

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
 Data File : VN084968.D
 Acq On : 20 Nov 2024 14:57
 Operator : JC\MD
 Sample : P4770-01 1000X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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_N\methods\82N103024W.M
 Title : SW846 8260

Signal : TIC: VN084968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	50	57	67	rBV	22410	51193	5.08%	0.461%
2	2.824	140	148	150	rBV4	6766	14840	1.47%	0.134%
3	2.906	150	162	163	rBV8	10160	27334	2.71%	0.246%
4	7.230	888	897	906	rBV4	4336	12530	1.24%	0.113%
5	8.165	1046	1056	1060	rBV	136813	318972	31.65%	2.871%
6	8.218	1060	1065	1079	rVB	235388	531752	52.76%	4.786%
7	8.441	1097	1103	1108	rBV4	5576	10585	1.05%	0.095%
8	8.577	1116	1126	1134	rBV	145912	335742	33.31%	3.022%
9	8.753	1134	1156	1180	rVB4	76543	539981	53.57%	4.860%
10	9.100	1206	1215	1226	rBV	355487	724642	71.89%	6.522%
11	9.588	1290	1298	1299	rBV2	8522	14641	1.45%	0.132%
12	10.012	1364	1370	1377	rBV2	14416	27127	2.69%	0.244%
13	10.147	1386	1393	1398	rVB3	19093	38123	3.78%	0.343%
14	10.488	1447	1451	1456	rBV2	6047	10149	1.01%	0.091%
15	10.565	1456	1464	1470	rVV	496054	910859	90.37%	8.199%
16	10.629	1470	1475	1485	rVB	133855	248463	24.65%	2.236%
17	11.865	1677	1685	1695	rBV	460337	820118	81.37%	7.382%
18	11.965	1695	1702	1711	rVV	70943	120227	11.93%	1.082%
19	12.065	1712	1719	1730	rVB	268478	520434	51.63%	4.684%
20	12.400	1769	1776	1786	rVB	139699	239839	23.79%	2.159%
21	12.694	1821	1826	1832	rVB2	32227	49031	4.86%	0.441%
22	12.847	1841	1852	1862	rVB	401307	671751	66.65%	6.046%
23	13.035	1878	1884	1889	rBV	57094	88632	8.79%	0.798%
24	13.094	1889	1894	1898	rVV	212804	371767	36.88%	3.346%
25	13.129	1898	1900	1903	rVV	98128	125881	12.49%	1.133%
26	13.170	1903	1907	1915	rVB	142618	234039	23.22%	2.107%
27	13.335	1927	1935	1942	rBV	94096	153090	15.19%	1.378%
28	13.482	1952	1960	1968	rBV	541042	849886	84.32%	7.650%
29	13.612	1974	1982	1987	rBV4	10452	23803	2.36%	0.214%
30	13.670	1987	1992	1998	rVB2	12721	19083	1.89%	0.172%
31	13.794	2005	2013	2024	rVB2	459777	1007941	100.00%	9.072%
32	13.988	2034	2046	2049	rBV2	114425	284902	28.27%	2.564%
33	14.017	2049	2051	2062	rVV5	117481	216510	21.48%	1.949%
34	14.112	2062	2067	2073	rVB3	6203	11674	1.16%	0.105%
35	14.182	2073	2079	2084	rBV	27391	45344	4.50%	0.408%
36	14.241	2084	2089	2092	rVV	56138	96341	9.56%	0.867%

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37	14.270	2092	2094	2099	rVV	55953	78376	7.78%	0.705%
38	14.329	2099	2104	2110	rVB	101821	159542	15.83%	1.436%
39	14.394	2110	2115	2118	rBV2	7957	10809	1.07%	0.097%
40	14.441	2118	2123	2128	rVB3	31144	54939	5.45%	0.495%
41	14.570	2139	2145	2152	rVB2	22779	38066	3.78%	0.343%
42	14.653	2152	2159	2162	rBV	67332	109905	10.90%	0.989%
43	14.694	2162	2166	2170	rVV	106499	169620	16.83%	1.527%
44	14.735	2170	2173	2177	rVV3	18340	28511	2.83%	0.257%
45	14.770	2177	2179	2182	rVV2	11156	15588	1.55%	0.140%
46	14.806	2182	2185	2192	rVV2	12530	21372	2.12%	0.192%
47	14.876	2192	2197	2201	rVV6	10356	16337	1.62%	0.147%
48	14.929	2201	2206	2211	rVV	40508	78741	7.81%	0.709%
49	14.970	2211	2213	2216	rVV2	11911	12983	1.29%	0.117%
50	15.047	2216	2226	2233	rVV3	75009	207953	20.63%	1.872%
51	15.100	2233	2235	2244	rVV5	12042	20722	2.06%	0.187%
52	15.206	2248	2253	2261	rBV6	8177	17139	1.70%	0.154%
53	15.317	2261	2272	2285	rVV6	23410	71545	7.10%	0.644%
54	15.429	2285	2291	2300	rVB5	14607	34454	3.42%	0.310%
55	15.641	2321	2327	2335	rVB	66250	122290	12.13%	1.101%
56	15.753	2340	2346	2351	rBV5	5331	13149	1.30%	0.118%
57	15.941	2373	2378	2385	rBV3	8016	14917	1.48%	0.134%
58	16.135	2398	2411	2412	rBV6	5115	10341	1.03%	0.093%
59	16.782	2514	2521	2522	rBV2	20777	35478	3.52%	0.319%

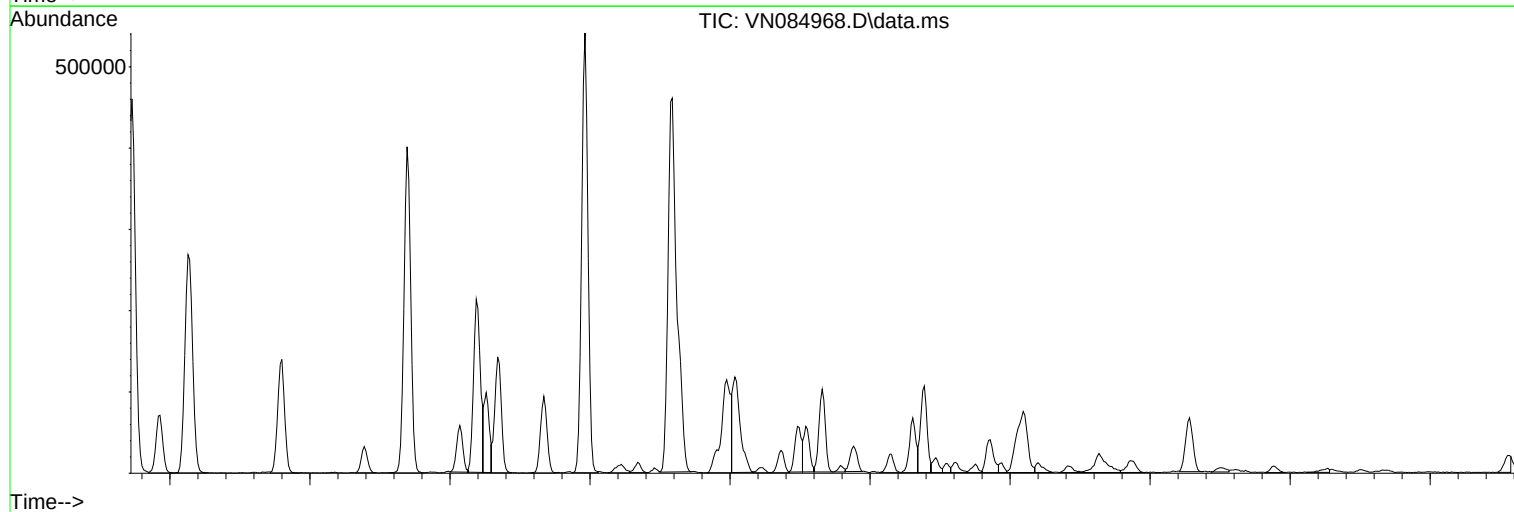
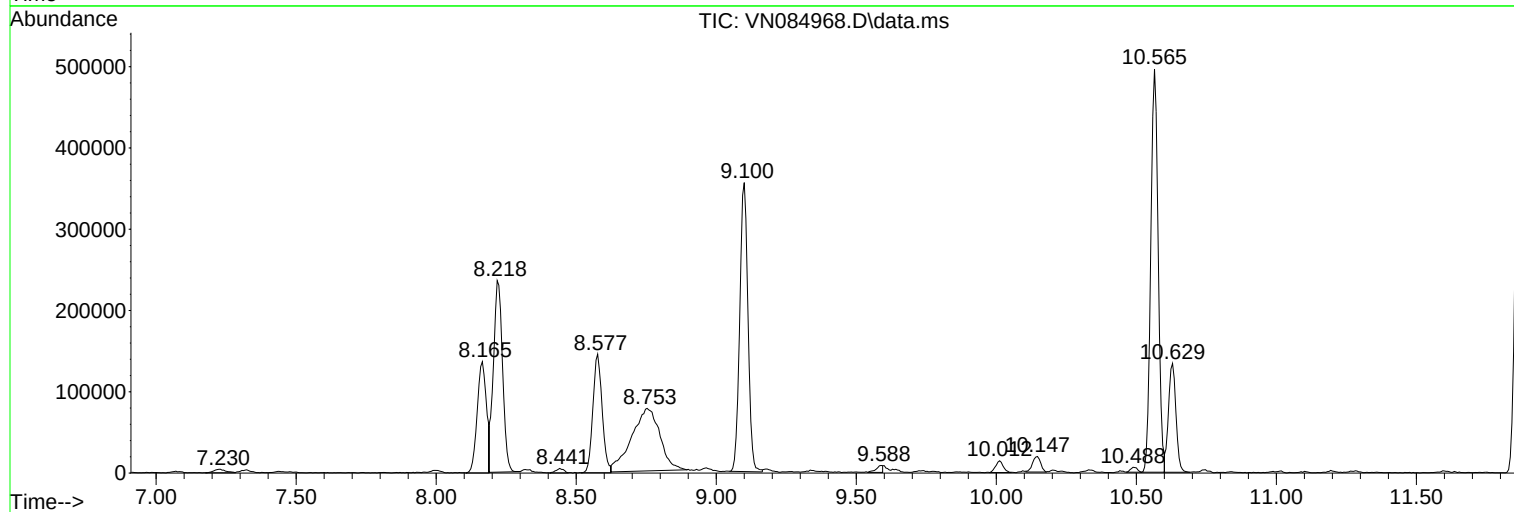
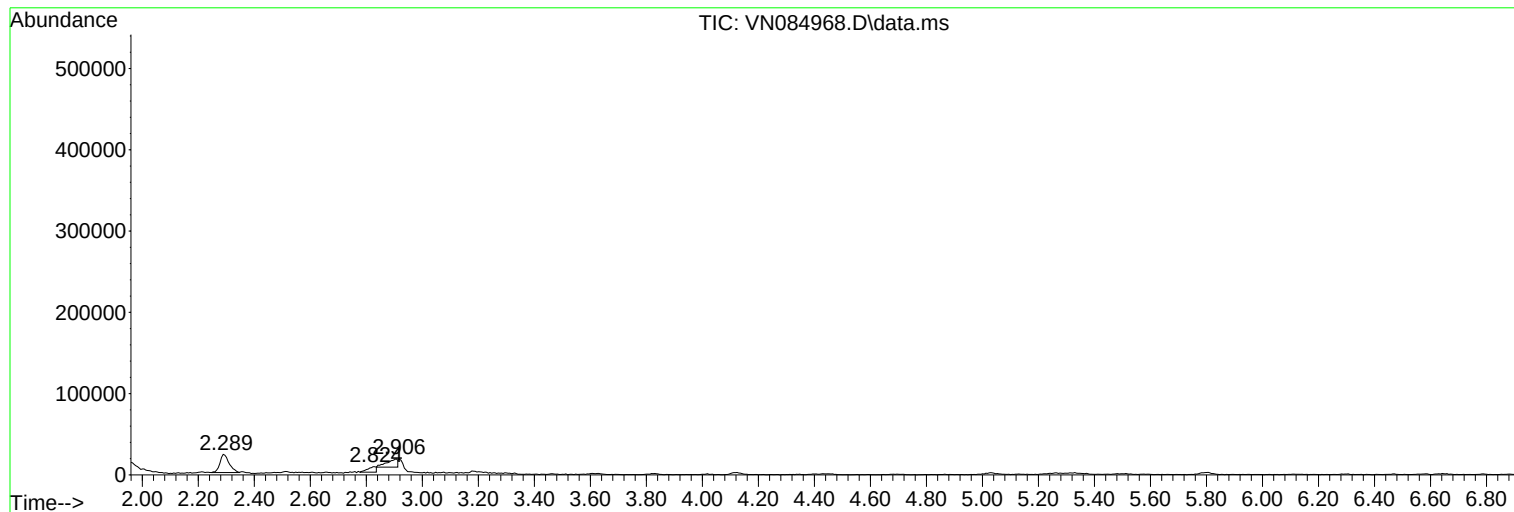
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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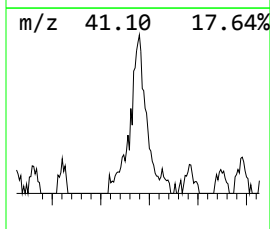
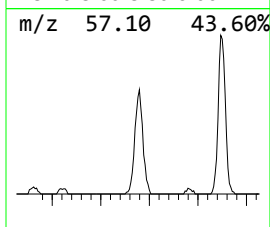
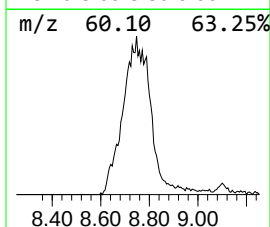
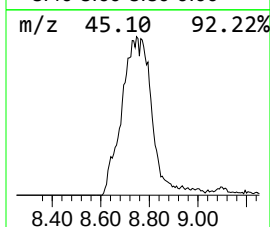
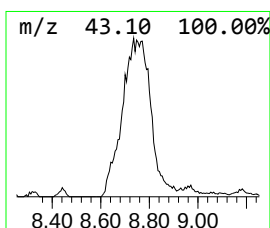
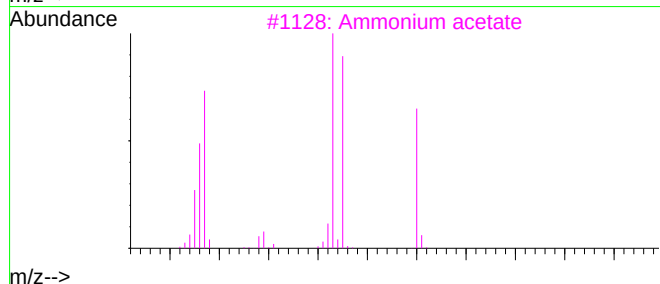
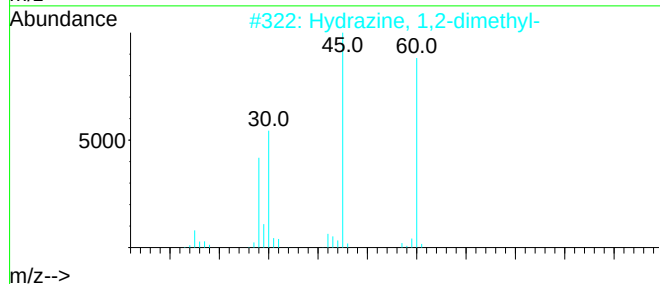
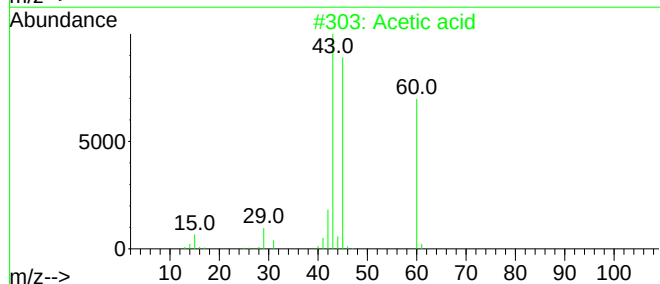
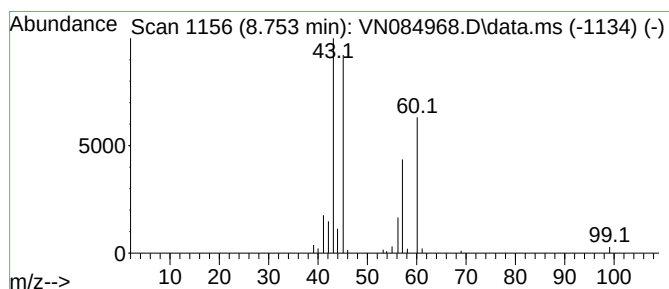
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	37.26 ug/l	539981	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	80
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	42
3	Ammonium acetate	77	C2H7NO2	000631-61-8	39
4	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	38
5	Propanal, 3-methoxy-	88	C4H8O2	002806-84-0	38



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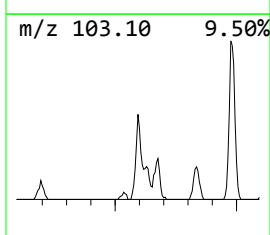
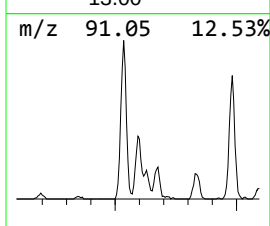
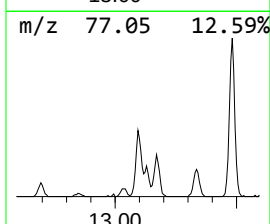
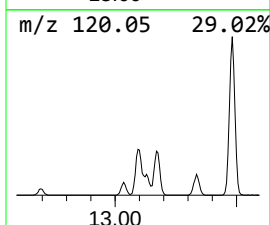
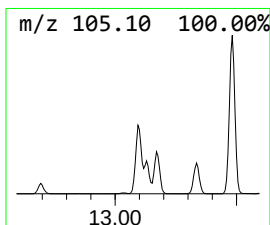
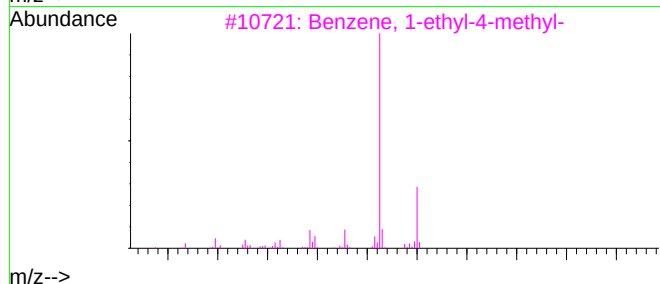
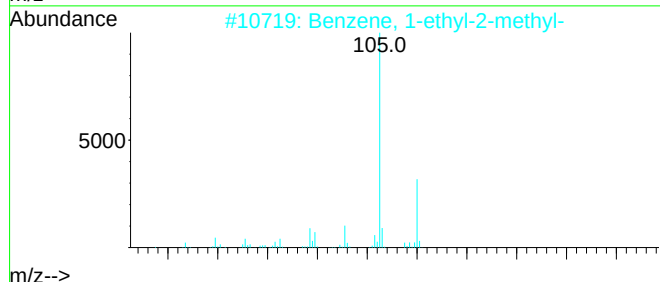
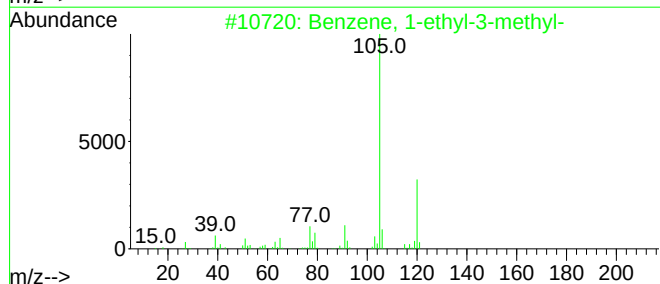
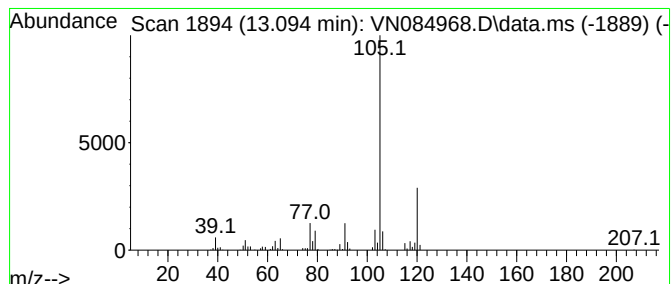
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	18.44 ug/l	371767	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

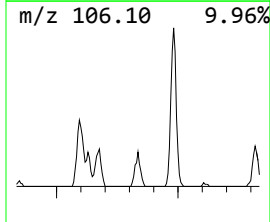
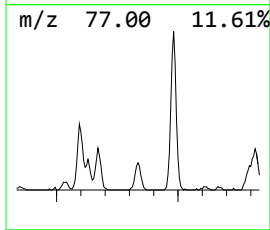
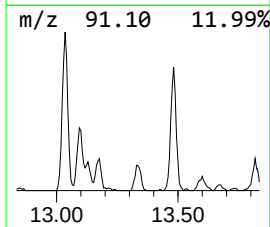
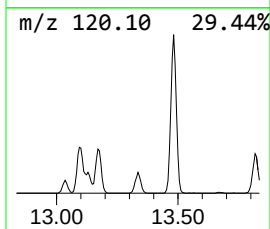
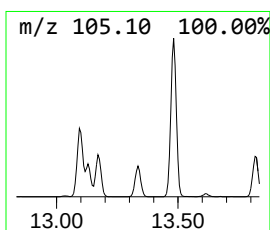
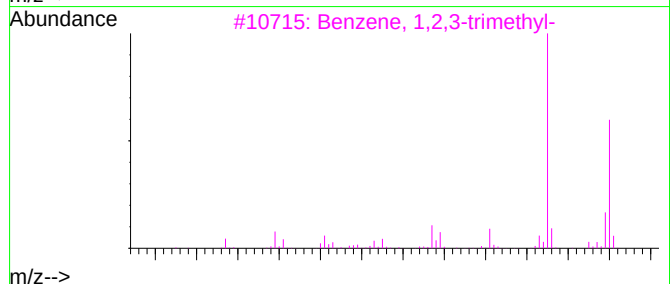
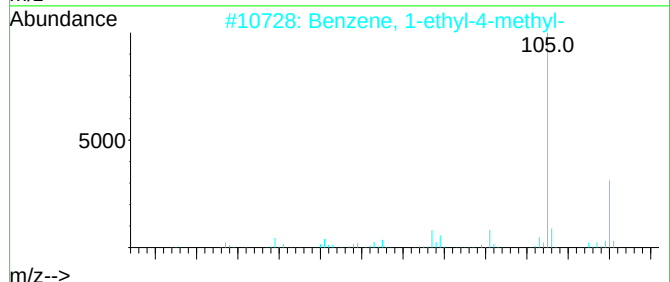
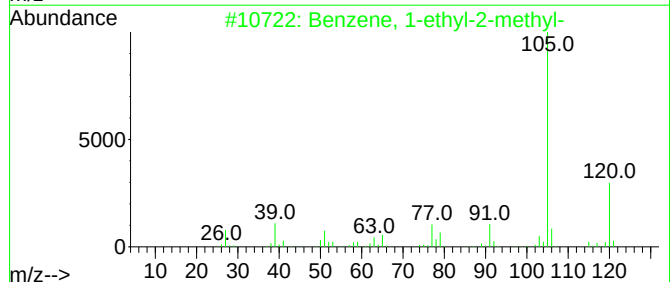
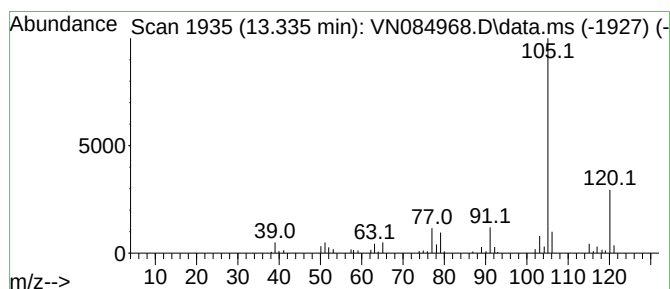
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	7.59 ug/l	153090	1,4-Dichlorobenzene-d4	13.794

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	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91



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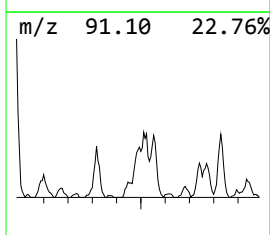
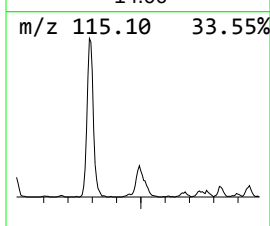
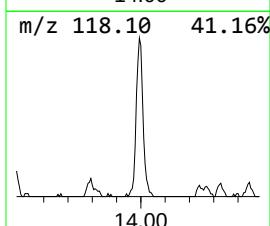
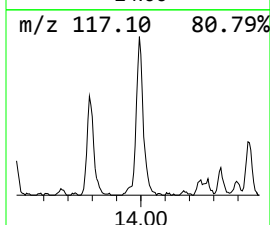
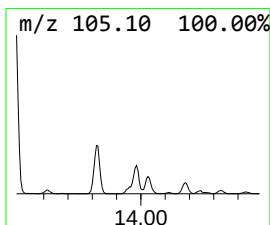
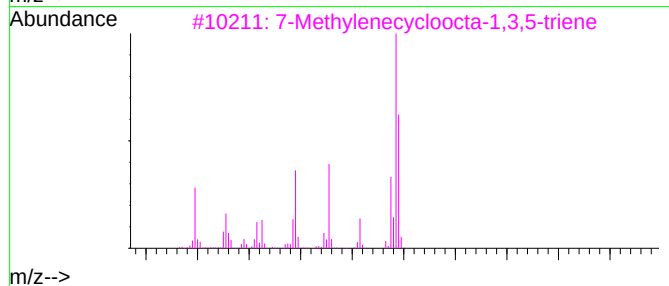
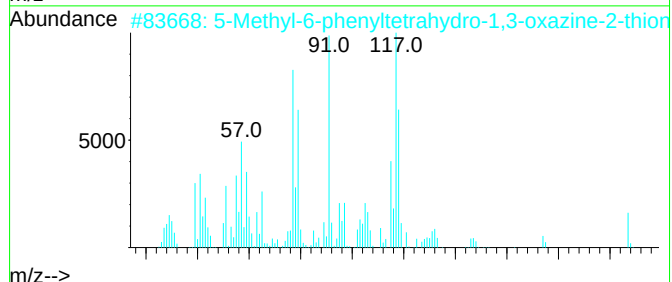
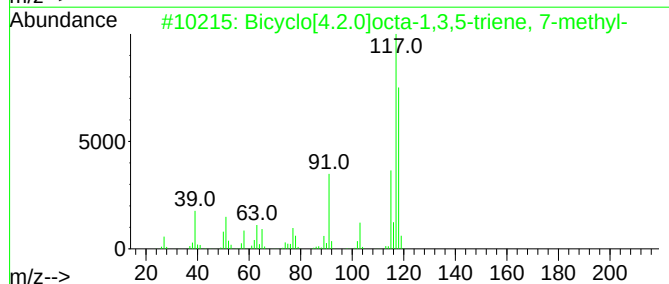
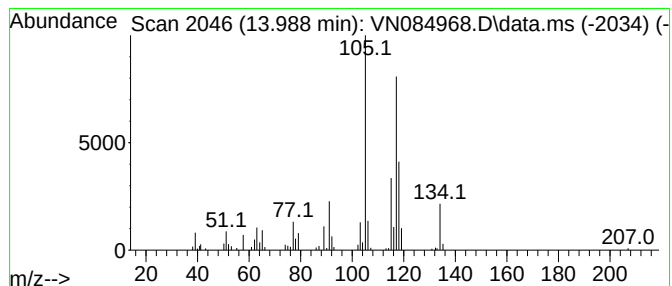
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.988	14.13 ug/l	284902	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	83
2	5-Methyl-6-phenyltetrahydro-1,3-...	207	C11H13NOS	086071-95-6	74
3	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	64
4	Indane	118	C9H10	000496-11-7	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

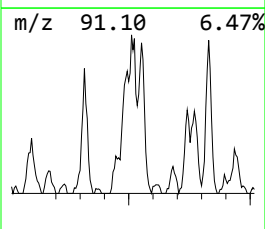
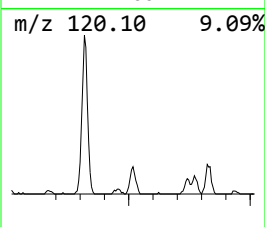
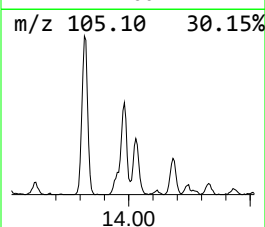
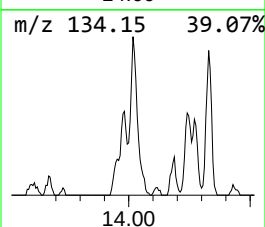
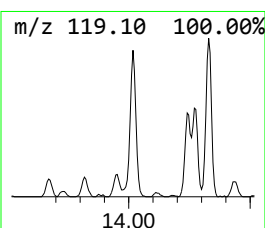
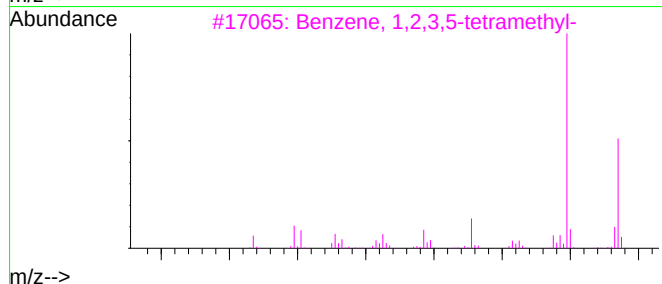
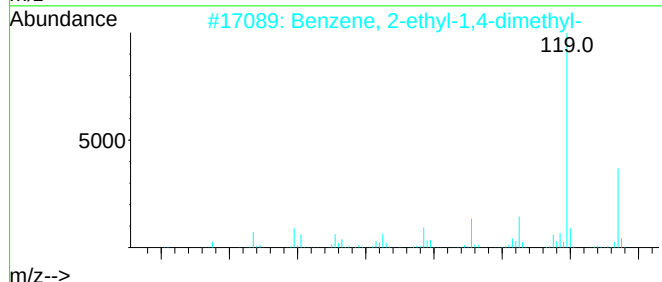
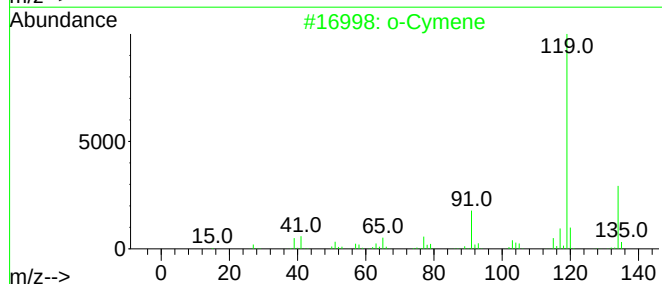
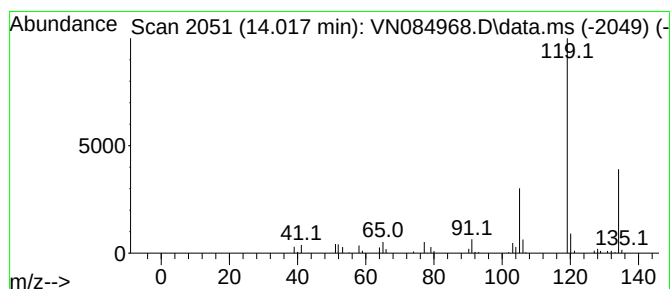
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 o-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.018	10.74 ug/l	216510	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	72
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	72
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
Data File : VN084968.D
Acq On : 20 Nov 2024 14:57
Operator : JC\MD
Sample : P4770-01 1000X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

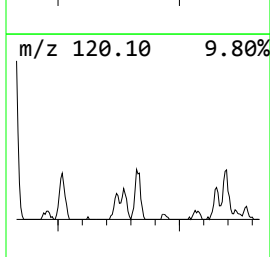
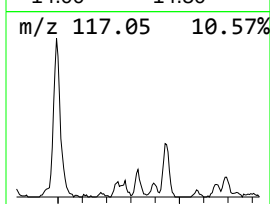
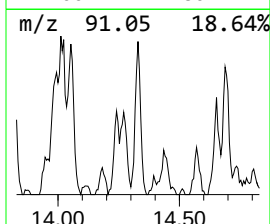
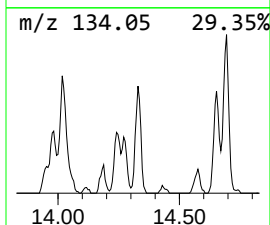
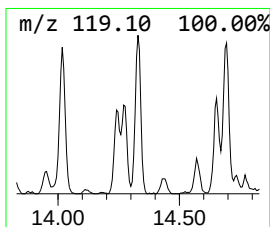
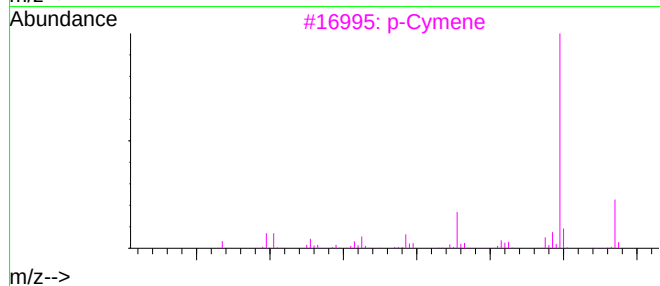
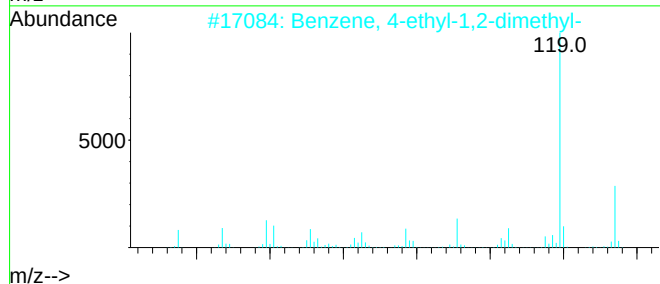
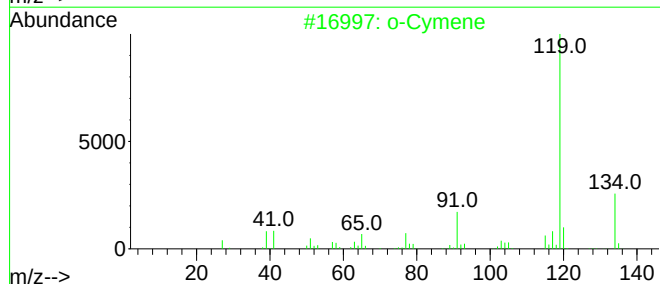
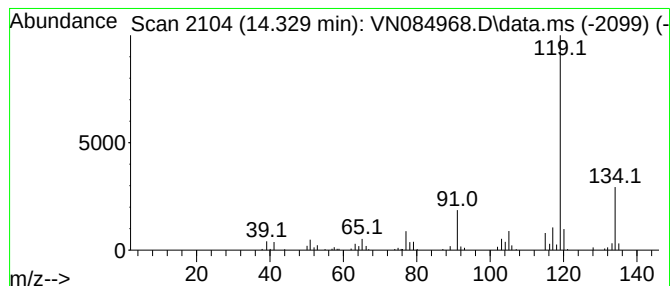
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	7.91 ug/l	159542	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
Data File : VN084968.D
Acq On : 20 Nov 2024 14:57
Operator : JC\MD
Sample : P4770-01 1000X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

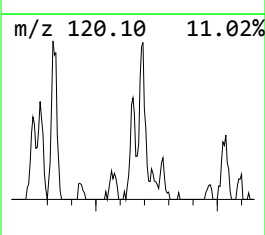
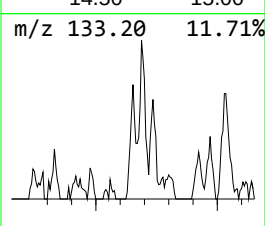
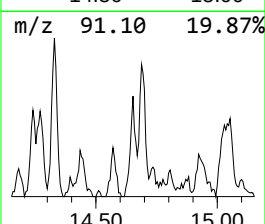
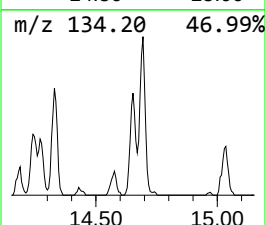
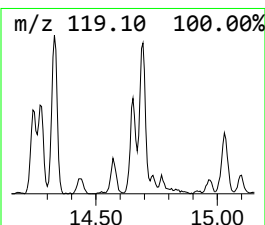
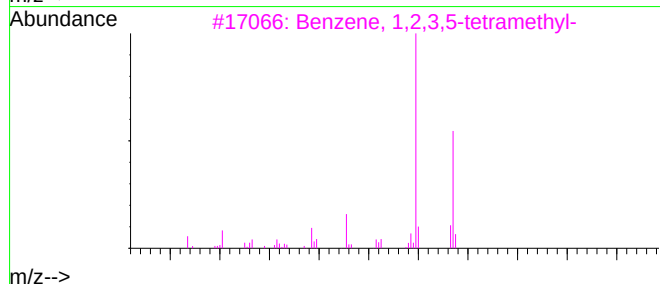
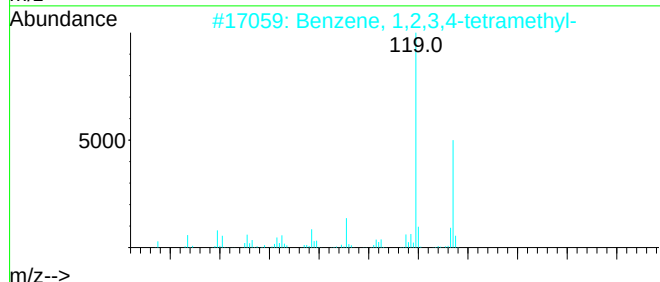
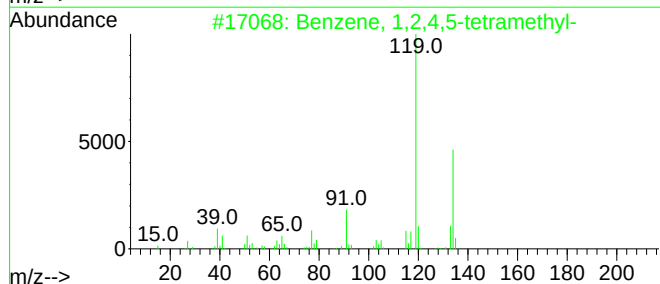
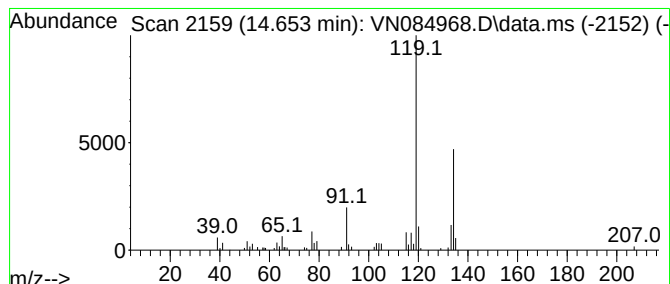
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.653	5.45 ug/l	109905	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
Data File : VN084968.D
Acq On : 20 Nov 2024 14:57
Operator : JC\MD
Sample : P4770-01 1000X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

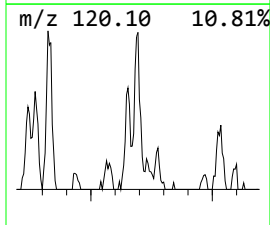
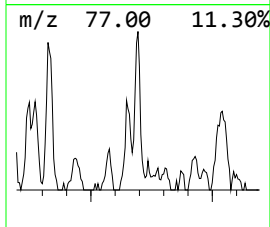
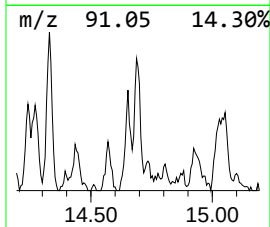
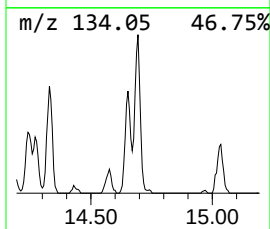
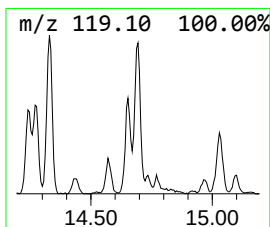
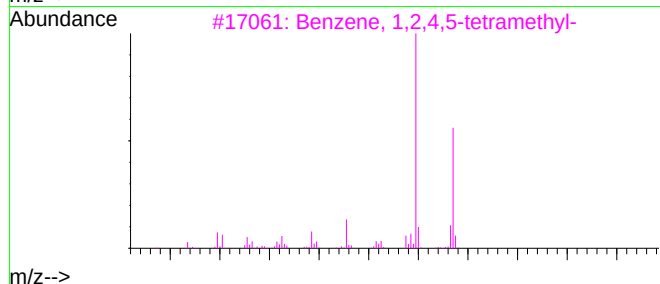
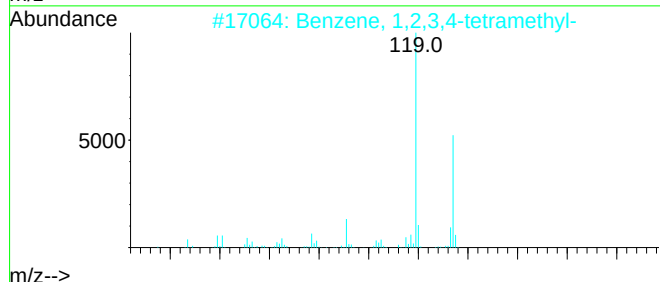
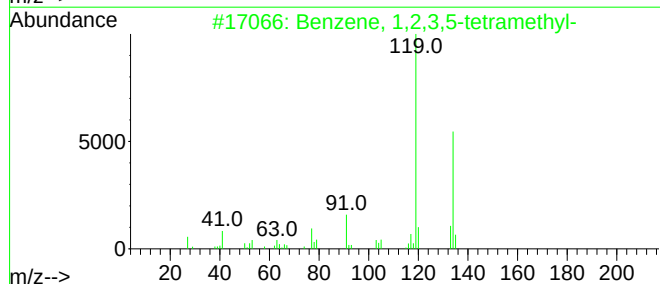
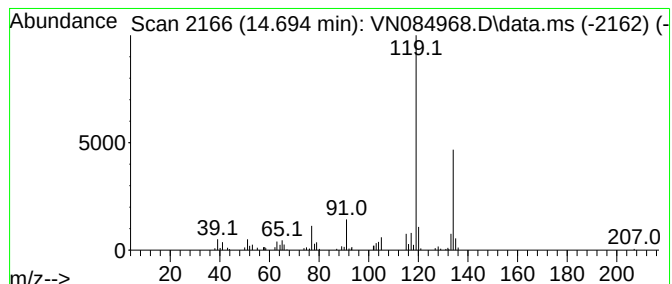
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.694	8.41 ug/l	169620	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
Data File : VN084968.D
Acq On : 20 Nov 2024 14:57
Operator : JC\MD
Sample : P4770-01 1000X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

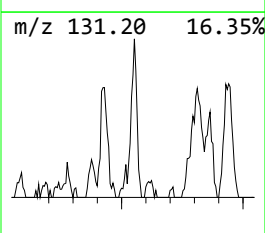
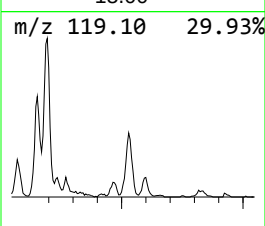
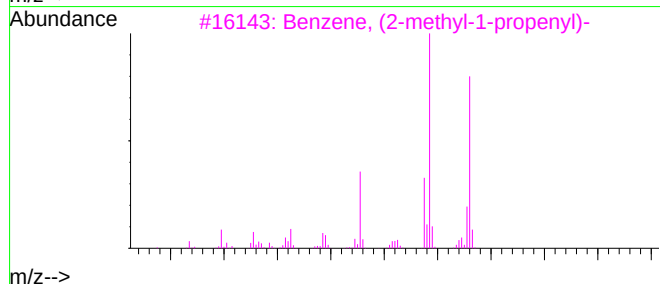
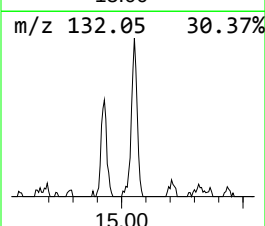
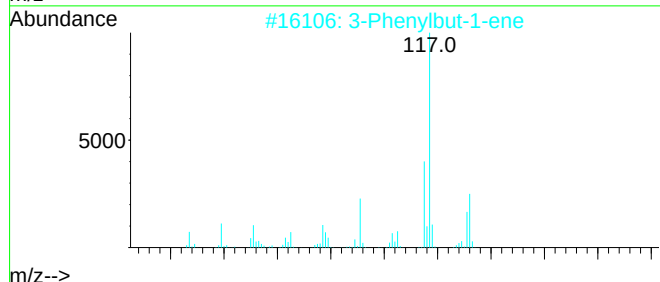
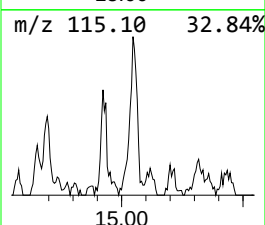
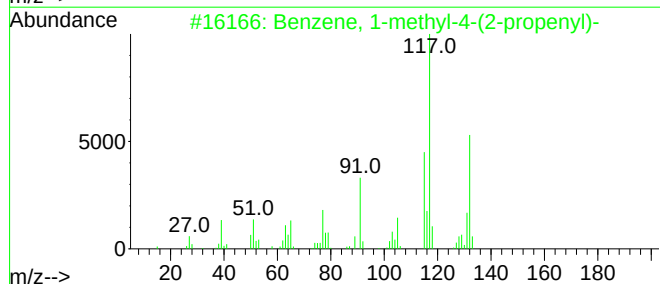
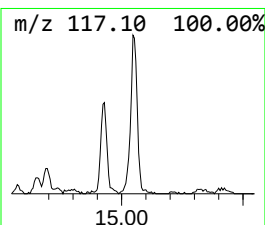
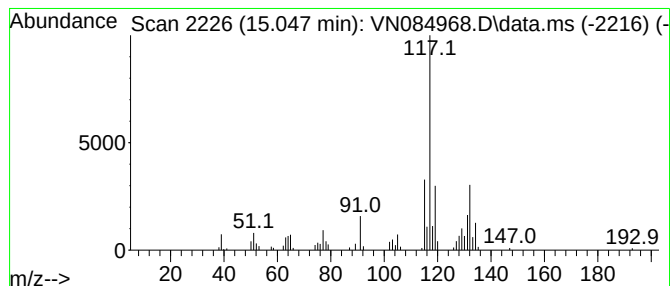
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-methyl-4-(2-prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	10.32 ug/l	207953	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	81
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112024\
Data File : VN084968.D
Acq On : 20 Nov 2024 14:57
Operator : JC\MD
Sample : P4770-01 1000X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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
Acetic acid	8.753	37.3	ug/l	539981	2	9.100	724642	50.0
Benzene, 1-ethy...	13.094	18.4	ug/l	371767	4	13.794	1007940	50.0
Benzene, 1-ethy...	13.335	7.6	ug/l	153090	4	13.794	1007940	50.0
Bicyclo[4.2.0]o...	13.988	14.1	ug/l	284902	4	13.794	1007940	50.0
o-Cymene	14.018	10.7	ug/l	216510	4	13.794	1007940	50.0
Benzene, 4-ethy...	14.329	7.9	ug/l	159542	4	13.794	1007940	50.0
Benzene, 1,2,4,...	14.653	5.5	ug/l	109905	4	13.794	1007940	50.0
Benzene, 1,2,3,...	14.694	8.4	ug/l	169620	4	13.794	1007940	50.0
Benzene, 1-meth...	15.047	10.3	ug/l	207953	4	13.794	1007940	50.0