

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
 Data File : VN084952.D
 Acq On : 19 Nov 2024 17:16
 Operator : JC\MD
 Sample : P4843-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SW-WTS-01

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: VN084952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.453	415	425	447	rBV4	26344	106578	3.89%	0.711%
2	7.965	1011	1022	1033	rBV	27254	70929	2.59%	0.473%
3	8.165	1044	1056	1060	rBV	153939	363872	13.29%	2.428%
4	8.224	1060	1066	1077	rVB	265801	600407	21.93%	4.007%
5	8.594	1116	1129	1136	rBV3	284489	960503	35.09%	6.410%
6	9.100	1206	1215	1227	rBV	405638	819686	29.94%	5.470%
7	9.312	1241	1251	1267	rBV	51527	174897	6.39%	1.167%
8	10.565	1456	1464	1471	rBV	582003	1052174	38.43%	7.022%
9	10.629	1471	1475	1483	rVB	23019	40102	1.46%	0.268%
10	11.865	1677	1685	1694	rBV	513250	900811	32.91%	6.012%
11	11.965	1694	1702	1712	rVV	423588	725869	26.52%	4.844%
12	12.070	1712	1720	1730	rVB2	67184	133099	4.86%	0.888%
13	12.394	1769	1775	1782	rBV	77117	132644	4.85%	0.885%
14	12.694	1820	1826	1834	rVB	80839	132824	4.85%	0.886%
15	12.847	1843	1852	1860	rBV	437594	731556	26.72%	4.882%
16	13.035	1878	1884	1890	rBV	34796	56070	2.05%	0.374%
17	13.129	1890	1900	1904	rVV	37994	75026	2.74%	0.501%
18	13.170	1904	1907	1913	rVB	33063	51612	1.89%	0.344%
19	13.335	1925	1935	1942	rVB	107988	175176	6.40%	1.169%
20	13.482	1949	1960	1967	rBV	196900	328191	11.99%	2.190%
21	13.788	2005	2012	2022	rBV2	503574	1043699	38.13%	6.966%
22	13.870	2022	2026	2034	rVB	56263	94020	3.43%	0.627%
23	13.953	2034	2040	2041	rBV2	18970	28700	1.05%	0.192%
24	13.994	2041	2047	2057	rVB	1504088	2535777	92.63%	16.924%
25	14.176	2072	2078	2084	rVB2	18541	35025	1.28%	0.234%
26	14.329	2099	2104	2111	rVB	27138	41295	1.51%	0.276%
27	14.447	2117	2124	2135	rVB	94220	170072	6.21%	1.135%
28	14.553	2135	2142	2152	rVB6	18190	41882	1.53%	0.280%
29	14.929	2199	2206	2212	rBV	52110	87082	3.18%	0.581%
30	15.053	2218	2227	2233	rBV3	55155	126257	4.61%	0.843%
31	15.117	2233	2238	2245	rVB4	18448	32724	1.20%	0.218%
32	15.206	2246	2253	2261	rVB2	74503	134725	4.92%	0.899%
33	15.311	2264	2271	2277	rBV6	17021	34919	1.28%	0.233%
34	15.429	2285	2291	2298	rBV4	22733	42713	1.56%	0.285%
35	15.641	2318	2327	2336	rBV	1424854	2737543	100.00%	18.270%
36	15.741	2338	2344	2352	rVB	34875	65643	2.40%	0.438%

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

37	16.782	2513	2521	2522	rbV	63169	99653	3.64%	0.665%
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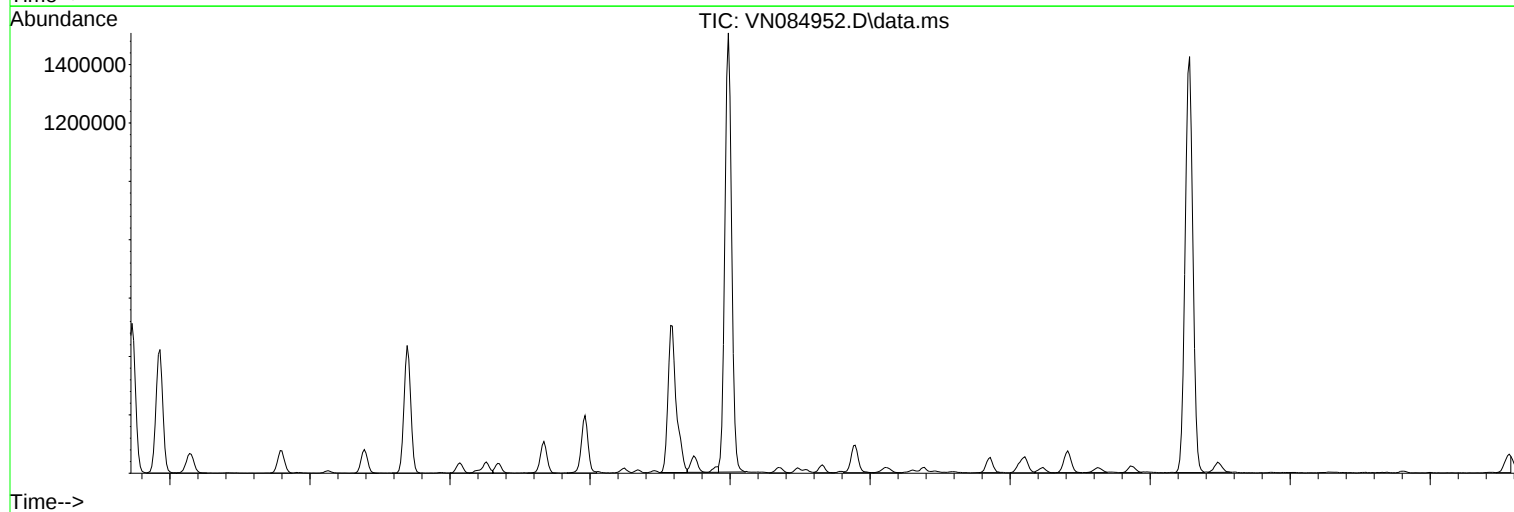
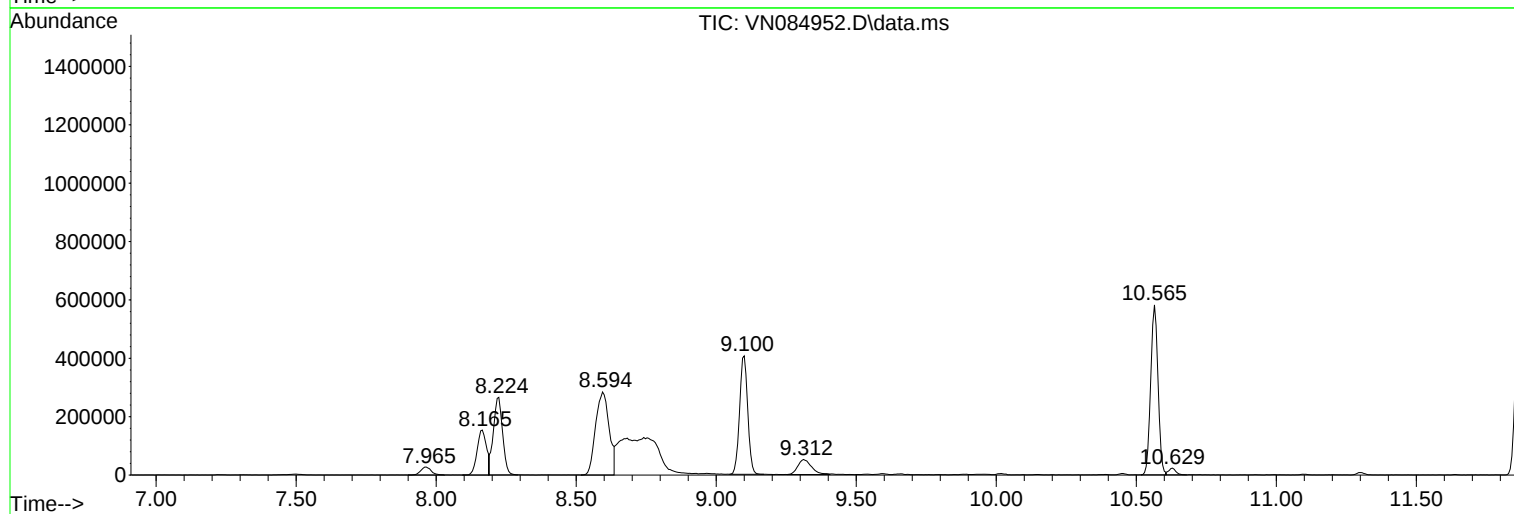
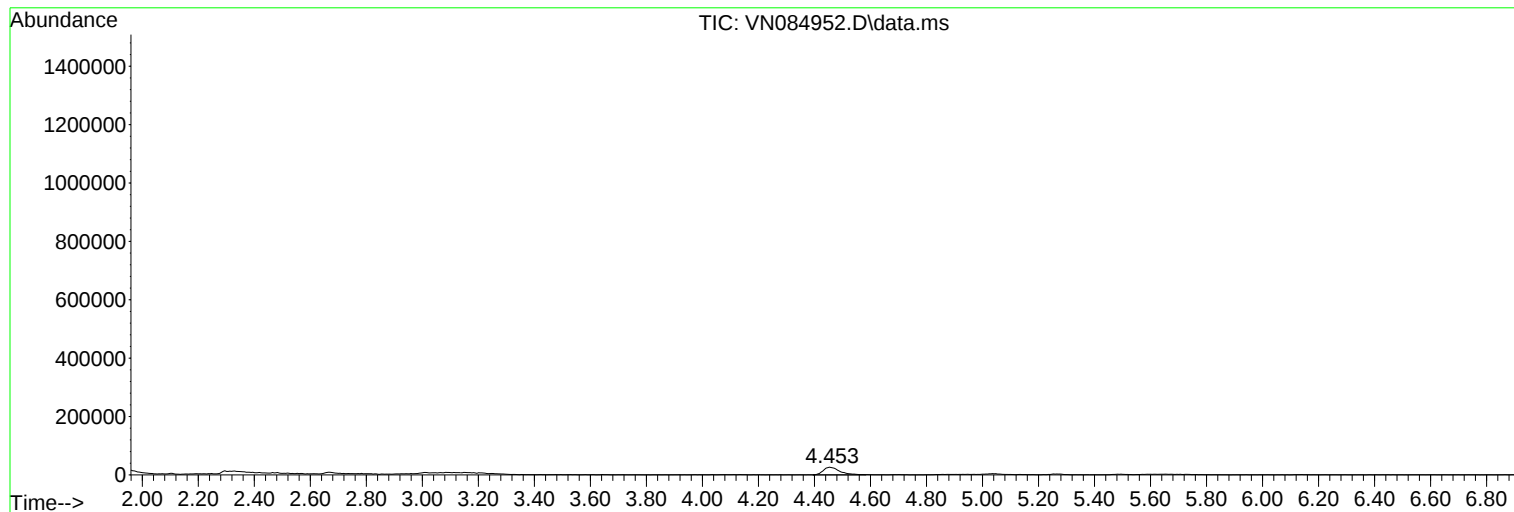
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Quant Title : SW846 8260

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



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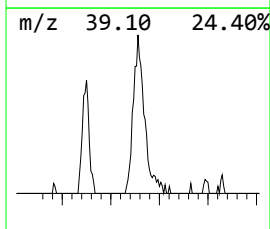
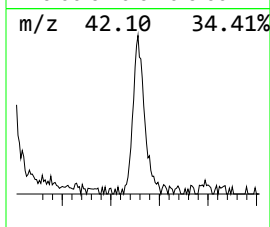
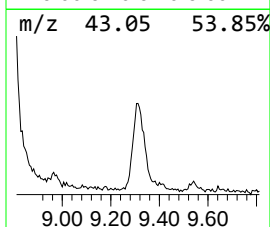
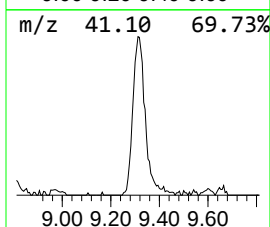
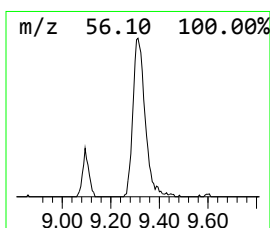
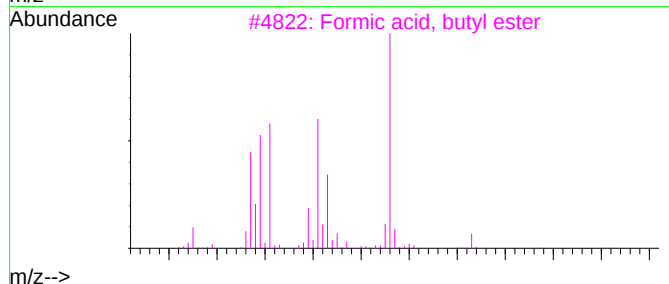
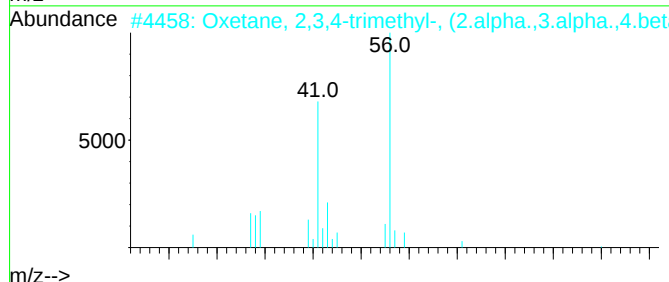
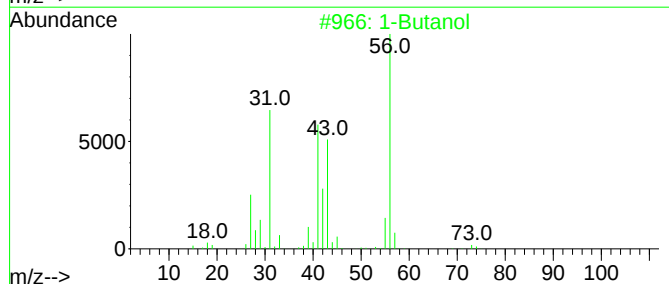
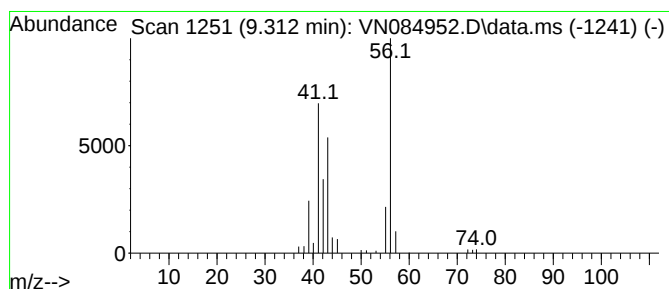
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.312	10.67 ug/l	174897	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	9
3	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	2-Butene, (Z)-	56	C4H8	000590-18-1	9



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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
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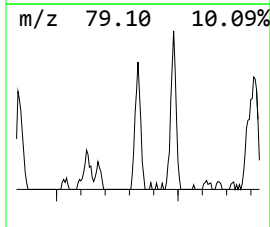
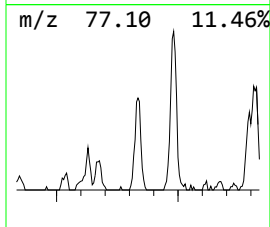
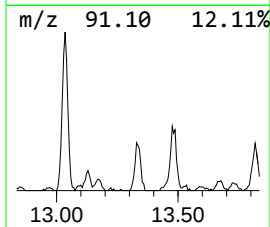
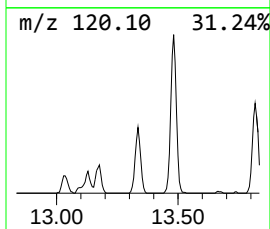
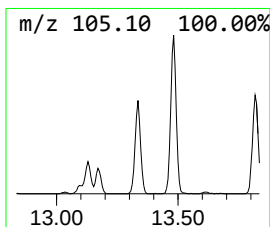
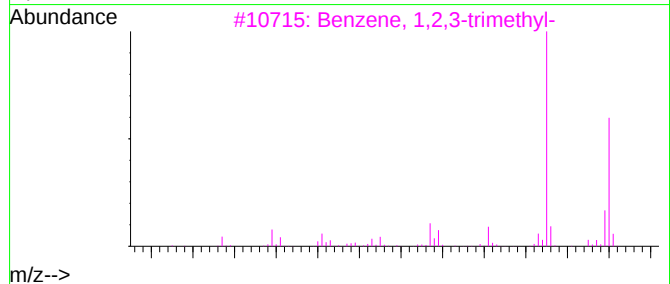
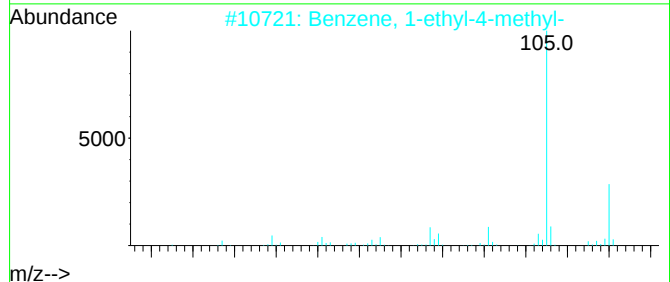
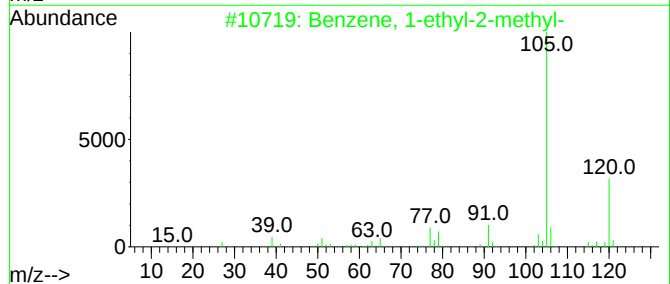
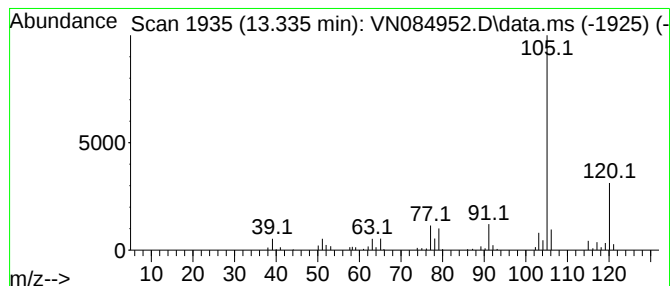
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	8.39 ug/l	175176	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	95
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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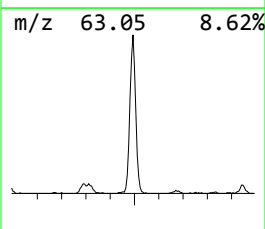
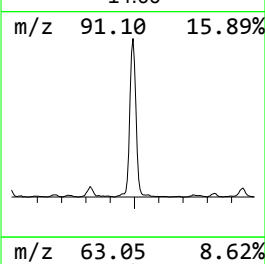
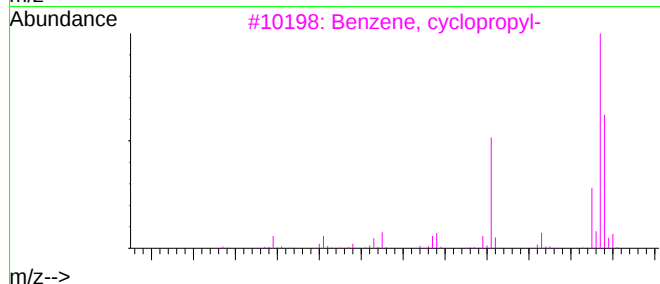
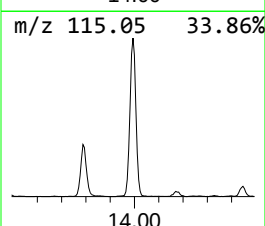
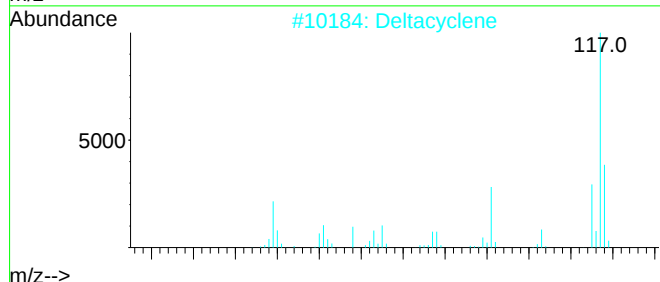
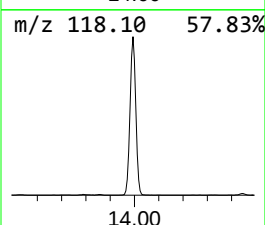
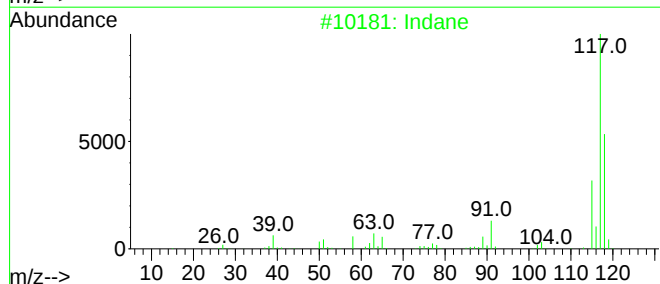
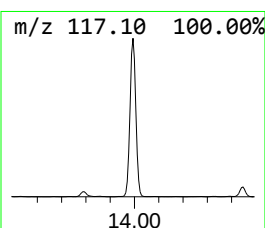
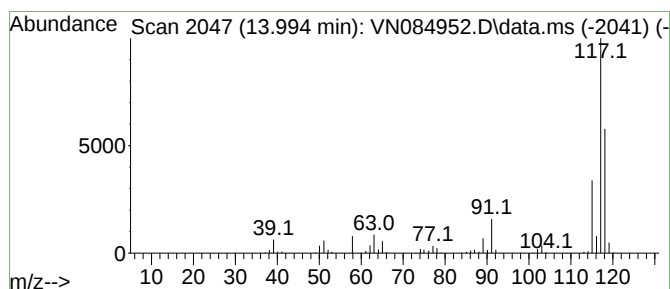
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	121.48 ug/l	2535780	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Deltacyclene	118	C9H10	007785-10-6	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-	118	C9H10	1000191-13-7	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60



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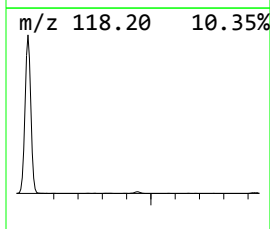
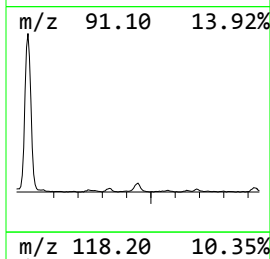
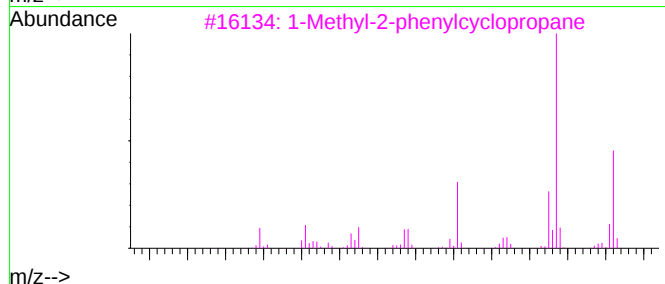
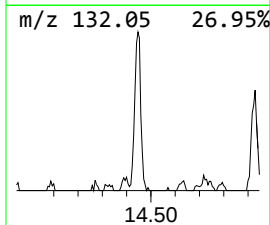
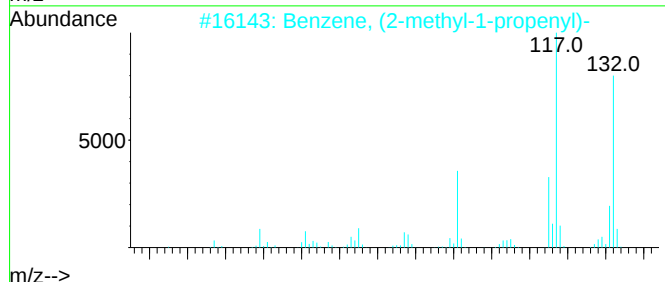
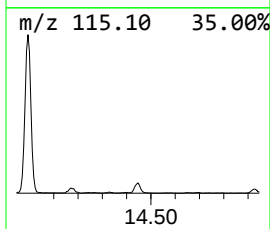
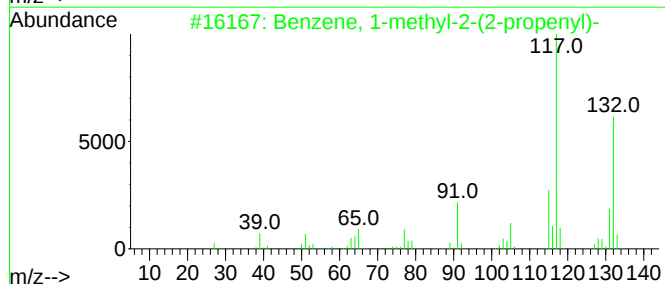
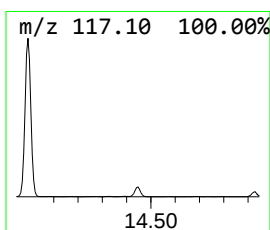
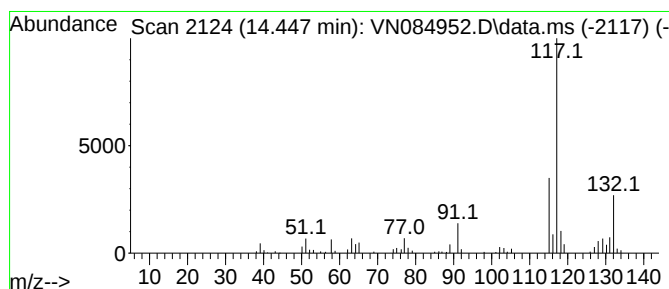
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	8.15 ug/l	170072	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	78
2	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	78
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	78
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	78
5	Indan, 1-methyl-	132	C10H12	000767-58-8	76



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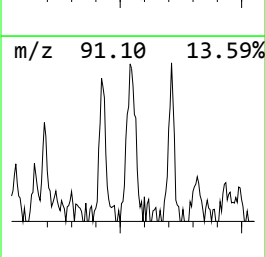
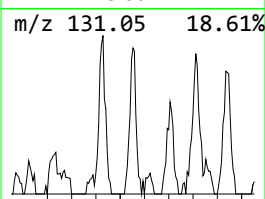
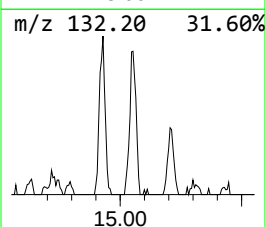
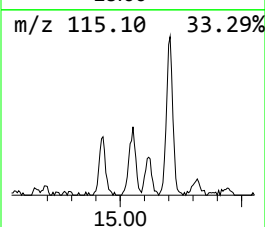
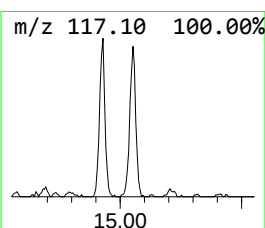
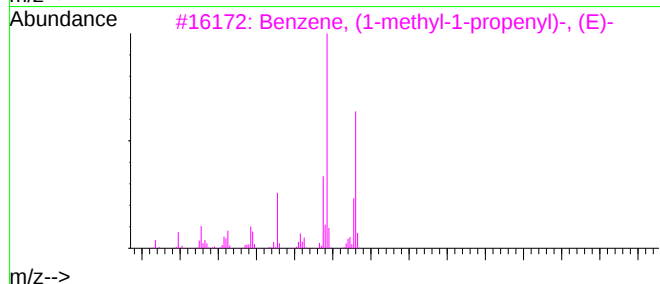
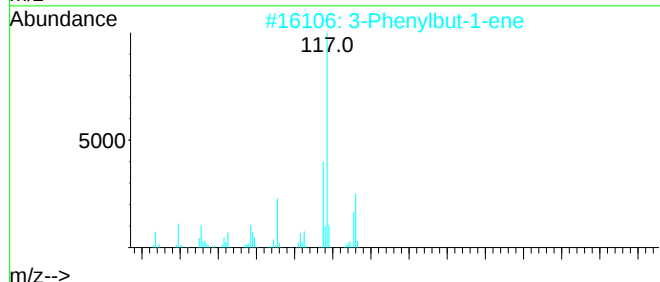
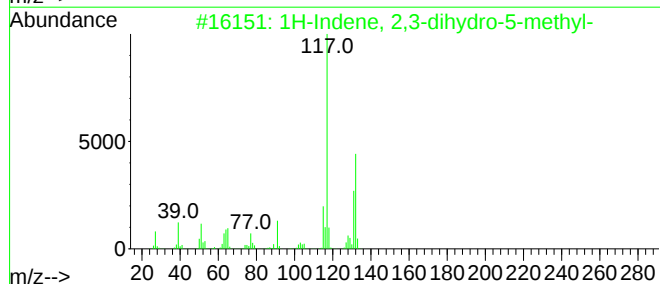
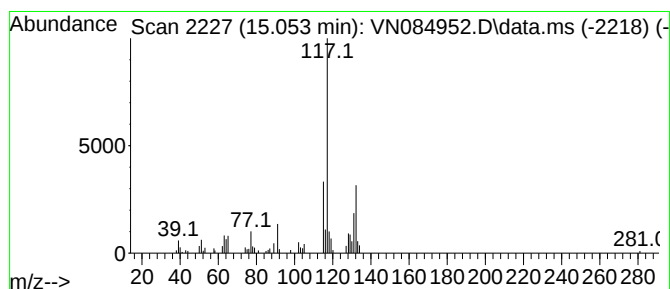
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.053	6.05 ug/l	126257	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
Data File : VN084952.D
Acq On : 19 Nov 2024 17:16
Operator : JC\MD
Sample : P4843-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SW-WTS-01

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

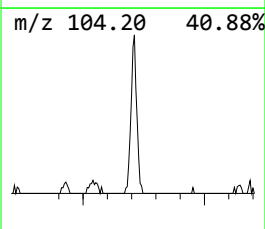
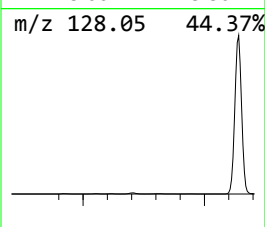
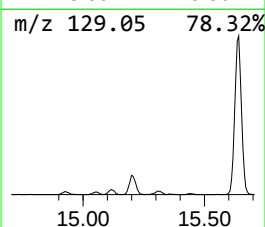
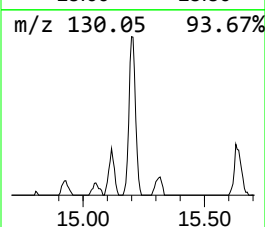
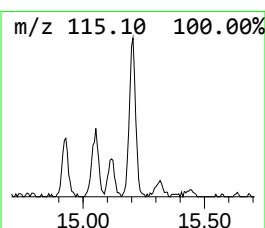
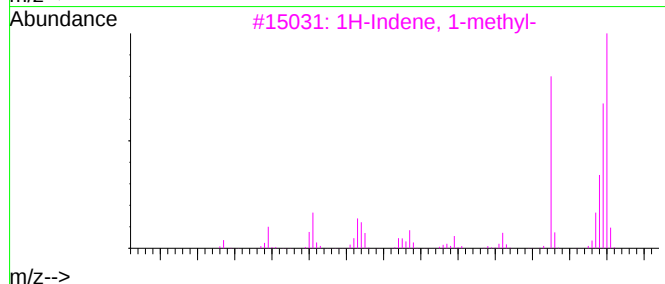
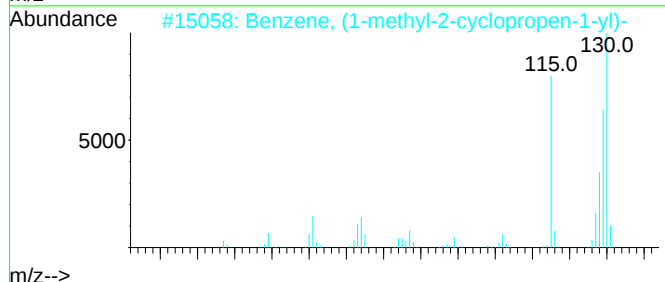
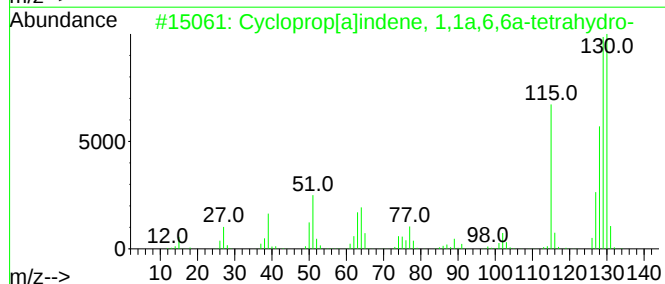
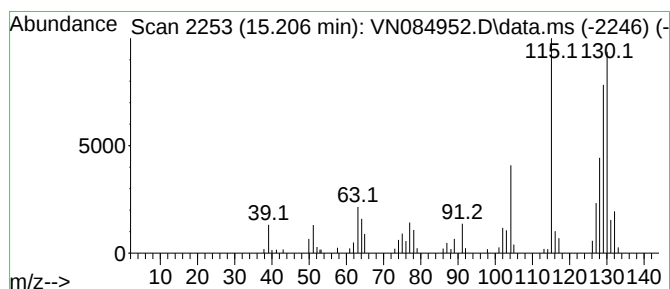
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	6.45 ug/l	134725	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	92
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	92
4	2-Methylindene	130	C10H10	002177-47-1	92
5	Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
Data File : VN084952.D
Acq On : 19 Nov 2024 17:16
Operator : JC\MD
Sample : P4843-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SW-WTS-01

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
1-Butanol	9.312	10.7	ug/l	174897	2	9.100	819686	50.0
Benzene, 1-ethy...	13.335	8.4	ug/l	175176	4	13.794	1043700	50.0
Indane	13.994	121.5	ug/l	2535780	4	13.794	1043700	50.0
Benzene, 1-meth...	14.447	8.2	ug/l	170072	4	13.794	1043700	50.0
1H-Indene, 2,3-...	15.053	6.0	ug/l	126257	4	13.794	1043700	50.0
Cycloprop[a]ind...	15.206	6.5	ug/l	134725	4	13.794	1043700	50.0