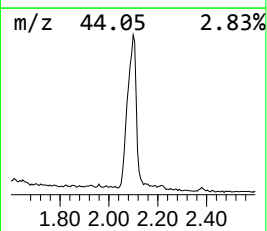
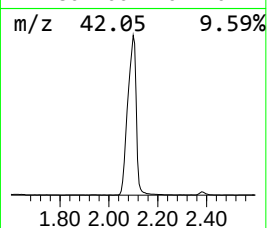
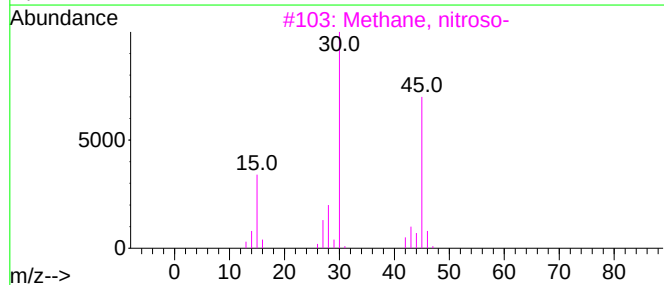
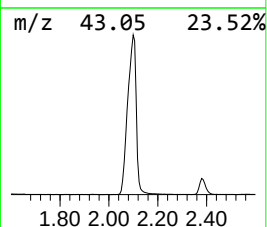
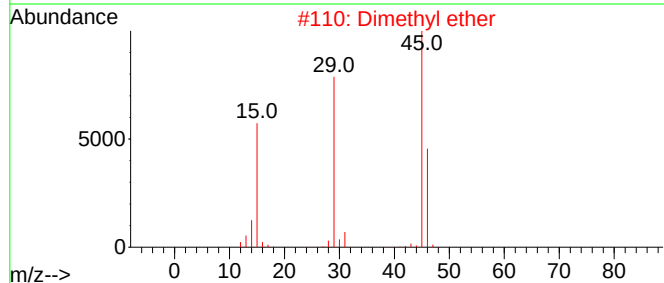
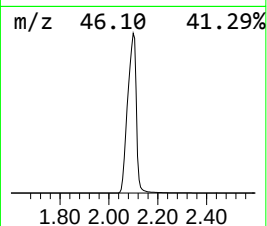
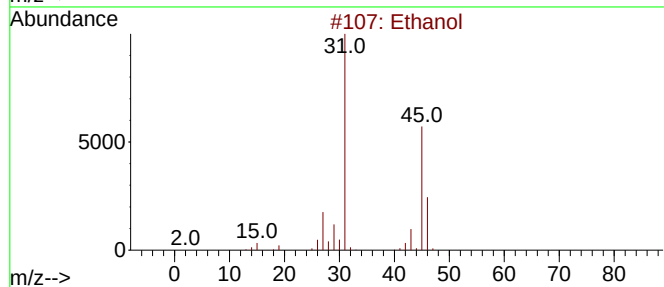
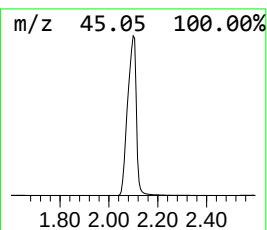
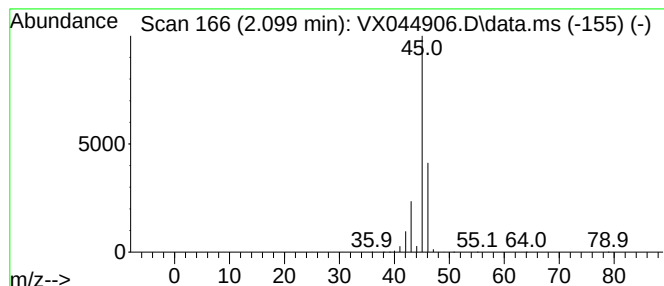
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	837.87 ug/l	4528440	Pentafluorobenzene	5.544

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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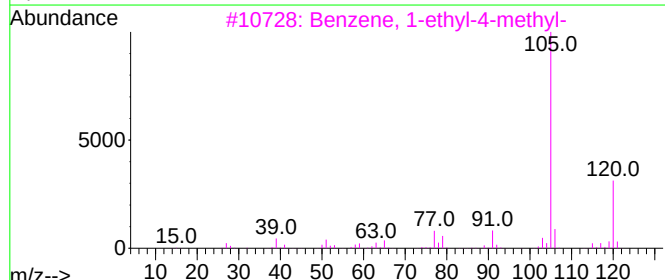
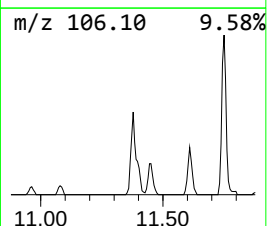
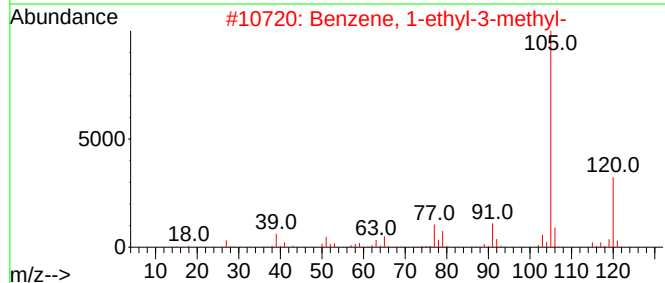
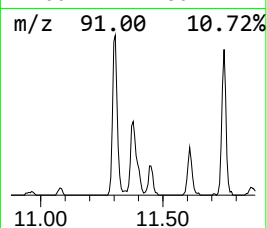
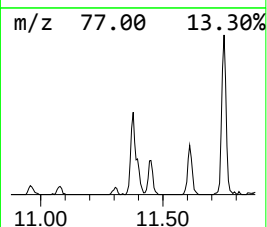
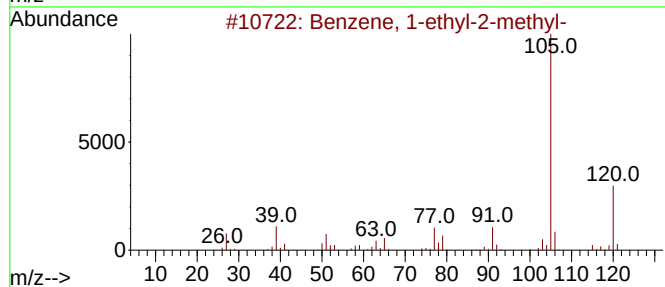
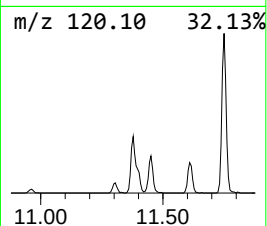
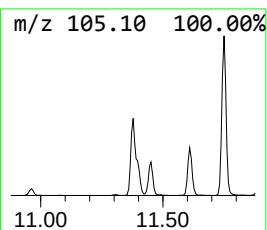
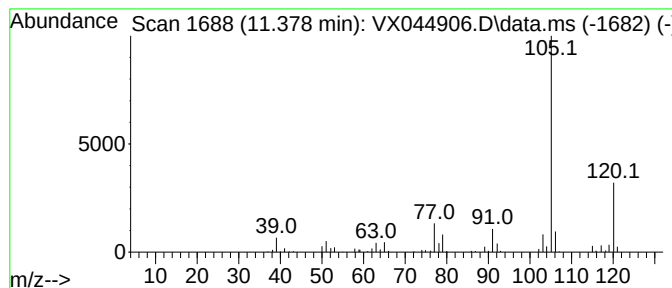
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	13.96 ug/l	138199	1,4-Dichlorobenzene-d4	12.018

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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ALS Vial : 15 Sample Multiplier: 1

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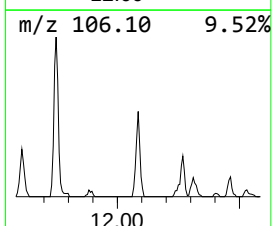
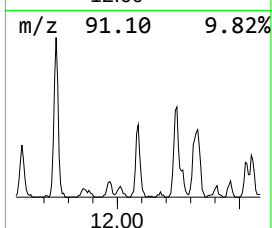
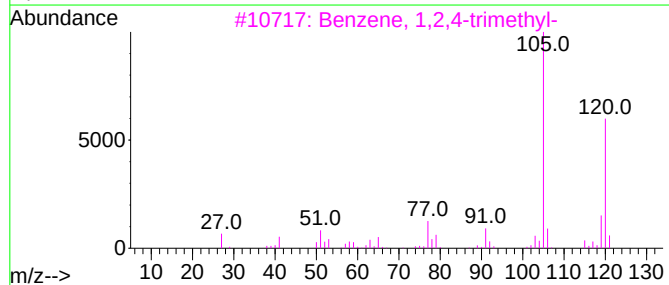
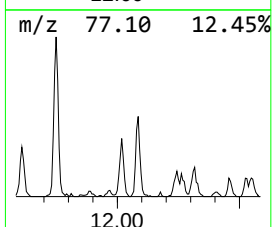
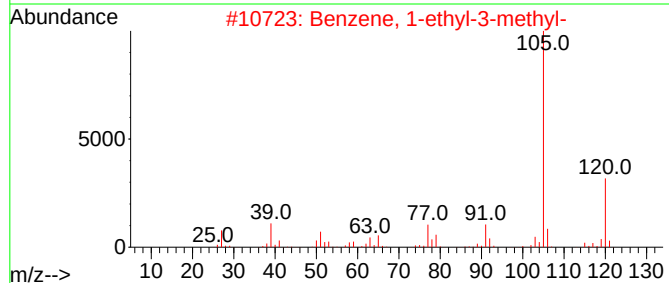
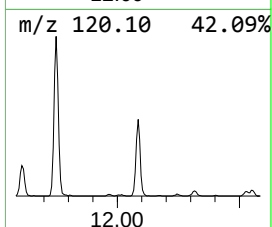
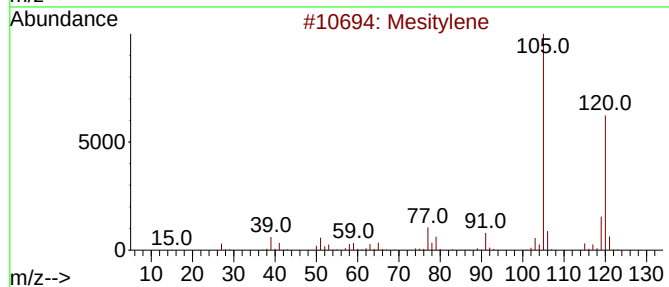
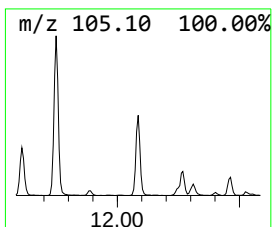
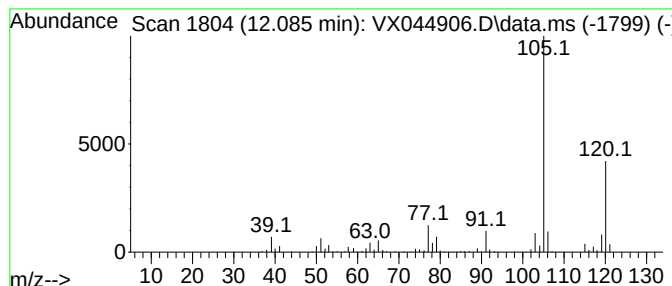
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Mesitylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	11.61 ug/l	114975	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
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			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



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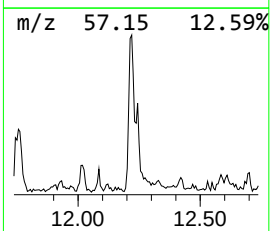
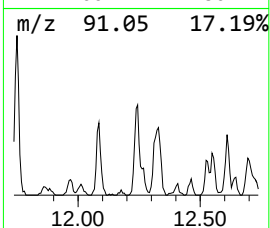
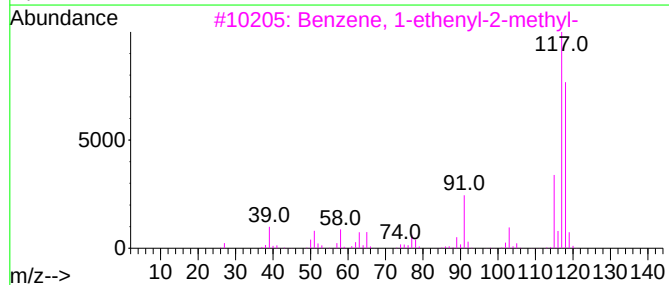
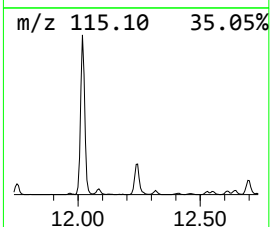
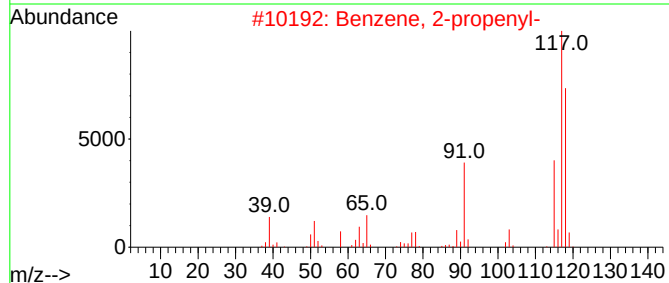
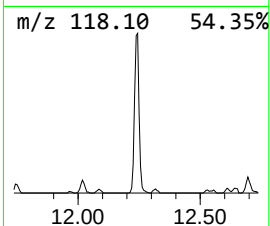
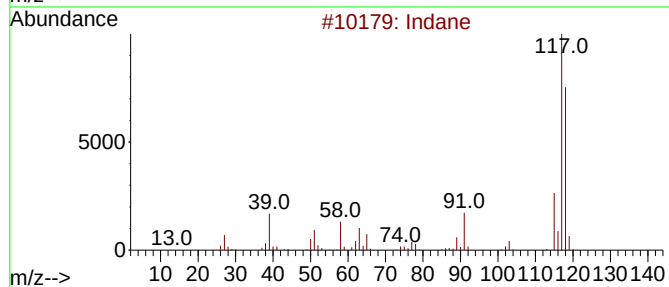
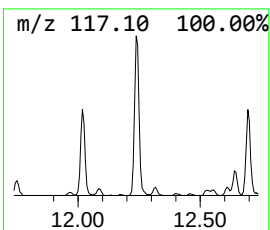
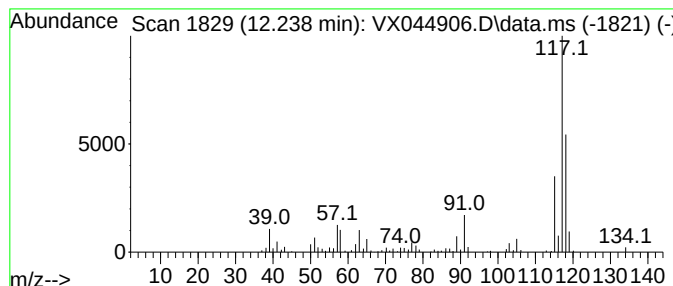
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.238	14.42 ug/l	142841	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	96
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
5			Deltacyclene	118	C9H10	007785-10-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021125\
Data File : VX044906.D
Acq On : 11 Feb 2025 15:15
Operator : JC/MD
Sample : Q1293-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2123

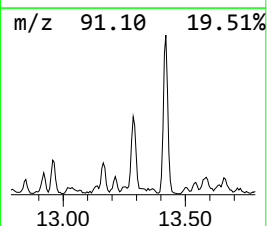
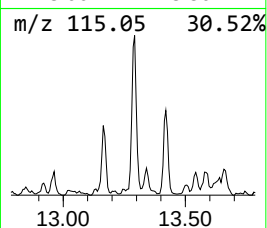
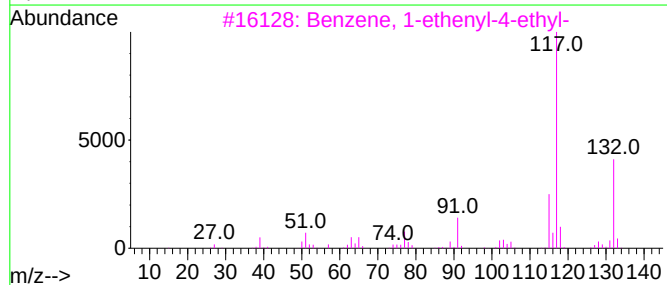
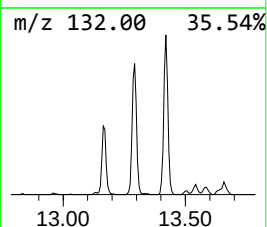
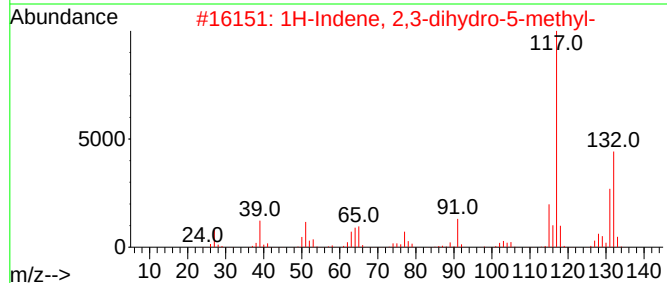
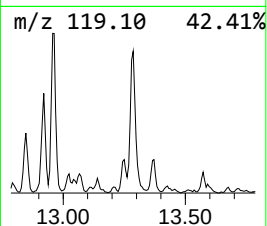
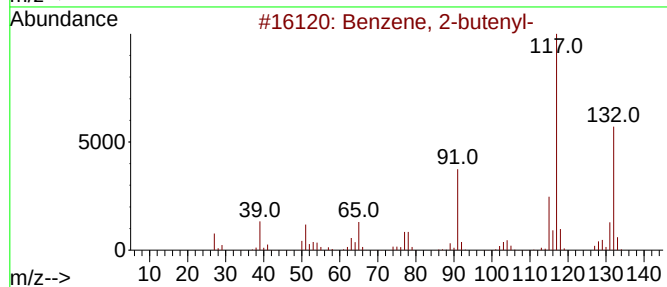
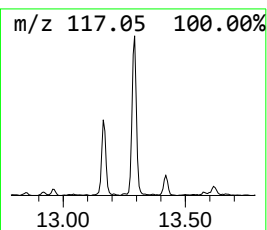
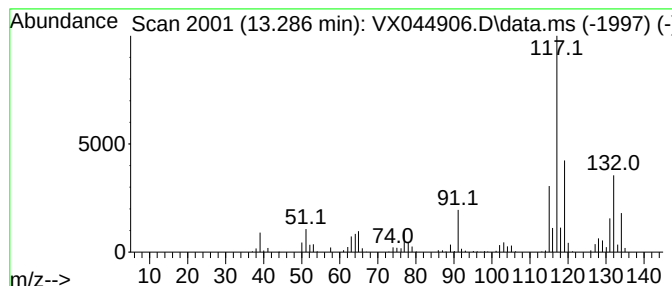
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-butenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	17.93 ug/l	177504	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	76
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021125\
Data File : VX044906.D
Acq On : 11 Feb 2025 15:15
Operator : JC/MD
Sample : Q1293-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2123

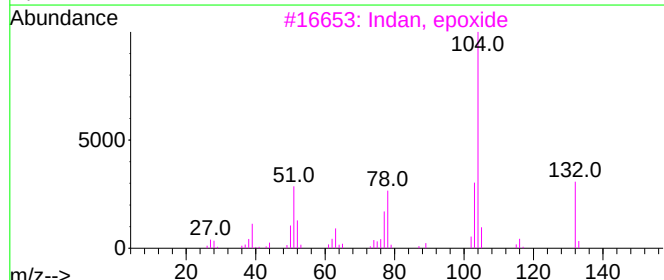
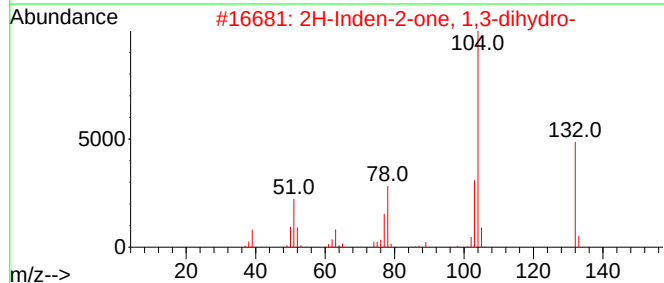
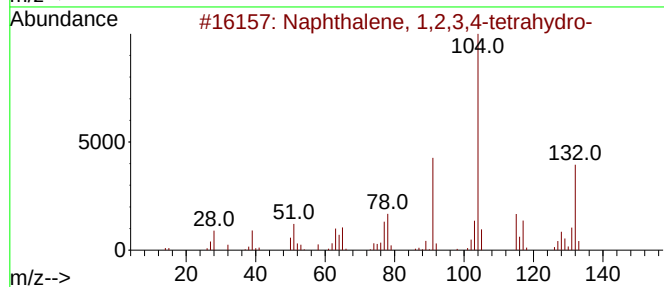
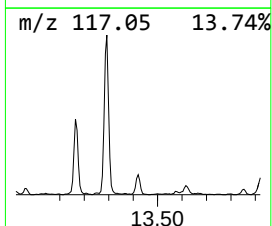
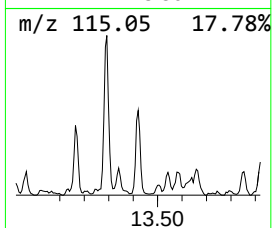
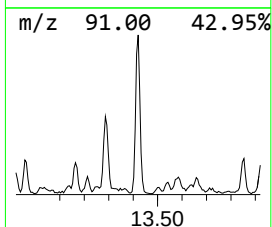
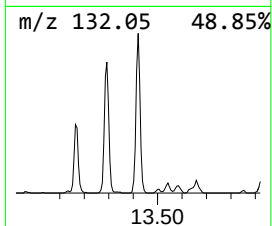
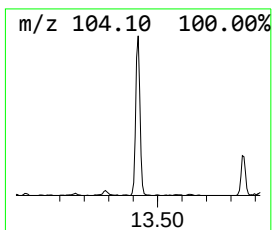
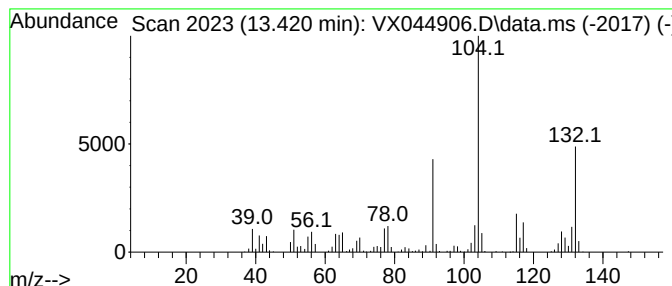
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	19.08 ug/l	188982	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	62
3			Indan, epoxide	132	C9H8O	000768-22-9	62
4			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46
5			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021125\
Data File : VX044906.D
Acq On : 11 Feb 2025 15:15
Operator : JC/MD
Sample : Q1293-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2123

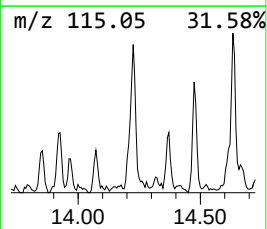
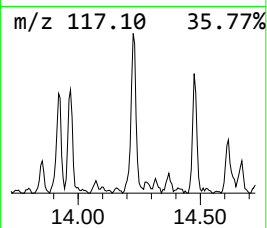
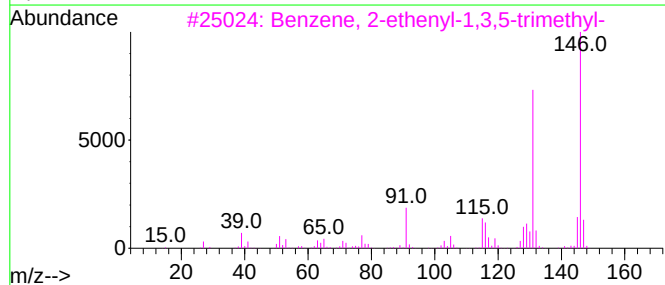
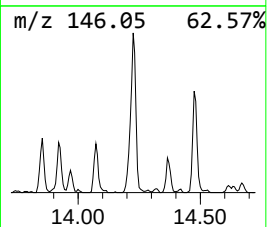
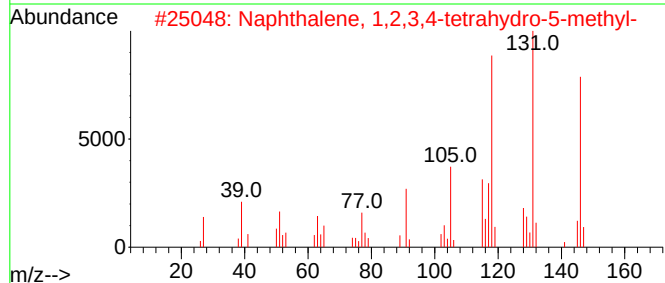
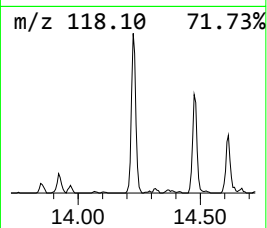
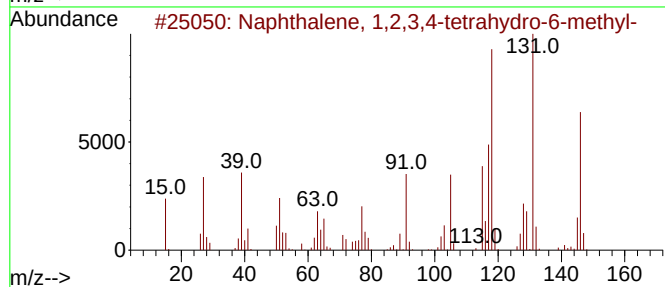
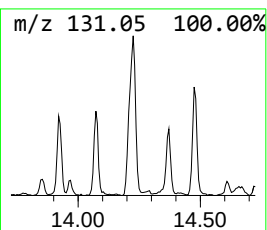
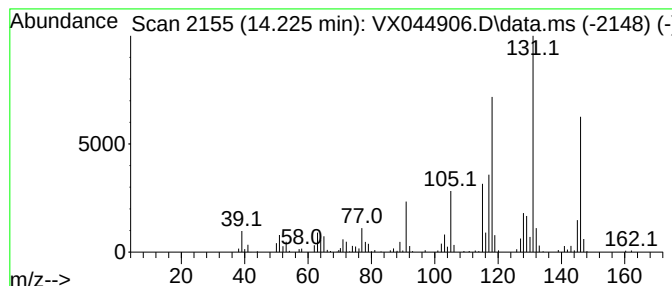
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	16.02 ug/l	158644	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	70
4			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	68
5			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021125\
Data File : VX044906.D
Acq On : 11 Feb 2025 15:15
Operator : JC/MD
Sample : Q1293-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2123

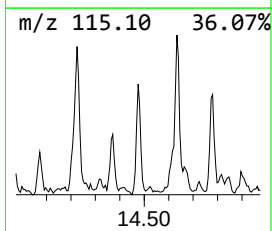
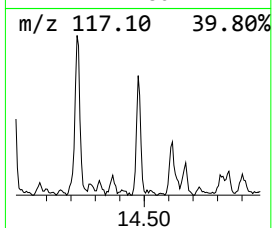
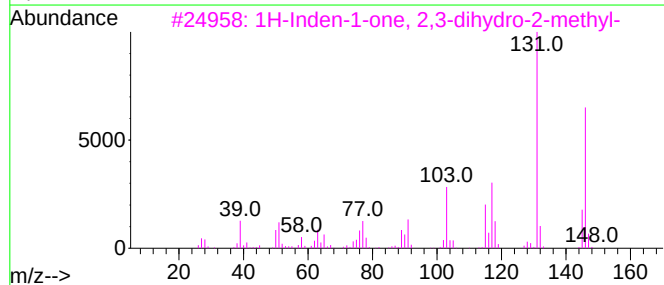
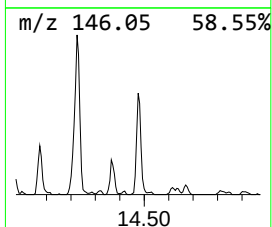
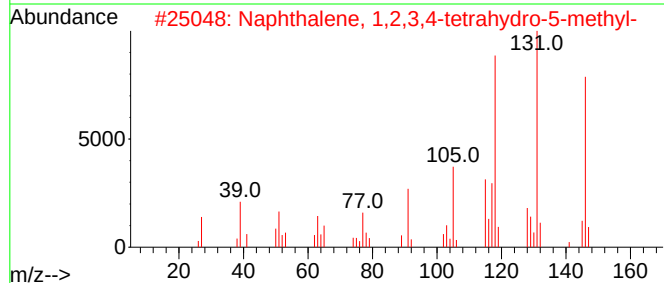
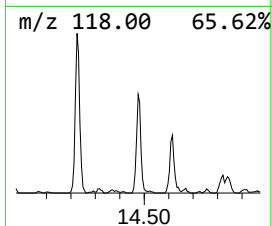
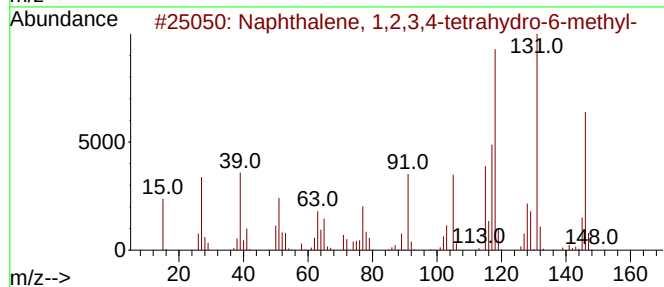
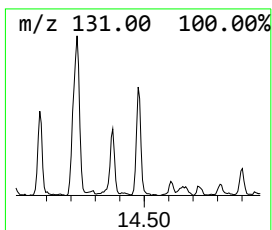
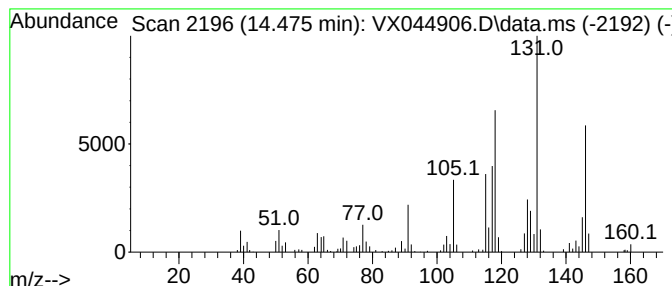
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.475	9.69 ug/l	95999	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	76
4			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	60
5			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021125\
Data File : VX044906.D
Acq On : 11 Feb 2025 15:15
Operator : JC/MD
Sample : Q1293-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2123

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.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	1.508	9.0	ug/l	48440	1	5.544	270235	50.0
Ethanol	2.099	837.9	ug/l	4528440	1	5.544	270235	50.0
Benzene, 1-ethy...	11.378	14.0	ug/l	138199	4	12.018	495122	50.0
Mesitylene	12.085	11.6	ug/l	114975	4	12.018	495122	50.0
Indane	12.238	14.4	ug/l	142841	4	12.018	495122	50.0
Benzene, 2-bute...	13.286	17.9	ug/l	177504	4	12.018	495122	50.0
Naphthalene, 1,...	13.420	19.1	ug/l	188982	4	12.018	495122	50.0
Naphthalene, 1,...	14.225	16.0	ug/l	158644	4	12.018	495122	50.0
Naphthalene, 1,...	14.475	9.7	ug/l	95999	4	12.018	495122	50.0