

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
 Data File : VN081499.D
 Acq On : 20 Mar 2024 17:22
 Operator : JC\MD
 Sample : P1799-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 50295

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\82N031824W.M
 Title : SW846 8260

Signal : TIC: VN081499.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.248	214	220	230	rVB5	19087	55996	1.74%	0.105%
2	4.430	412	421	431	rBV	12715	33242	1.04%	0.062%
3	8.171	1047	1057	1061	rBV	368247	901874	28.08%	1.690%
4	8.224	1061	1066	1078	rVB	722308	1604481	49.96%	3.007%
5	8.583	1117	1127	1140	rBV	399293	967925	30.14%	1.814%
6	9.100	1206	1215	1229	rBV	999900	2046641	63.73%	3.835%
7	10.571	1456	1465	1471	rBV	1460109	2753978	85.76%	5.160%
8	10.629	1471	1475	1484	rVB	451711	833422	25.95%	1.562%
9	11.865	1676	1685	1695	rBV	1343884	2359395	73.47%	4.421%
10	11.965	1695	1702	1712	rVB	623084	1058573	32.96%	1.984%
11	12.071	1712	1720	1730	rBV	1681645	3211321	100.00%	6.017%
12	12.400	1765	1776	1784	rBV	1457198	2438371	75.93%	4.569%
13	12.694	1820	1826	1833	rVB2	36485	59288	1.85%	0.111%
14	12.853	1845	1853	1863	rVB	1013259	1769120	55.09%	3.315%
15	13.035	1878	1884	1888	rBV	78516	123883	3.86%	0.232%
16	13.100	1888	1895	1898	rVV	1275331	2140797	66.66%	4.011%
17	13.129	1898	1900	1904	rVV	652015	946762	29.48%	1.774%
18	13.176	1904	1908	1915	rVB	779776	1236439	38.50%	2.317%
19	13.335	1928	1935	1943	rBV	735218	1209436	37.66%	2.266%
20	13.482	1953	1960	1971	rVB	1521217	2420213	75.37%	4.535%
21	13.617	1974	1983	1987	rBV4	31222	61995	1.93%	0.116%
22	13.676	1987	1993	1998	rBV	144739	240774	7.50%	0.451%
23	13.729	1998	2002	2006	rVB2	62570	82578	2.57%	0.155%
24	13.794	2006	2013	2016	rBV	1342485	2524892	78.62%	4.731%
25	13.882	2024	2028	2034	rVB5	30994	57619	1.79%	0.108%
26	13.953	2034	2040	2041	rBV	195564	259717	8.09%	0.487%
27	13.994	2041	2047	2050	rBV2	606359	1225270	38.15%	2.296%
28	14.117	2063	2068	2073	rVB4	91242	151543	4.72%	0.284%
29	14.182	2073	2079	2084	rBV	248874	405123	12.62%	0.759%
30	14.247	2084	2090	2092	rBV	334459	524772	16.34%	0.983%
31	14.276	2092	2095	2099	rVB	325490	466376	14.52%	0.874%
32	14.329	2099	2104	2110	rVB	582134	936157	29.15%	1.754%
33	14.400	2110	2116	2119	rBV2	151026	255779	7.96%	0.479%
34	14.447	2119	2124	2133	rVB2	470252	819520	25.52%	1.536%
35	14.523	2133	2137	2140	rVB4	27748	34540	1.08%	0.065%
36	14.576	2140	2146	2151	rVB3	218378	348860	10.86%	0.654%

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37	14.653	2151	2159	2162	rBV	361988	592117	18.44%	1.110%
38	14.694	2162	2166	2171	rVB	499497	714193	22.24%	1.338%
39	14.735	2171	2173	2177	rVB	116253	133955	4.17%	0.251%
40	14.776	2177	2180	2184	rVB	66801	76954	2.40%	0.144%
41	14.876	2188	2197	2201	rBV3	122875	251047	7.82%	0.470%
42	14.929	2201	2206	2211	rBV	560528	992320	30.90%	1.859%
43	15.053	2218	2227	2233	rBV2	1143328	2625747	81.77%	4.920%
44	15.100	2233	2235	2247	rVB4	93687	198092	6.17%	0.371%
45	15.211	2247	2254	2261	rBV	872584	1555924	48.45%	2.916%
46	15.323	2261	2273	2277	rBV3	336160	908721	28.30%	1.703%
47	15.441	2285	2293	2302	rVB4	350180	927507	28.88%	1.738%
48	15.600	2314	2320	2322	rBV6	47364	94548	2.94%	0.177%
49	15.641	2322	2327	2332	rVV	160581	320149	9.97%	0.600%
50	15.700	2332	2337	2342	rVV	290787	560920	17.47%	1.051%
51	15.759	2342	2347	2348	rVV4	169719	299811	9.34%	0.562%
52	15.782	2348	2351	2370	rVB5	236423	819533	25.52%	1.536%
53	15.947	2370	2379	2387	rBV2	288736	617442	19.23%	1.157%
54	16.023	2387	2392	2397	rBV7	23975	50833	1.58%	0.095%
55	16.129	2400	2410	2411	rVV3	240052	478683	14.91%	0.897%
56	16.170	2411	2417	2427	rVV2	735095	1684653	52.46%	3.157%
57	16.258	2427	2432	2438	rVV3	87839	196894	6.13%	0.369%
58	16.347	2438	2447	2460	rVB2	200555	651379	20.28%	1.221%
59	16.506	2463	2474	2486	rBV2	468928	1152784	35.90%	2.160%
60	16.717	2498	2510	2515	rBV2	230856	605594	18.86%	1.135%
61	16.782	2515	2521	2522	rBV	216047	290502	9.05%	0.544%

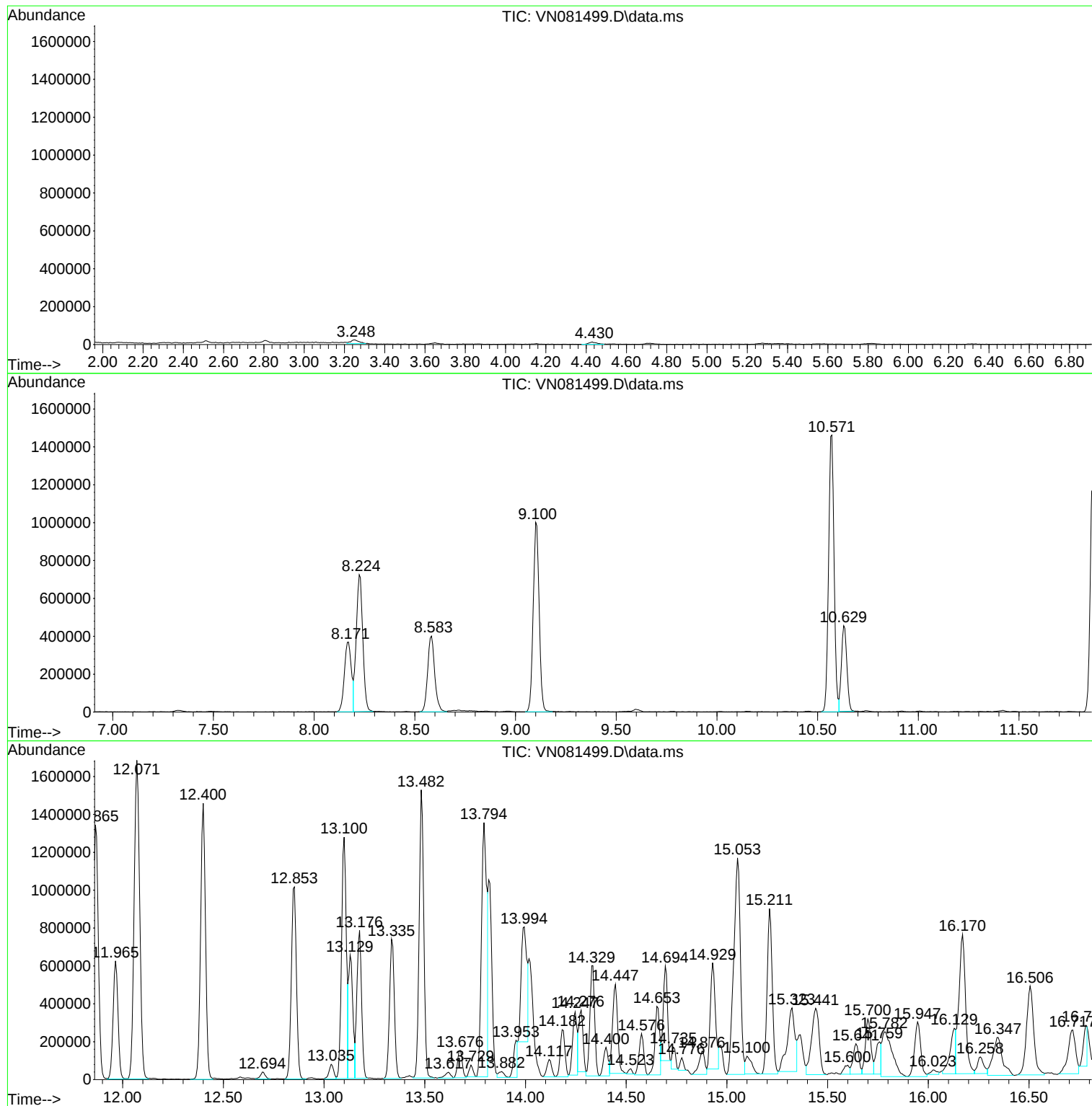
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Quant Title : SW846 8260

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



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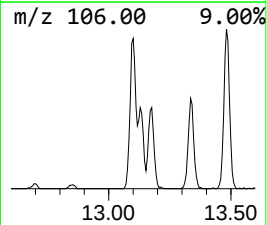
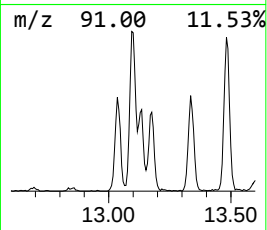
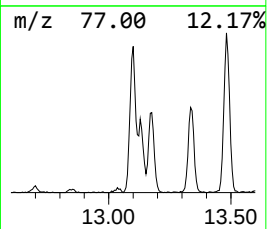
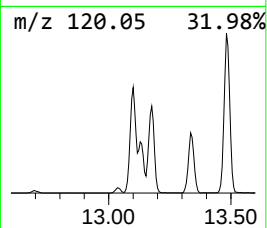
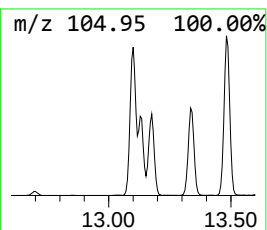
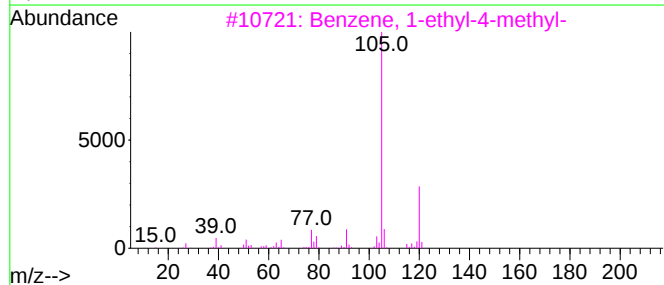
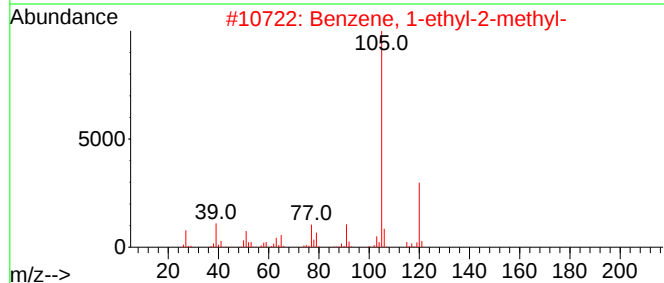
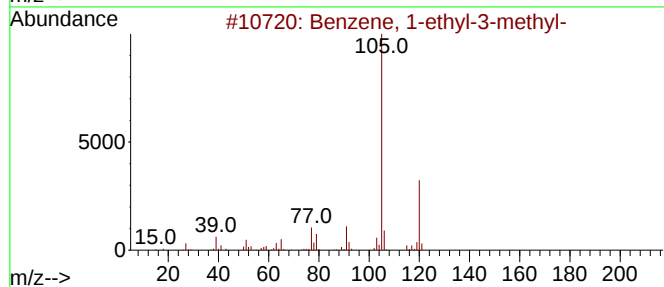
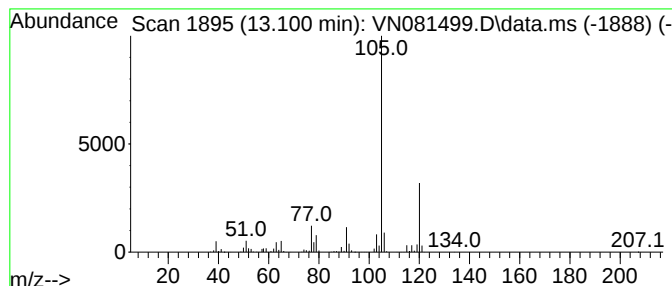
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	42.39 ug/l	2140800	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	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	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			Mesitylene	120	C9H12	000108-67-8	91



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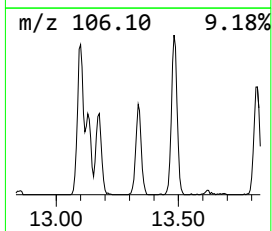
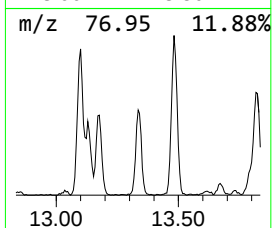
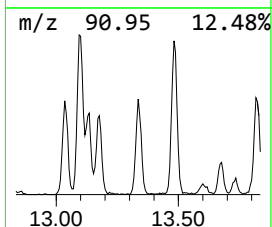
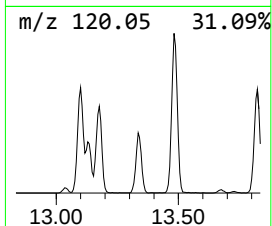
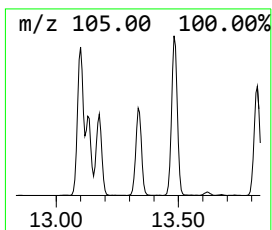
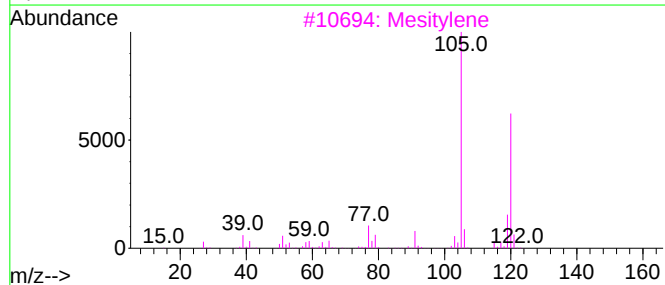
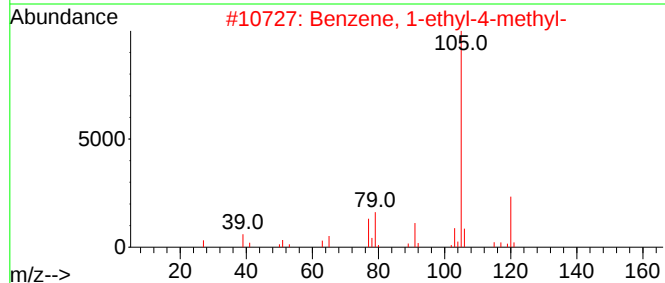
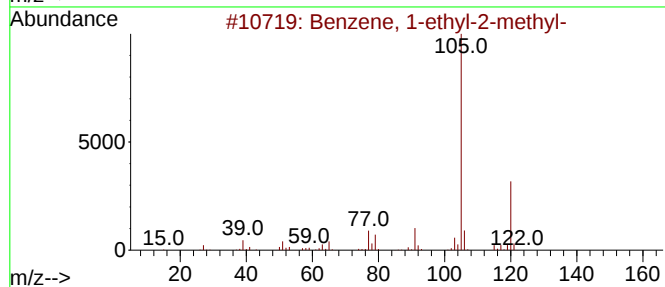
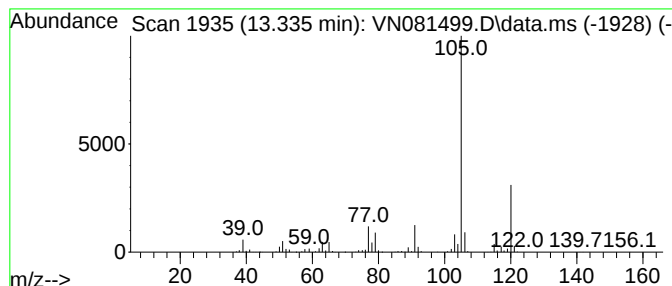
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	23.95 ug/l	1209440	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	93
3			Mesitylene	120	C9H12	000108-67-8	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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ALS Vial : 15 Sample Multiplier: 1

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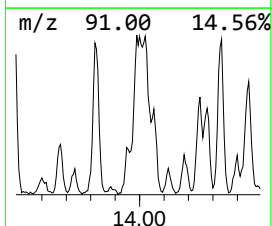
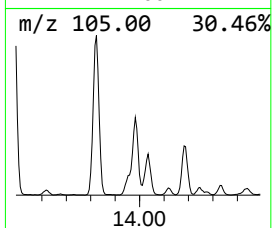
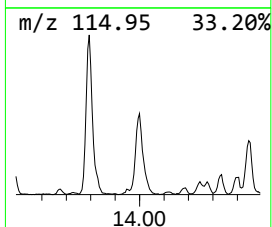
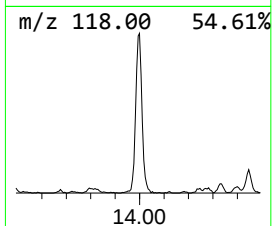
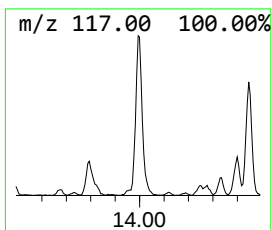
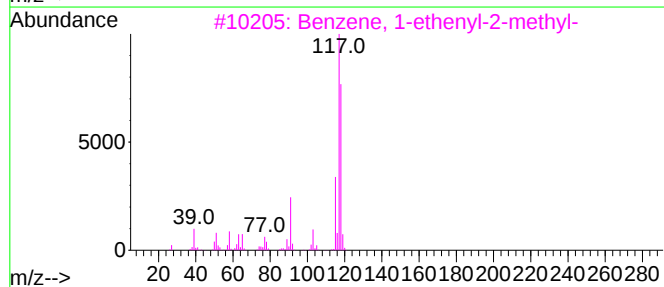
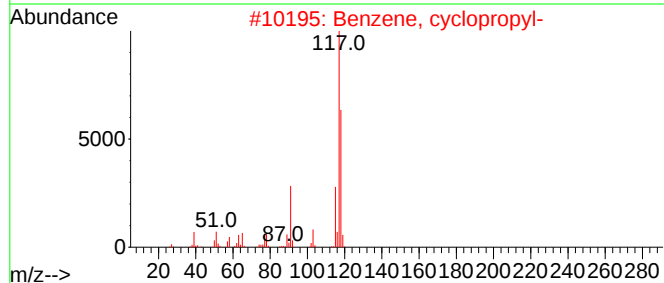
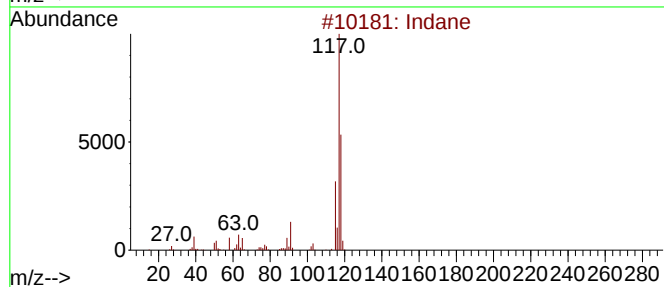
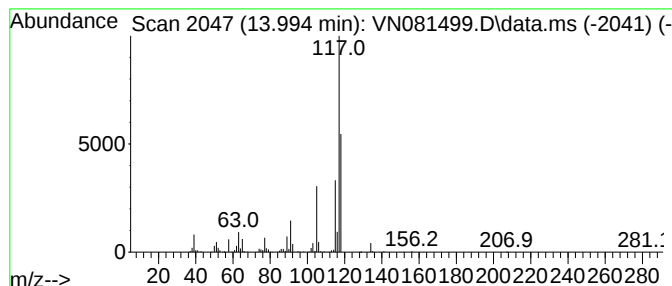
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	24.26 ug/l	1225270	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	92
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	62
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	62
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	58
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53



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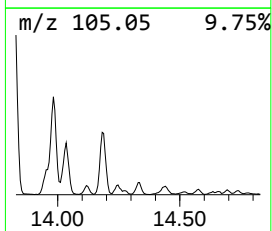
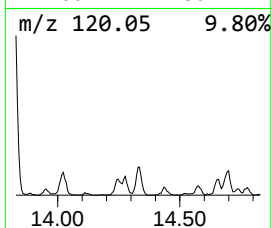
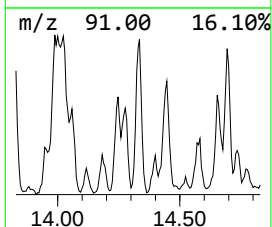
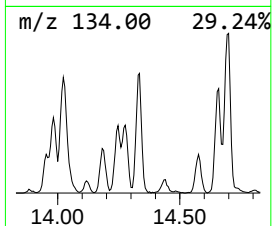
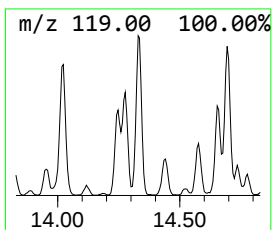
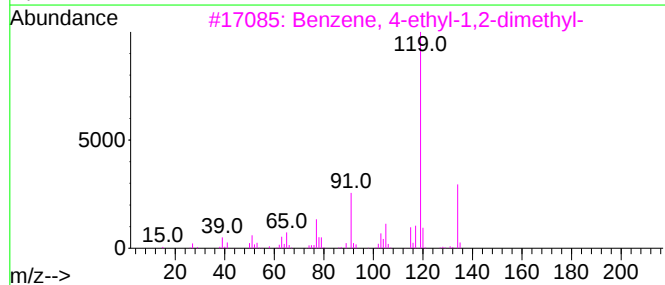
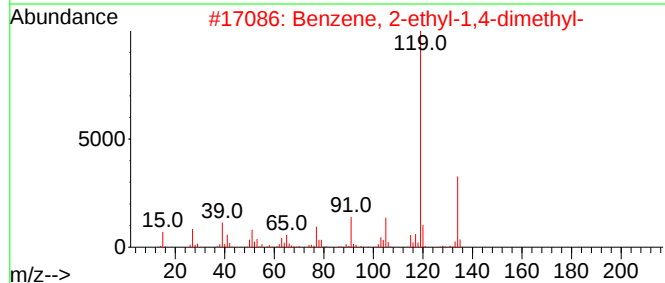
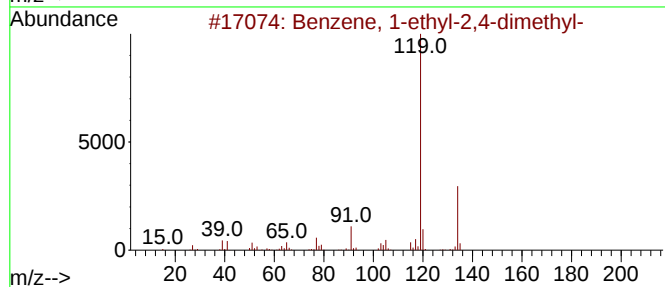
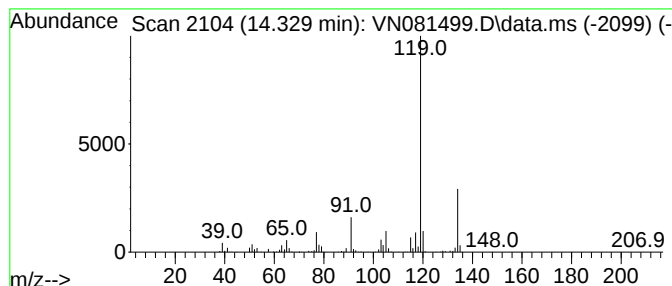
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	18.54 ug/l	936157	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5			o-Cymene	134	C10H14	000527-84-4	94



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ClientSampleId :
50295

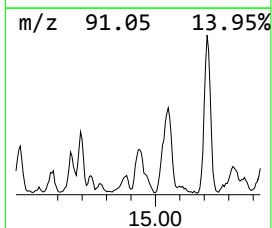
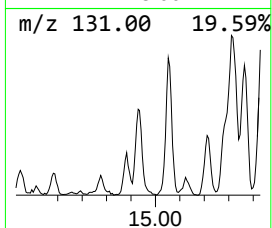
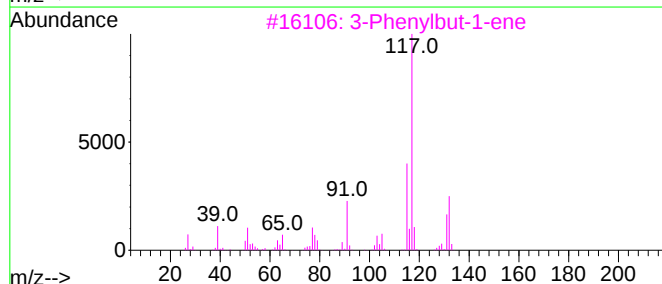
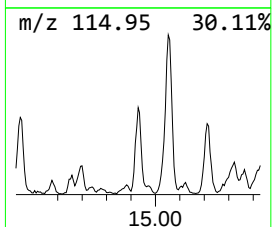
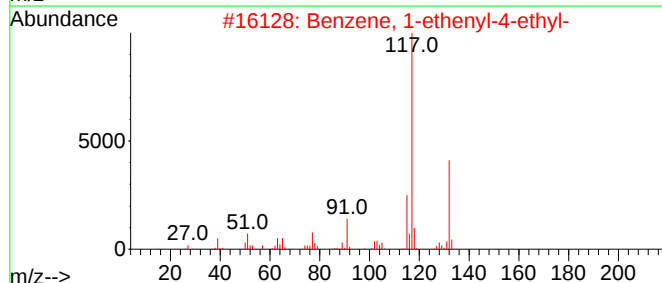
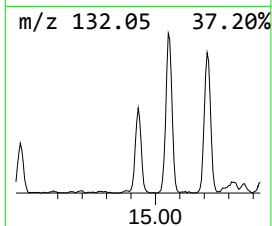
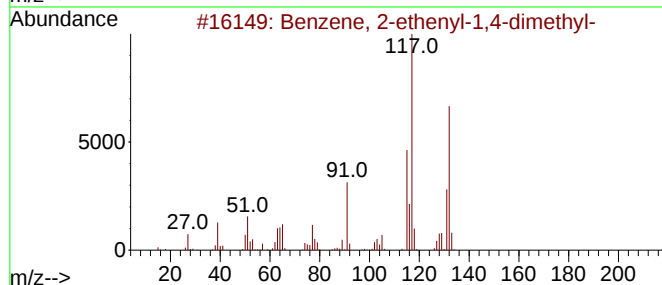
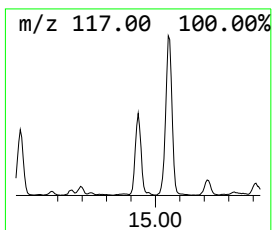
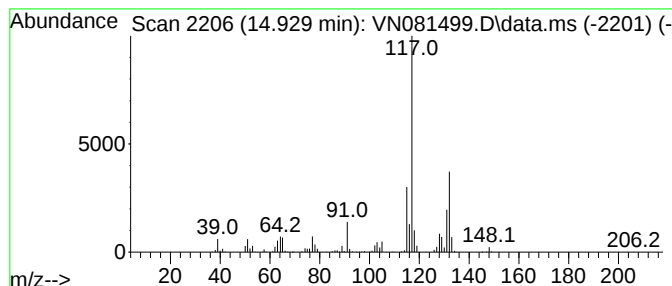
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	19.65 ug/l	992320	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	94
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081499.D
Acq On : 20 Mar 2024 17:22
Operator : JC\MD
Sample : P1799-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50295

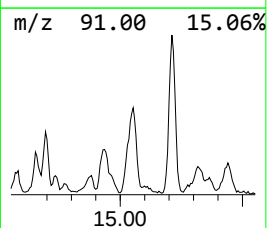
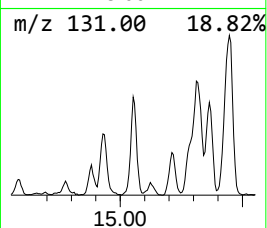
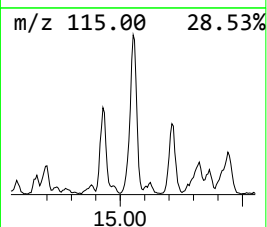
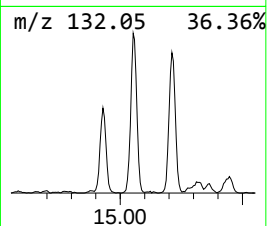
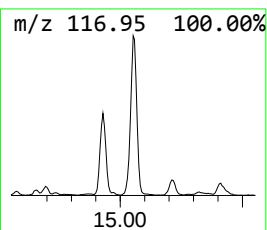
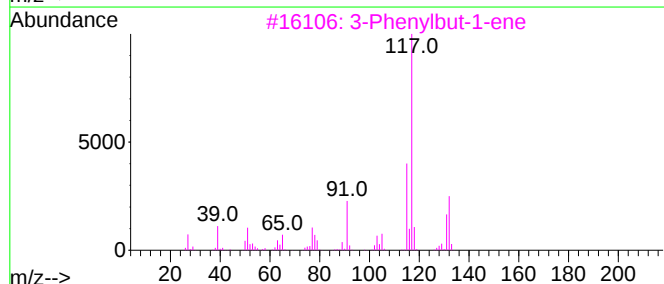
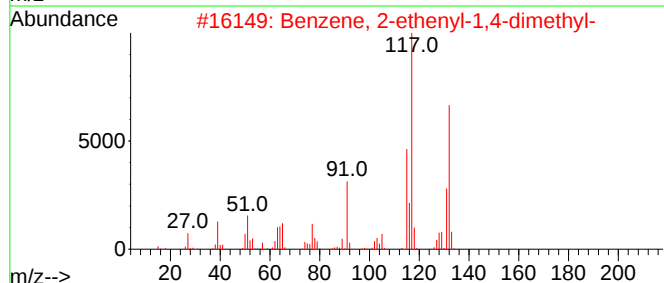
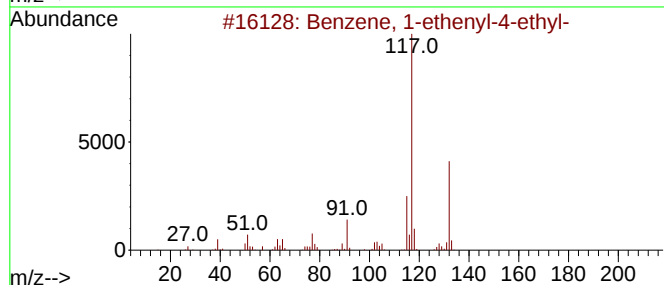
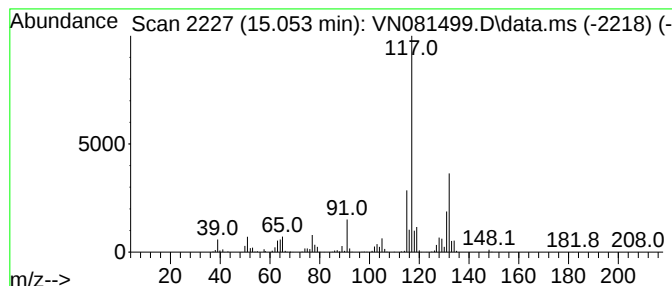
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	52.00 ug/l	2625750	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081499.D
Acq On : 20 Mar 2024 17:22
Operator : JC\MD
Sample : P1799-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50295

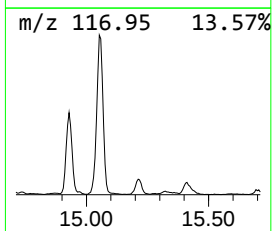
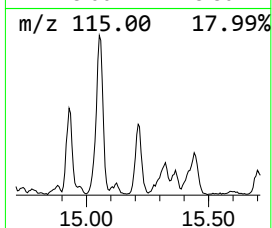
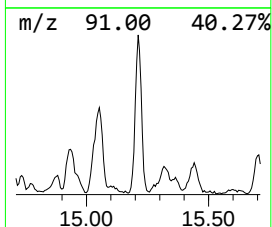
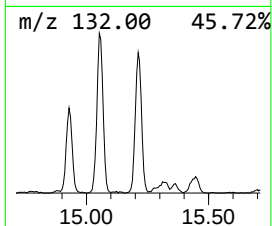
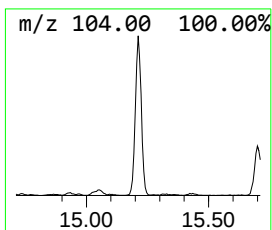
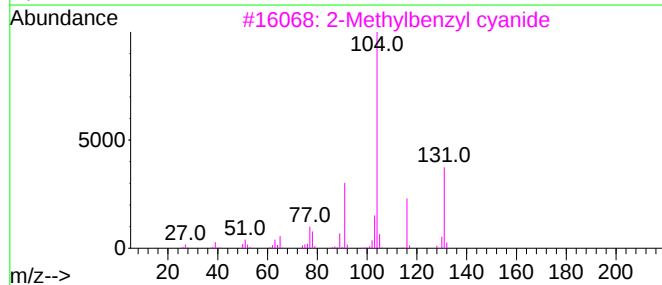
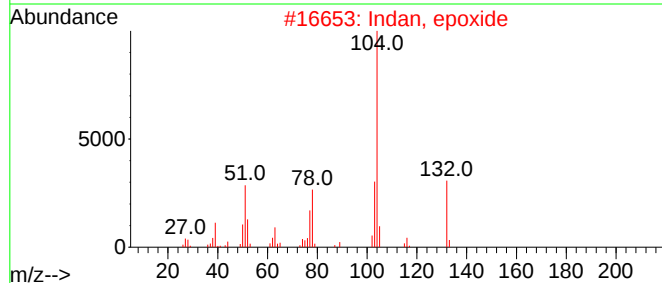
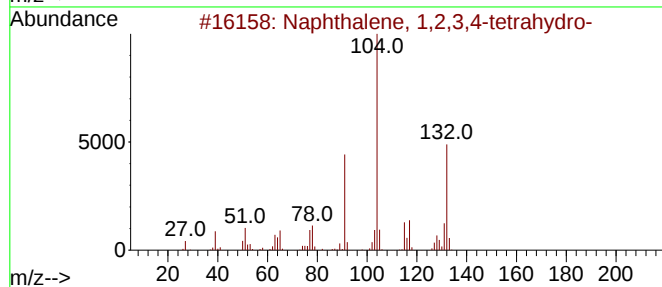
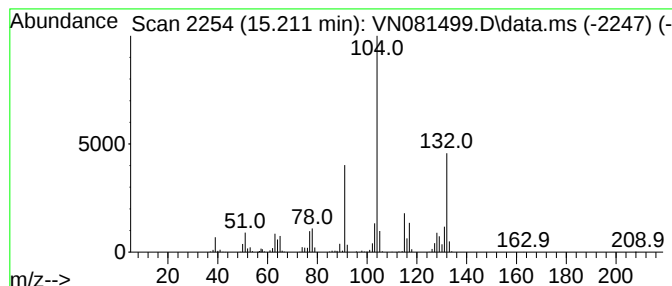
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	30.81 ug/l	1555920	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			Indan, epoxide	132	C9H8O	000768-22-9	58
3			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	49
4			Acetic acid, 2-phenylethyl ester	164	C10H12O2	000103-45-7	38
5			Styrene	104	C8H8	000100-42-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081499.D
Acq On : 20 Mar 2024 17:22
Operator : JC\MD
Sample : P1799-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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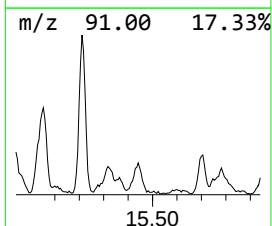
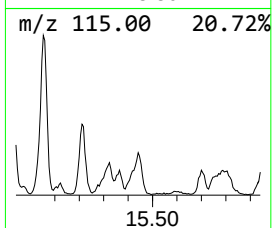
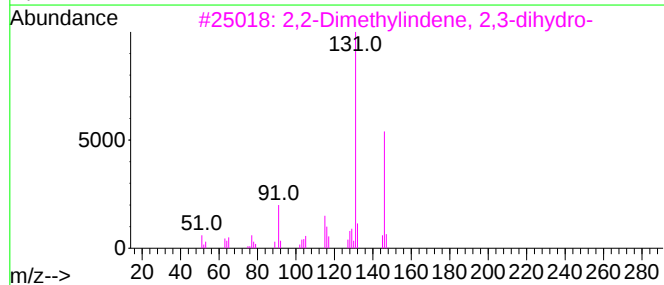
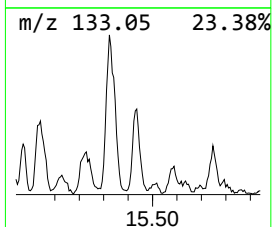
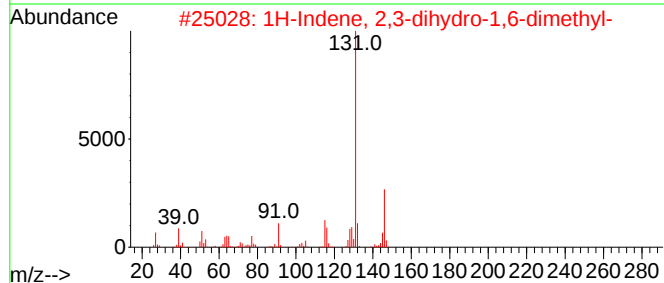
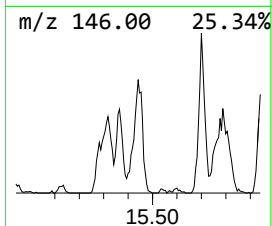
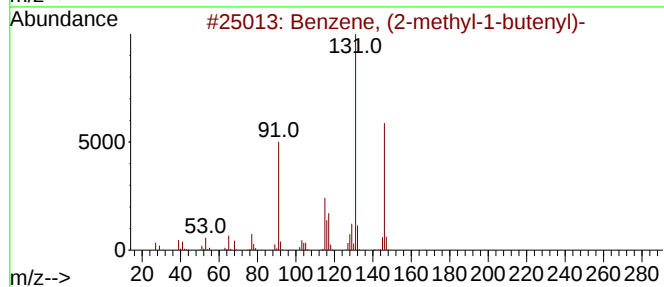
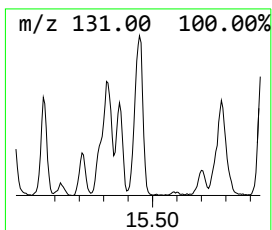
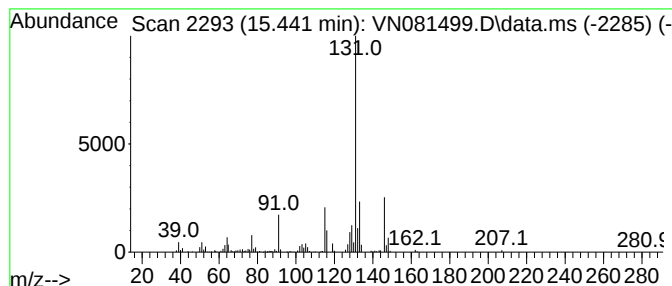
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (2-methyl-1-butenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.441	18.37 ug/l	927507	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	87
2			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	87
3			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	87
4			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87
5			1,3-Cyclopentadiene, 5-(trans-2-...	146	C11H14	079209-36-2	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081499.D
Acq On : 20 Mar 2024 17:22
Operator : JC\MD
Sample : P1799-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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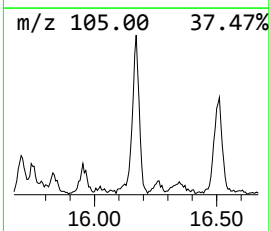
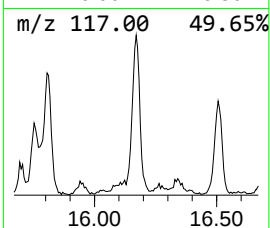
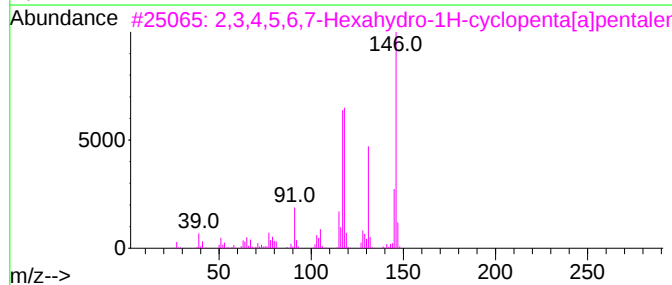
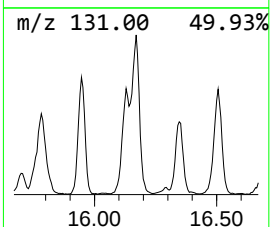
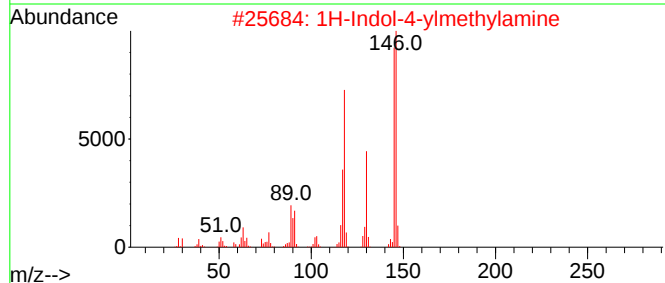
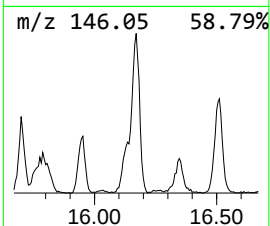
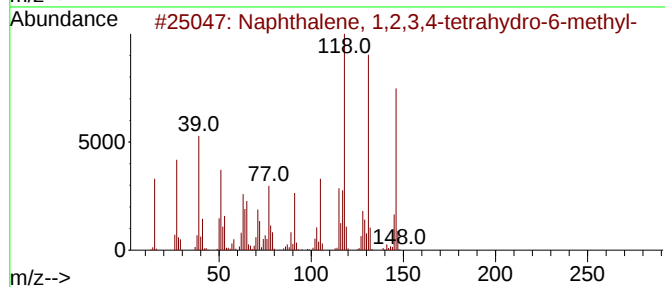
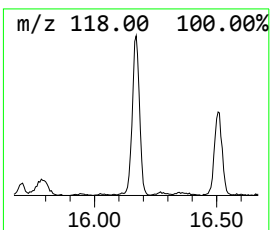
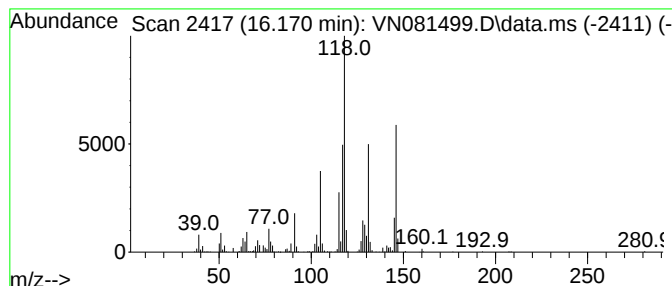
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	33.36 ug/l	1684650	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	64
2			1H-Indol-4-ylmethylamine	146	C9H10N2	003468-18-6	52
3			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	46
4			1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	46
5			5H-Benzocycloheptene,6,7,8,9-tet...	146	C11H14	001075-16-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081499.D
Acq On : 20 Mar 2024 17:22
Operator : JC\MD
Sample : P1799-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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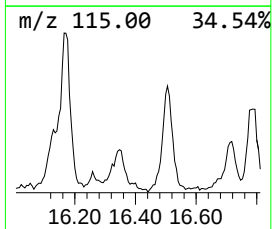
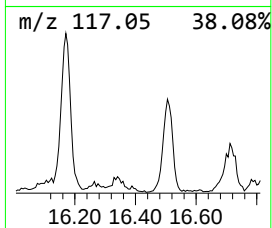
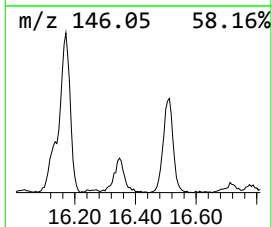
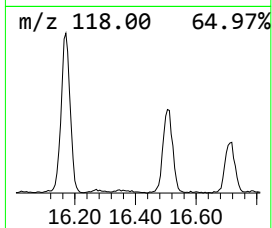
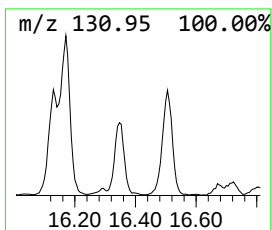
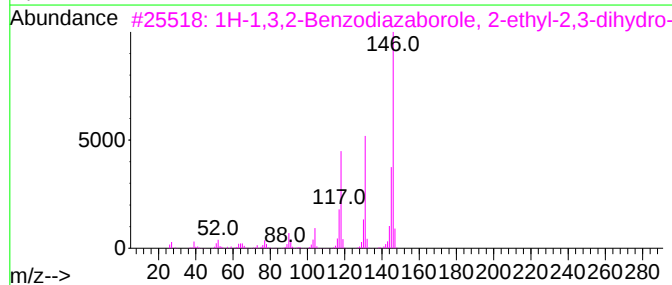
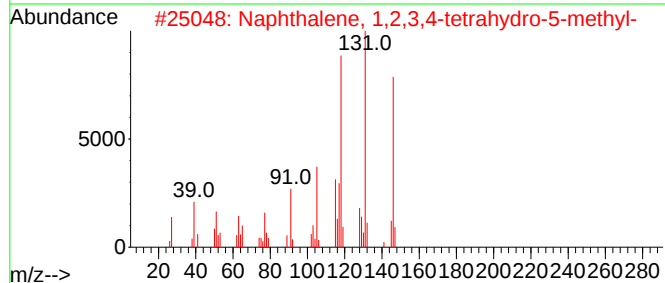
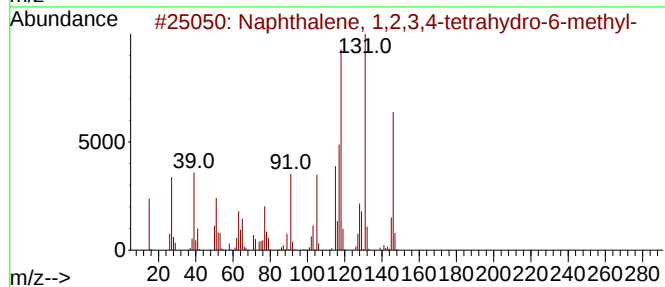
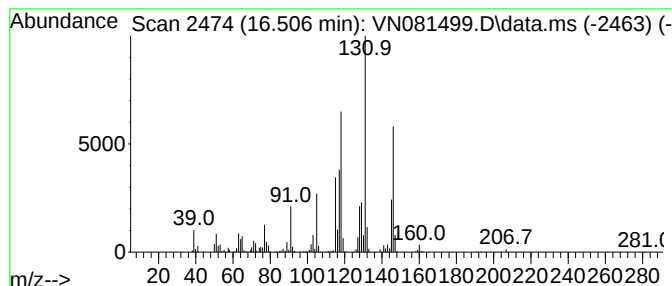
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	22.83 ug/l	1152780	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	81
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	64
5			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081499.D
Acq On : 20 Mar 2024 17:22
Operator : JC\MD
Sample : P1799-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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
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Benzene, 1-ethy...	13.335	23.9	ug/l	1209440	4	13.794	2524890	50.0
Indane	13.994	24.3	ug/l	1225270	4	13.794	2524890	50.0
Benzene, 1-ethy...	14.329	18.5	ug/l	936157	4	13.794	2524890	50.0
Benzene, 2-ethe...	14.929	19.6	ug/l	992320	4	13.794	2524890	50.0
Benzene, 1-ethe...	15.053	52.0	ug/l	2625750	4	13.794	2524890	50.0
Naphthalene, 1,...	15.211	30.8	ug/l	1555920	4	13.794	2524890	50.0
Benzene, (2-met...	15.441	18.4	ug/l	927507	4	13.794	2524890	50.0
Naphthalene, 1,...	16.170	33.4	ug/l	1684650	4	13.794	2524890	50.0
Naphthalene, 1,...	16.506	22.8	ug/l	1152780	4	13.794	2524890	50.0