

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
 Data File : VN068090.D
 Acq On : 12 Aug 2021 15:26
 Operator : JC/MD
 Sample : M3360-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41920

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\82N072921W.M
 Title : SW846 8260

Signal : TIC: VN068090.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.743	267	281	298	rBV6	16956	39682	1.28%	0.109%
2	8.024	2225	2250	2261	rBV2	243770	578930	18.71%	1.586%
3	8.088	2262	2274	2296	rVB2	398439	913236	29.51%	2.501%
4	8.440	2383	2405	2428	rBV2	267302	625216	20.21%	1.713%
5	8.971	2583	2603	2635	rBV	636250	1343579	43.42%	3.680%
6	10.446	3133	3153	3183	rBV	1043583	2008154	64.90%	5.501%
7	11.746	3621	3638	3661	rBV	987137	1802642	58.26%	4.938%
8	11.848	3662	3676	3695	rVB	224459	404840	13.08%	1.109%
9	11.953	3695	3715	3746	rBV	1536433	3019999	97.60%	8.272%
10	12.283	3809	3838	3858	rBV	704470	1223454	39.54%	3.351%
11	12.581	3937	3949	3961	rBV2	44664	72910	2.36%	0.200%
12	12.733	3978	4006	4027	rBV2	760712	1359045	43.92%	3.723%
13	12.924	4064	4077	4086	rBV2	69726	117481	3.80%	0.322%
14	12.986	4086	4100	4108	rBV	1261666	2131417	68.88%	5.838%
15	13.061	4120	4128	4146	rVB	801183	1315270	42.51%	3.603%
16	13.222	4169	4188	4207	rBV	714349	1209020	39.07%	3.312%
17	13.372	4228	4244	4273	rVB	1902618	3094230	100.00%	8.476%
18	13.503	4276	4293	4303	rBV2	39209	86881	2.81%	0.238%
19	13.562	4303	4315	4326	rBV2	101928	159476	5.15%	0.437%
20	13.619	4326	4336	4344	rBV2	36317	51799	1.67%	0.142%
21	13.678	4344	4358	4363	rBV	973324	1610871	52.06%	4.412%
22	13.774	4385	4394	4406	rVB5	31130	49936	1.61%	0.137%
23	13.841	4406	4419	4422	rBV2	196236	261810	8.46%	0.717%
24	13.876	4423	4432	4438	rVV3	571481	962411	31.10%	2.636%
25	13.911	4440	4445	4468	rVB2	626828	1034728	33.44%	2.834%
26	14.005	4468	4480	4492	rBV2	68825	112611	3.64%	0.308%
27	14.072	4492	4505	4516	rBV	198010	320060	10.34%	0.877%
28	14.133	4516	4528	4533	rBV2	283372	451375	14.59%	1.236%
29	14.219	4549	4560	4573	rVB	673965	1052243	34.01%	2.882%
30	14.281	4573	4583	4590	rBV2	95905	153708	4.97%	0.421%
31	14.329	4590	4601	4614	rVB3	384051	643084	20.78%	1.762%
32	14.407	4625	4630	4639	rVB8	28817	39350	1.27%	0.108%
33	14.461	4639	4650	4662	rVB	212270	338620	10.94%	0.928%
34	14.541	4664	4680	4687	rBV	403825	663294	21.44%	1.817%
35	14.581	4687	4695	4705	rVV	590940	916801	29.63%	2.511%
36	14.624	4705	4711	4719	rVV3	98388	135966	4.39%	0.372%

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	14.662	4719	4725	4735	rVB2	48753	64055	2.07%	0.175%
38	14.764	4752	4763	4770	rBV4	61266	95896	3.10%	0.263%
39	14.812	4771	4781	4791	rVV	293233	485127	15.68%	1.329%
40	14.855	4792	4797	4807	rVB	85653	119445	3.86%	0.327%
41	14.933	4807	4826	4839	rBV4	805015	1765611	57.06%	4.836%
42	14.989	4840	4847	4862	rVB6	78197	159157	5.14%	0.436%
43	15.086	4870	4883	4901	rBV	274625	489495	15.82%	1.341%
44	15.198	4902	4925	4934	rBV5	205119	494265	15.97%	1.354%
45	15.314	4954	4968	4986	rVB4	207794	507829	16.41%	1.391%
46	15.458	5011	5022	5030	rBV6	20739	42429	1.37%	0.116%
47	15.507	5032	5040	5051	rVB2	51068	84039	2.72%	0.230%
48	15.566	5051	5062	5071	rBV3	80926	139756	4.52%	0.383%
49	15.622	5073	5083	5088	rBV7	61472	109185	3.53%	0.299%
50	15.807	5135	5152	5171	rBV2	111373	228693	7.39%	0.626%
51	15.984	5195	5218	5223	rBV7	97857	231678	7.49%	0.635%
52	16.022	5226	5232	5256	rVV3	169711	346444	11.20%	0.949%
53	16.113	5256	5266	5278	rVV3	45016	93874	3.03%	0.257%
54	16.193	5282	5296	5324	rVB3	69167	205552	6.64%	0.563%
55	16.349	5335	5354	5373	rBV3	130295	297810	9.62%	0.816%
56	16.553	5405	5430	5444	rBV5	52597	140690	4.55%	0.385%
57	16.620	5445	5455	5485	rVB9	33877	102381	3.31%	0.280%

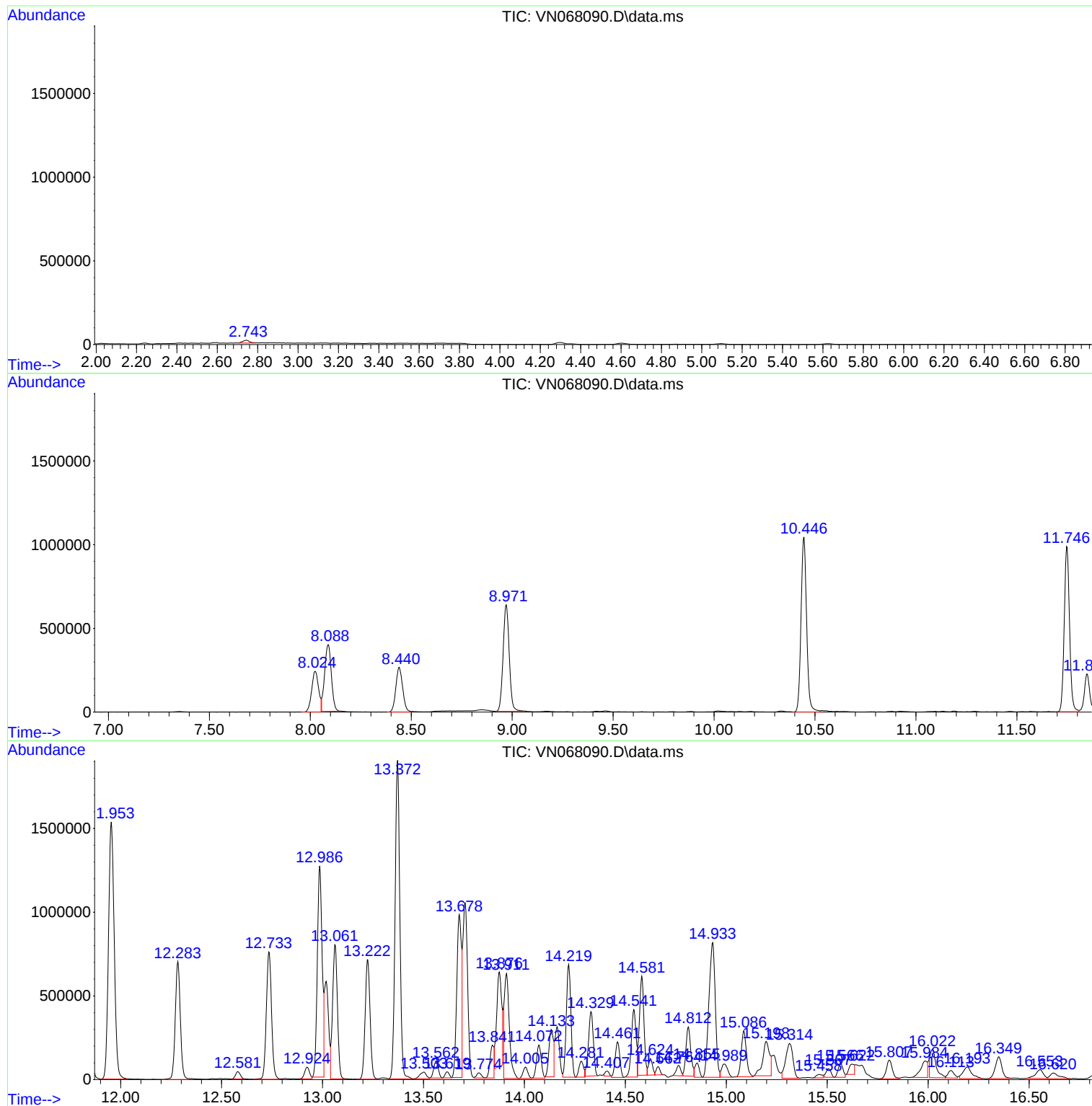
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Quant Title : SW846 8260

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



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Instrument :
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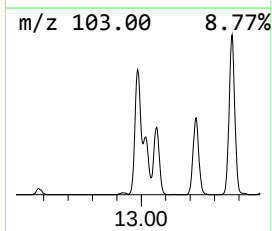
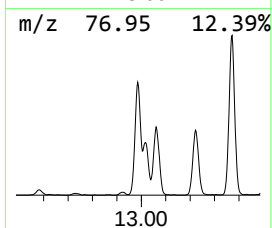
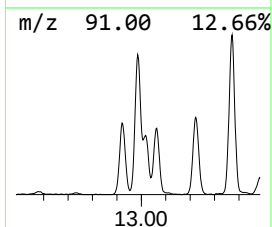
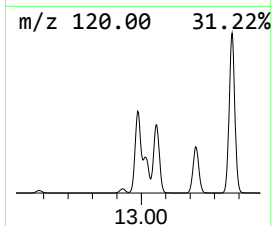
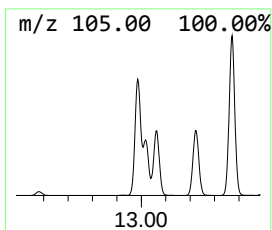
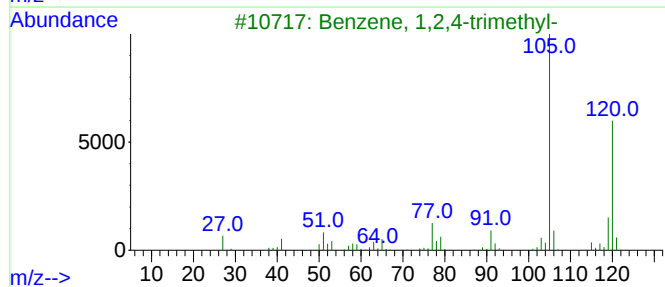
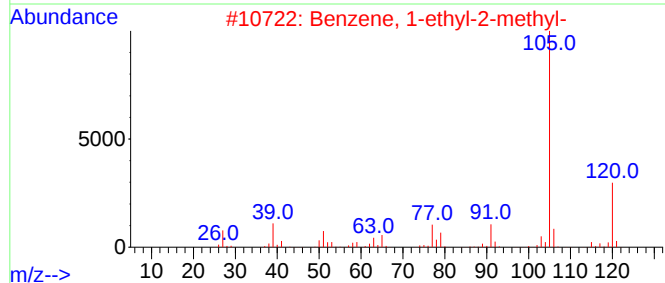
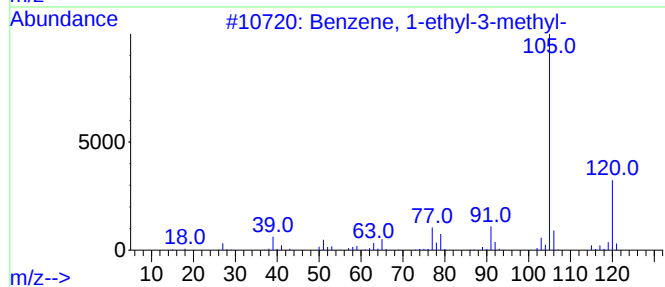
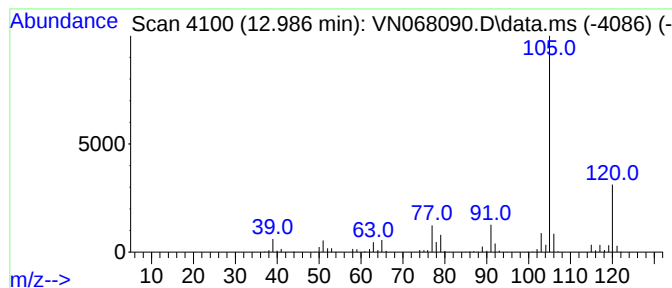
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	66.16 ug/l	2131420	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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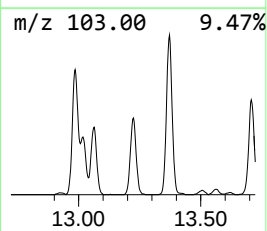
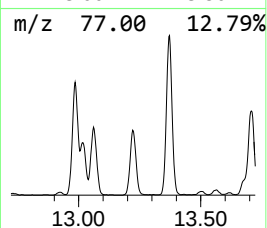
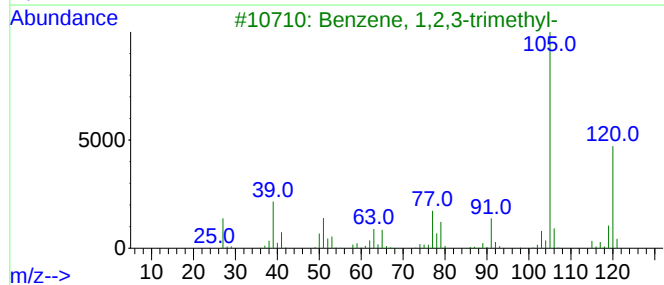
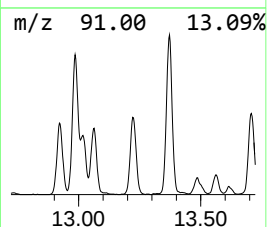
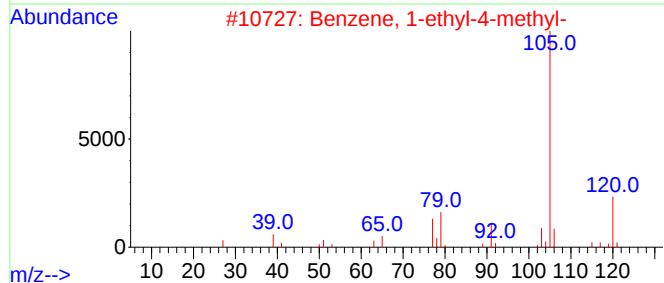
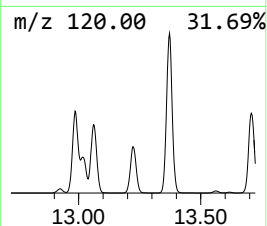
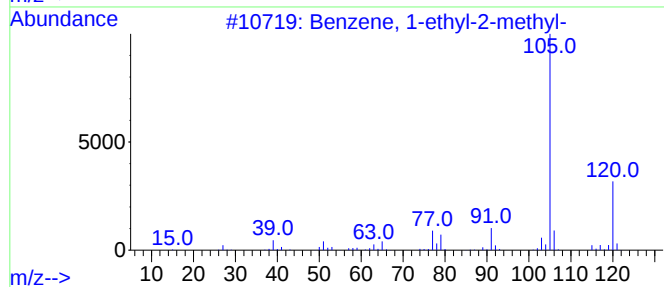
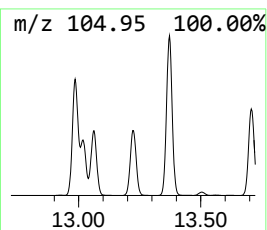
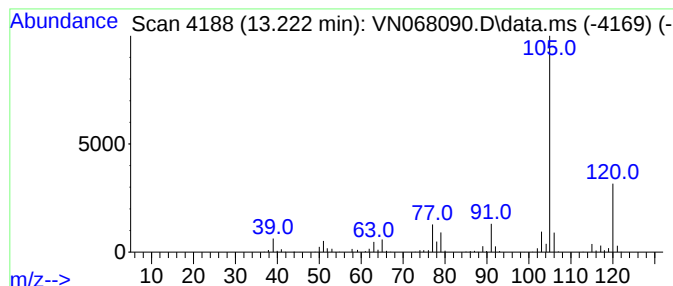
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	37.53 ug/l	1209020	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Mesitylene	120	C9H12	000108-67-8	91



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

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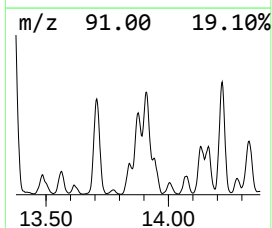
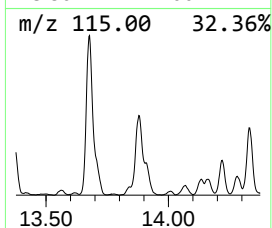
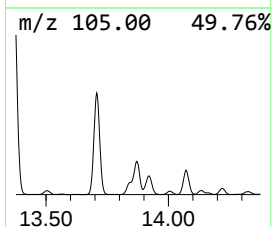
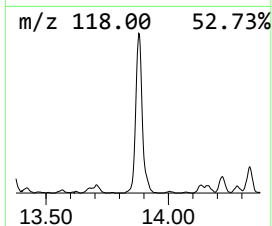
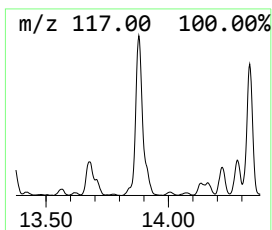
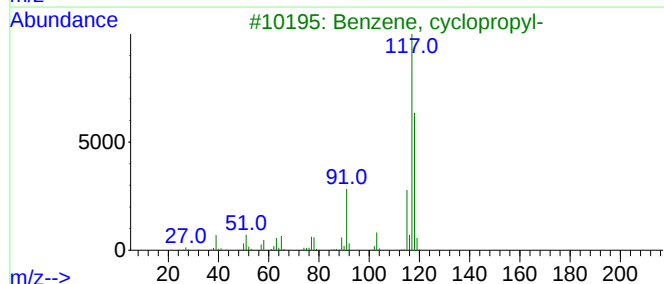
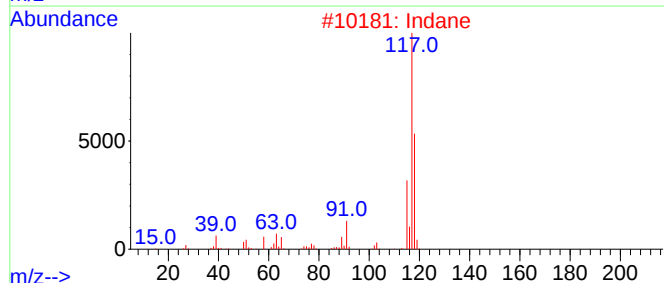
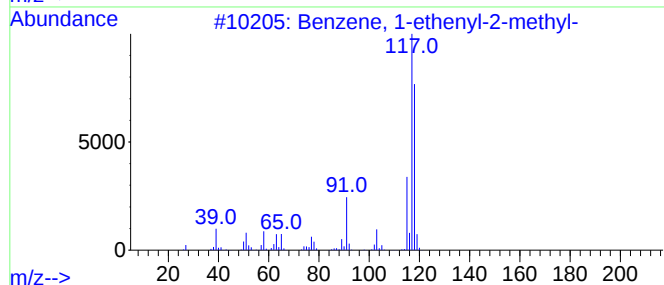
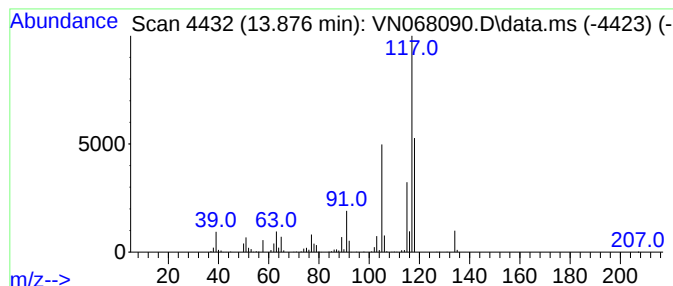
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethenyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	29.87 ug/l	962411	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
2			Indane	118	C9H10	000496-11-7	70
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



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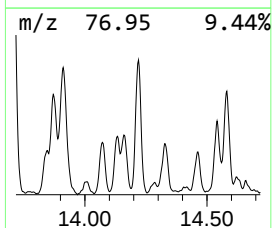
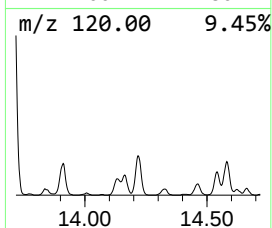
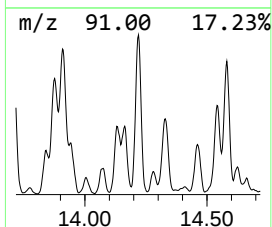
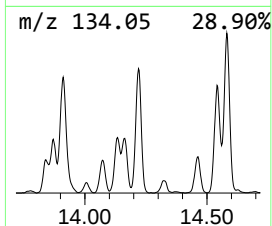
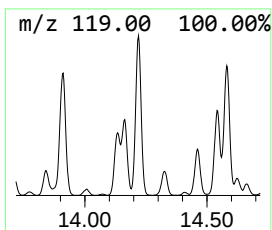
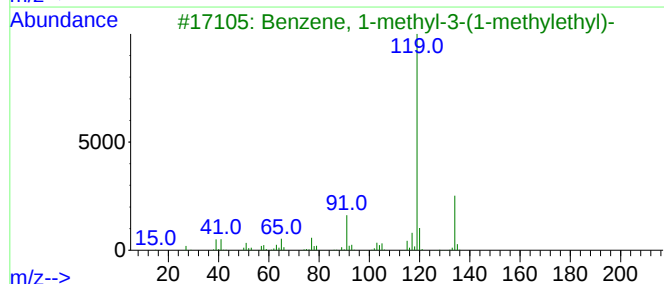
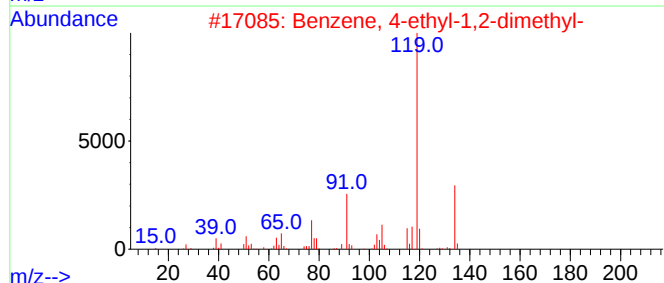
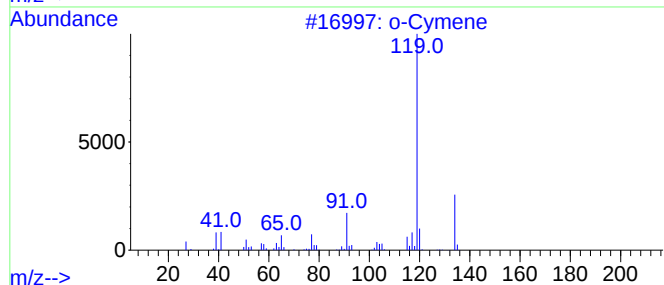
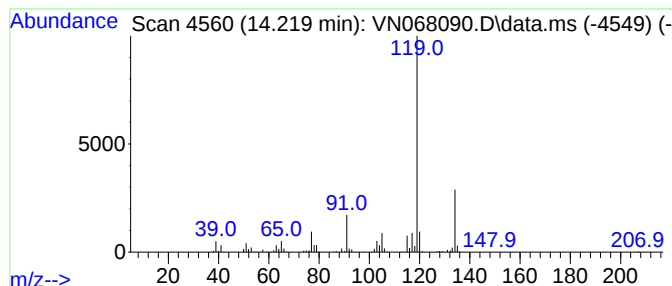
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

Peak Number 4 o-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	32.66 ug/l	1052240	1,4-Dichlorobenzene-d4	13.678

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	96
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



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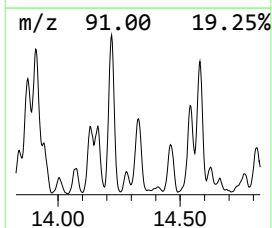
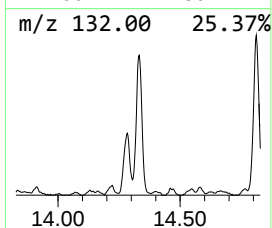
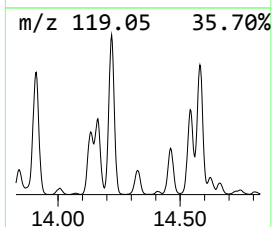
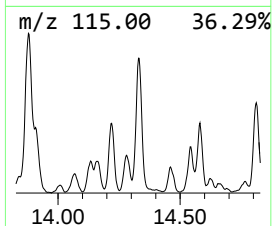
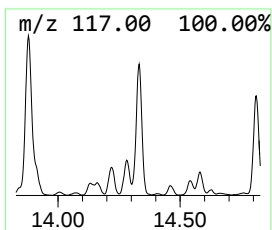
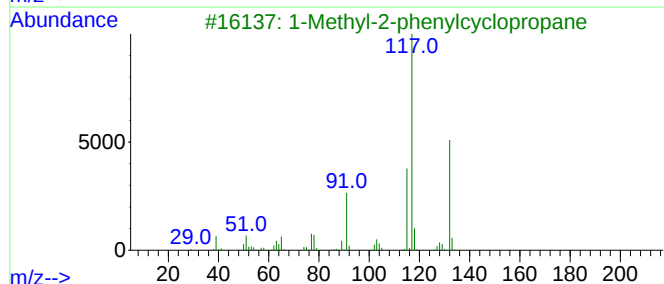
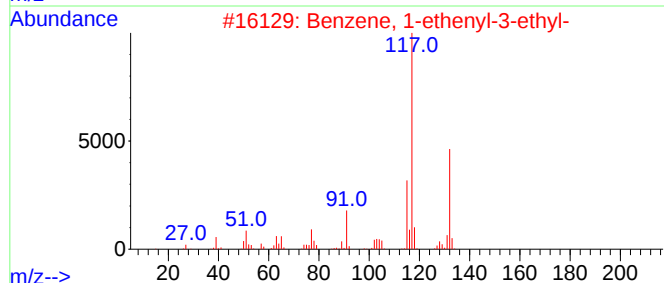
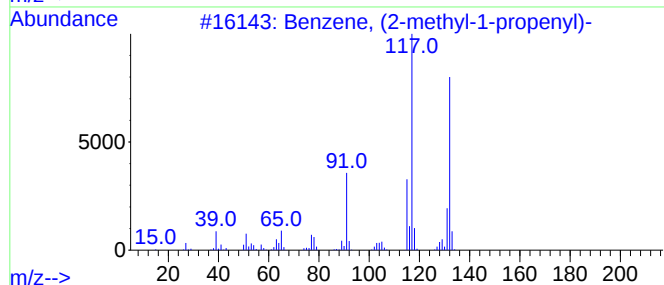
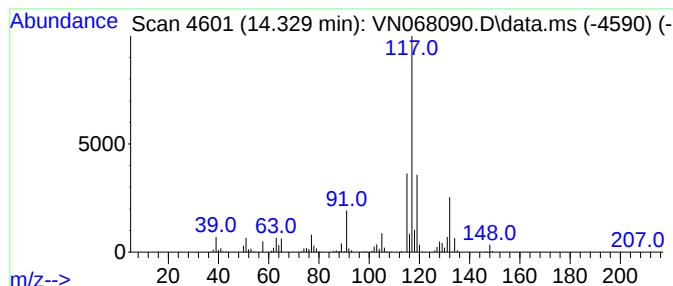
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, (2-methyl-1-propen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	19.96 ug/l	643084	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	72
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	68
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	68
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
5			Indan, 1-methyl-	132	C10H12	000767-58-8	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
Data File : VN068090.D
Acq On : 12 Aug 2021 15:26
Operator : JC/MD
Sample : M3360-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41920

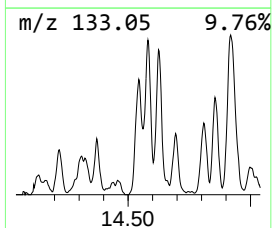
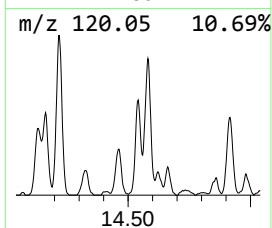
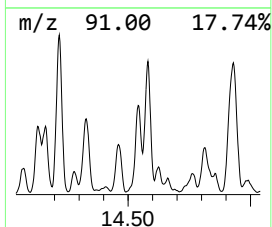
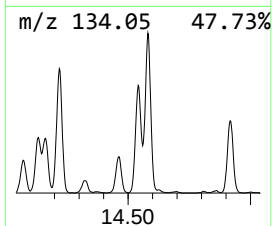
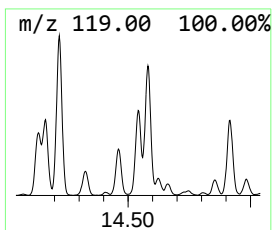
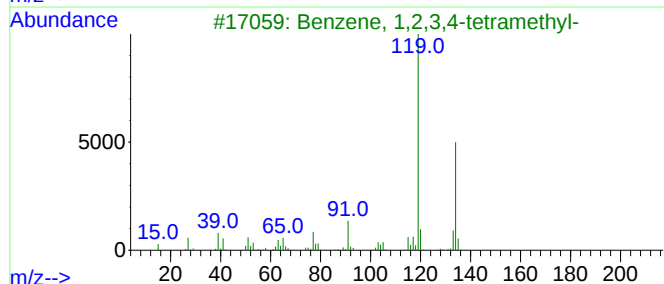
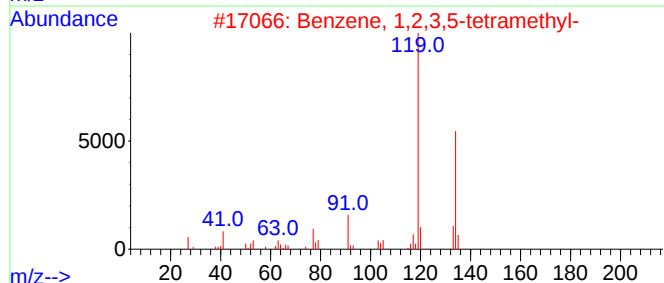
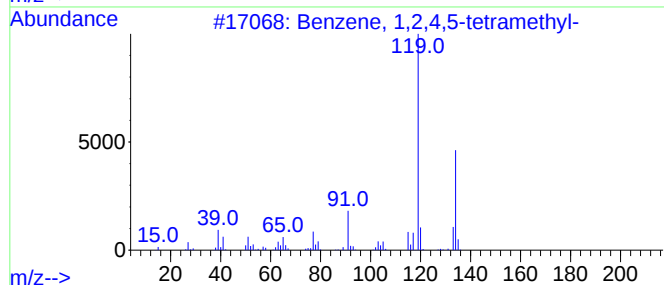
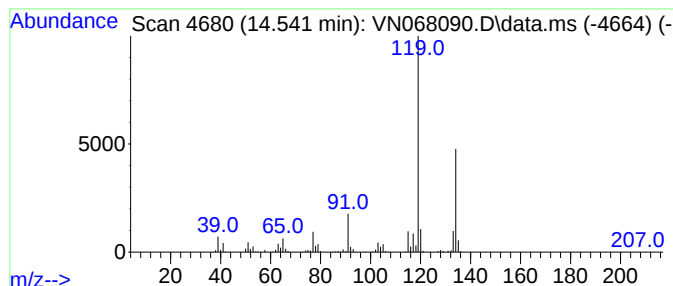
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	20.59 ug/l	663294	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	96
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
Data File : VN068090.D
Acq On : 12 Aug 2021 15:26
Operator : JC/MD
Sample : M3360-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41920

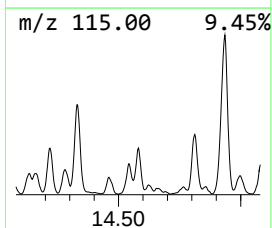
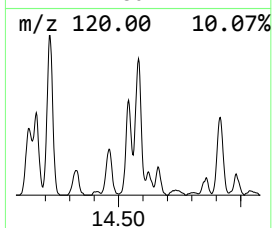
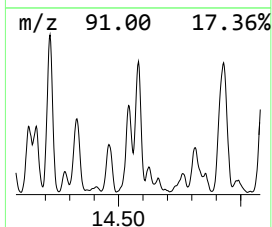
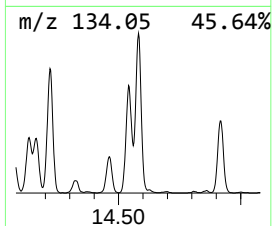
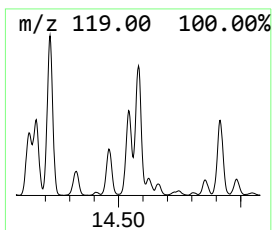
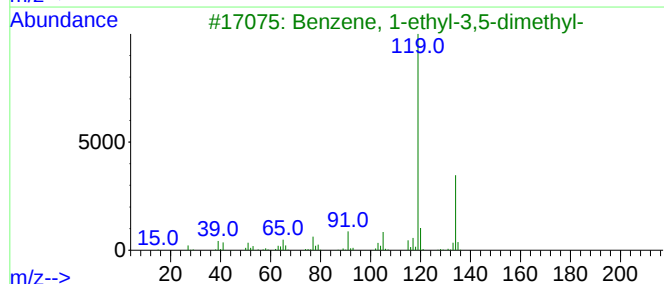
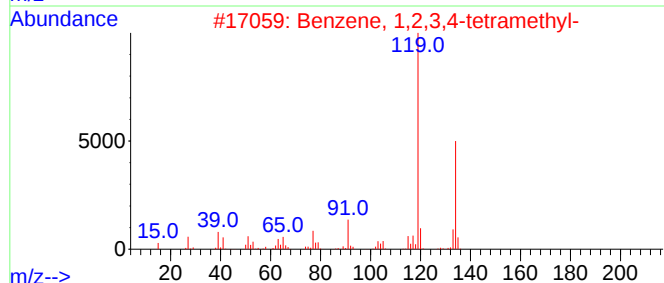
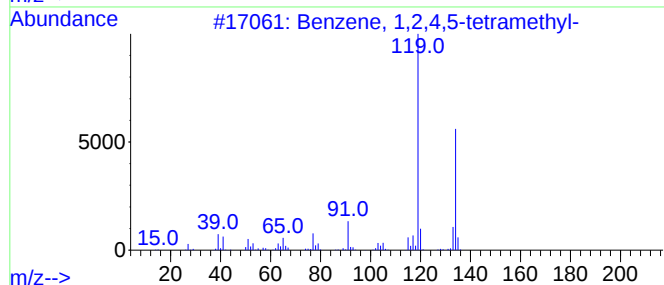
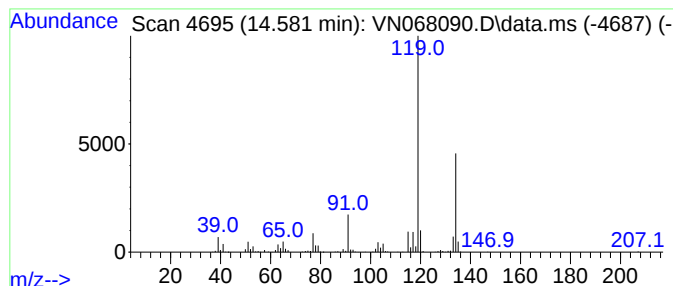
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.581	28.46 ug/l	916801	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5			o-Cymene	134	C10H14	000527-84-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
Data File : VN068090.D
Acq On : 12 Aug 2021 15:26
Operator : JC/MD
Sample : M3360-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41920

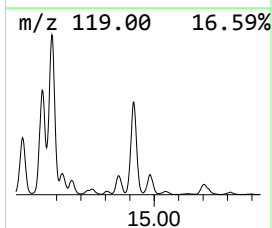
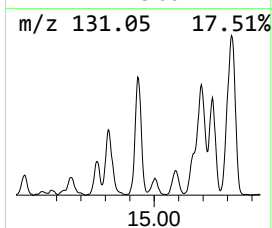
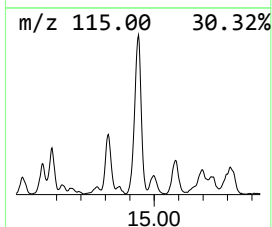
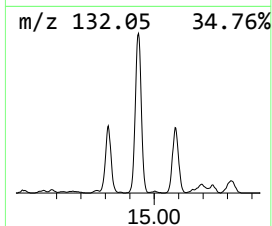
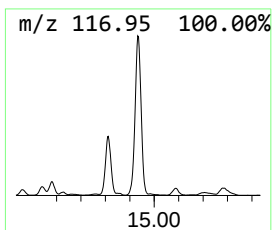
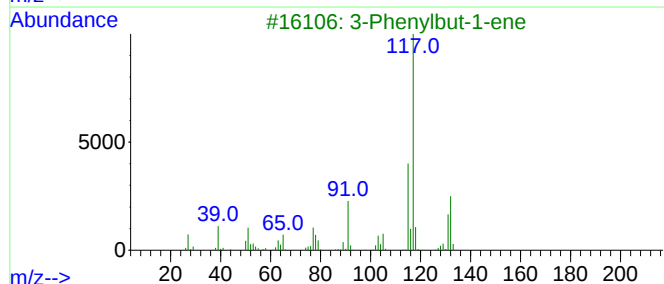
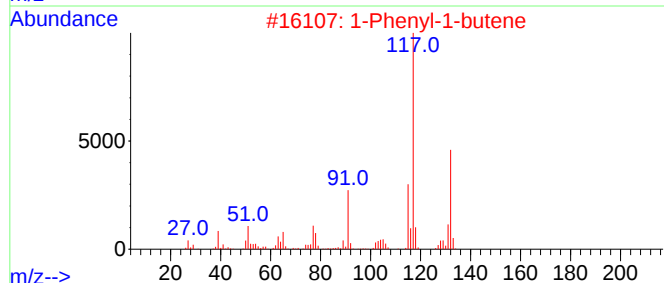
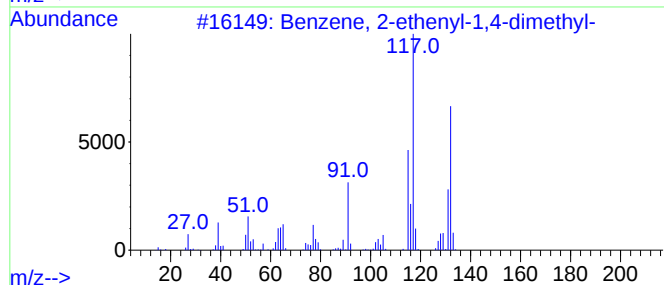
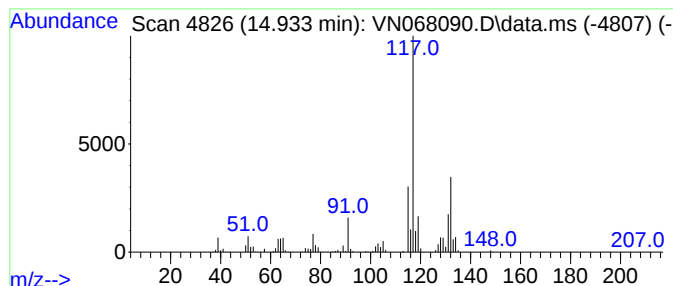
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	54.80 ug/l	1765610	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	90
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
Data File : VN068090.D
Acq On : 12 Aug 2021 15:26
Operator : JC/MD
Sample : M3360-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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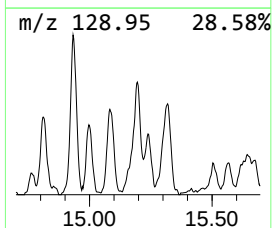
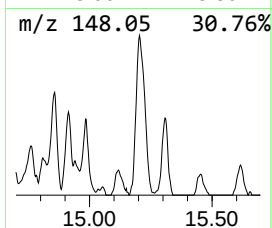
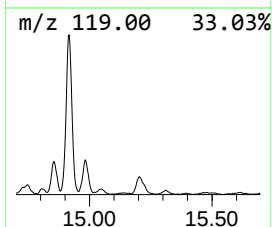
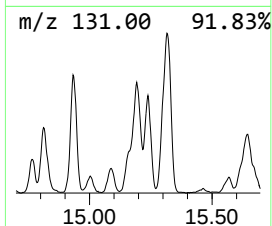
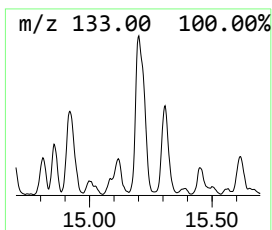
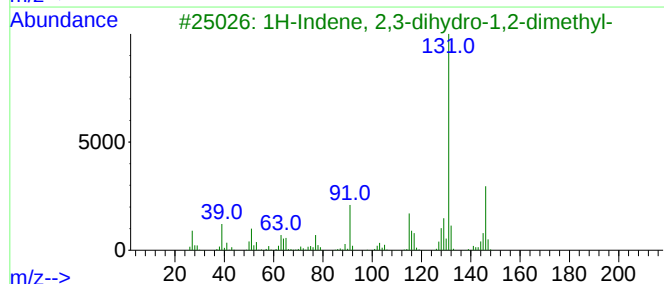
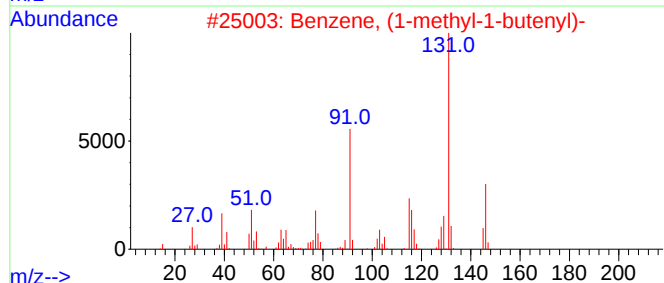
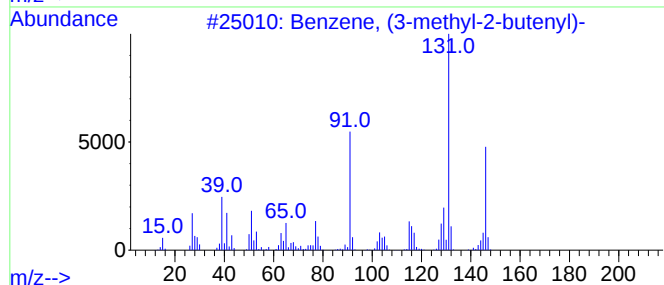
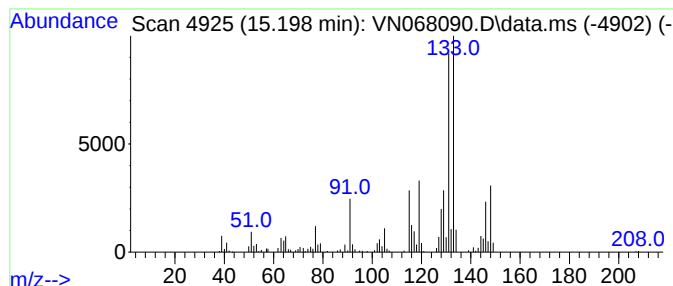
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.198 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	15.34 ug/l	494265	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	46
2			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	46
3			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	46
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	46
5			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
Data File : VN068090.D
Acq On : 12 Aug 2021 15:26
Operator : JC/MD
Sample : M3360-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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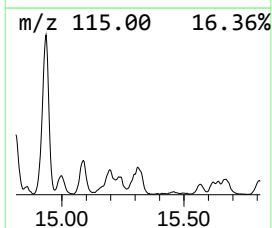
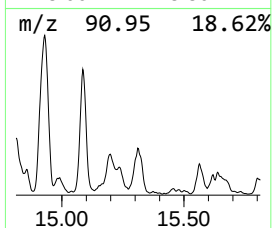
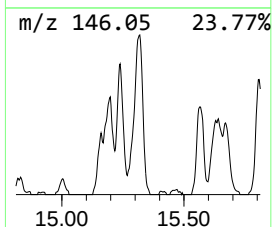
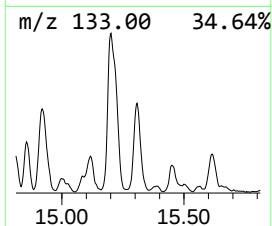
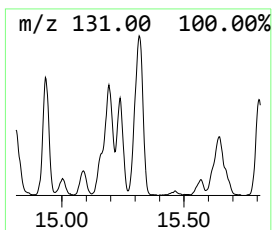
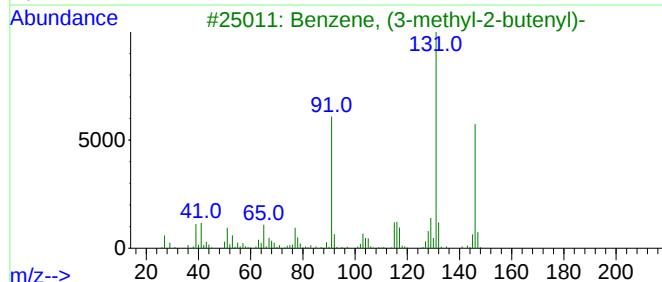
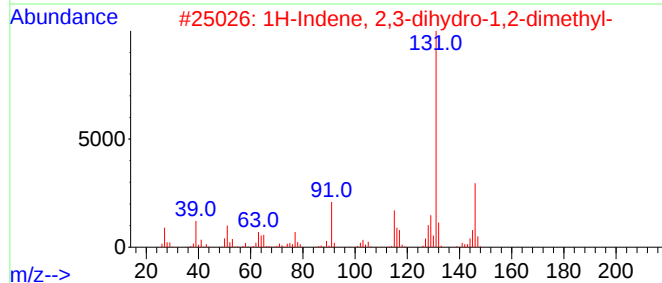
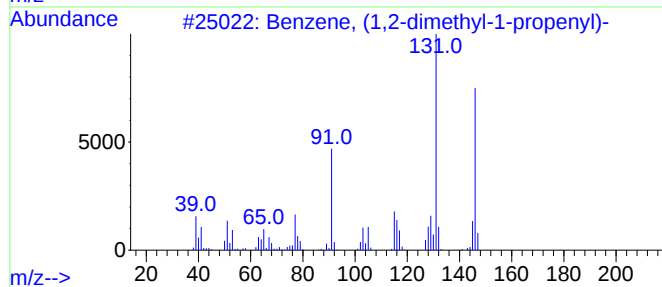
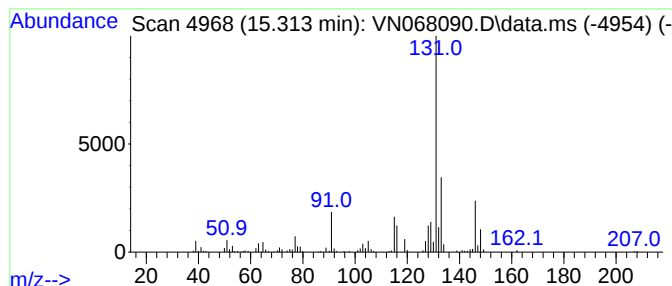
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, (1,2-dimethyl-1-propenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.313	15.76 ug/l	507829	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	89
2			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	81
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	81
4			1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	81
5			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081221\
Data File : VN068090.D
Acq On : 12 Aug 2021 15:26
Operator : JC/MD
Sample : M3360-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41920

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.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...	13.222	37.5	ug/l	1209020	4	13.678	1610870	50.0
Benzene, 1-ethe...	13.876	29.9	ug/l	962411	4	13.678	1610870	50.0
o-Cymene	14.219	32.7	ug/l	1052240	4	13.678	1610870	50.0
Benzene, (2-met...	14.329	20.0	ug/l	643084	4	13.678	1610870	50.0
Benzene, 1,2,4,...	14.541	20.6	ug/l	663294	4	13.678	1610870	50.0
Benzene, 1,2,3,...	14.581	28.5	ug/l	916801	4	13.678	1610870	50.0
Benzene, 2-ethe...	14.933	54.8	ug/l	1765610	4	13.678	1610870	50.0
unknown15.198	15.198	15.3	ug/l	494265	4	13.678	1610870	50.0
Benzene, (1,2-d...	15.313	15.8	ug/l	507829	4	13.678	1610870	50.0