

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
 Data File : VN067504.D
 Acq On : 25 Jun 2021 15:06
 Operator : JC/MD
 Sample : M2806-02 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2

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\82N062421W.M
 Title : SW846 8260

Signal : TIC: VN067504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.024	2228	2250	2261	rBV	197769	466069	6.75%	1.643%
2	8.086	2261	2273	2295	rVB3	343745	802109	11.62%	2.828%
3	8.440	2382	2405	2427	rBV2	273121	631402	9.15%	2.226%
4	8.971	2582	2603	2629	rBV	591228	1242520	18.01%	4.381%
5	10.443	3131	3152	3191	rBV	954808	1811460	26.25%	6.387%
6	11.747	3619	3638	3659	rBV	821759	1501430	21.76%	5.294%
7	11.846	3662	3675	3698	rVV	290539	528220	7.66%	1.862%
8	11.961	3698	3718	3757	rVB	256660	539556	7.82%	1.902%
9	12.581	3936	3949	3968	rVB	574205	995417	14.43%	3.509%
10	12.734	3992	4006	4025	rBV2	610548	1062041	15.39%	3.744%
11	12.921	4058	4076	4090	rBV	970769	1626243	23.57%	5.734%
12	12.986	4090	4100	4105	rVV	177085	281392	4.08%	0.992%
13	13.018	4106	4112	4121	rVV	302922	483558	7.01%	1.705%
14	13.061	4121	4128	4141	rVB	208635	324573	4.70%	1.144%
15	13.324	4202	4226	4229	rBV9	73499	159739	2.32%	0.563%
16	13.369	4230	4243	4267	rVB	4141814	6900056	100.00%	24.327%
17	13.501	4273	4292	4305	rBV3	235652	511927	7.42%	1.805%
18	13.562	4305	4315	4325	rVB3	66479	109339	1.58%	0.385%
19	13.619	4326	4336	4344	rBV2	52215	74659	1.08%	0.263%
20	13.678	4344	4358	4361	rBV	734711	1049111	15.20%	3.699%
21	13.707	4362	4369	4384	rVB	1435095	2328237	33.74%	8.209%
22	13.774	4384	4394	4406	rVB2	95254	154467	2.24%	0.545%
23	13.841	4406	4419	4424	rBV2	225530	359598	5.21%	1.268%
24	13.879	4424	4433	4443	rVB	548261	848368	12.30%	2.991%
25	14.002	4468	4479	4494	rVB3	118823	197953	2.87%	0.698%
26	14.134	4514	4528	4533	rBV	147564	242109	3.51%	0.854%
27	14.160	4534	4538	4549	rVV	147761	204147	2.96%	0.720%
28	14.219	4549	4560	4572	rVV	386207	606810	8.79%	2.139%
29	14.281	4572	4583	4590	rVV2	115656	199931	2.90%	0.705%
30	14.329	4590	4601	4614	rVV3	389453	686192	9.94%	2.419%
31	14.463	4637	4651	4662	rBV5	100929	174099	2.52%	0.614%
32	14.541	4662	4680	4687	rBV	154752	265251	3.84%	0.935%
33	14.579	4687	4694	4706	rVB	216748	326787	4.74%	1.152%
34	14.919	4805	4821	4839	rBV4	207828	460609	6.68%	1.624%
35	15.086	4871	4883	4897	rBV3	48325	81962	1.19%	0.289%
36	15.507	5024	5040	5056	rVB2	67442	126189	1.83%	0.445%

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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\82N062421W.M
Title : SW846 8260

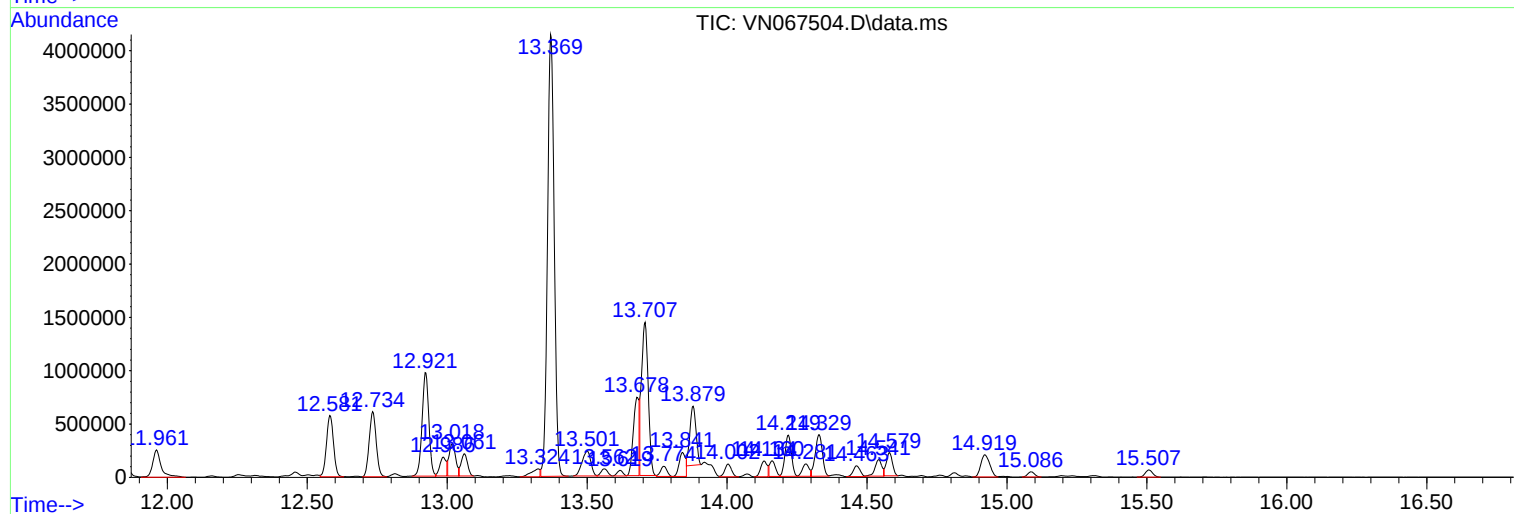
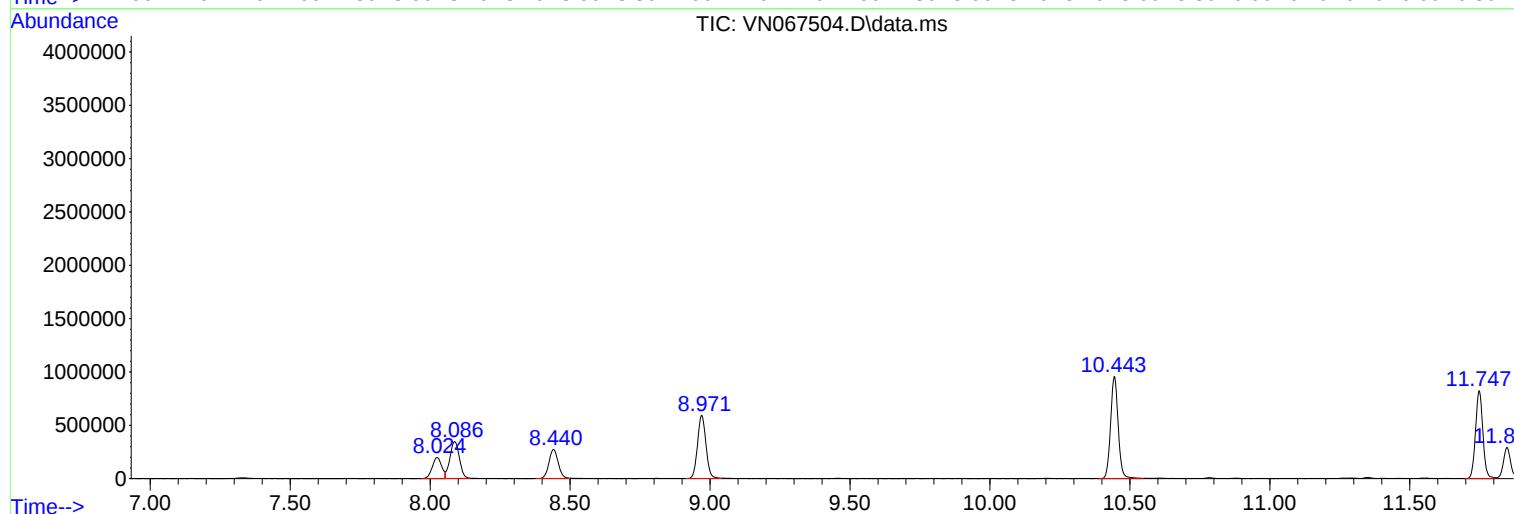
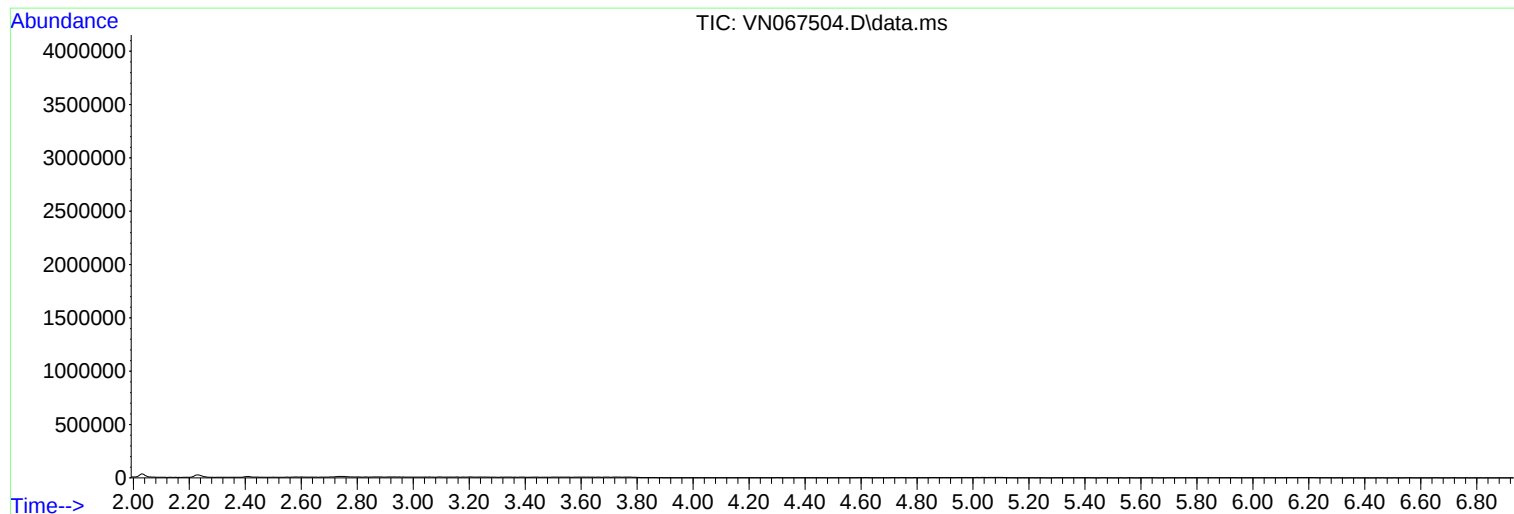
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
MW-2

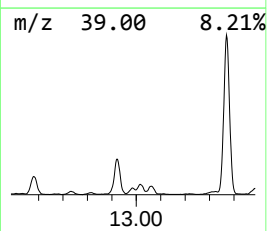
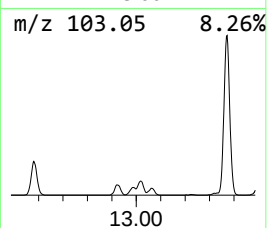
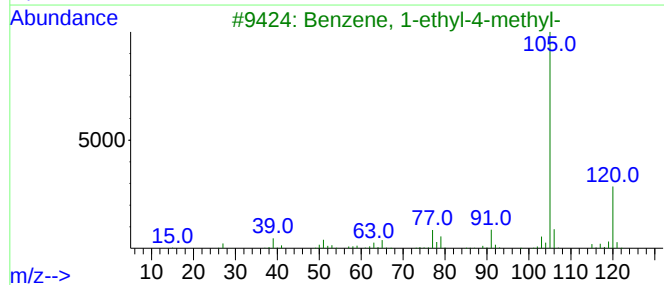
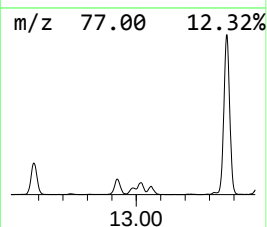
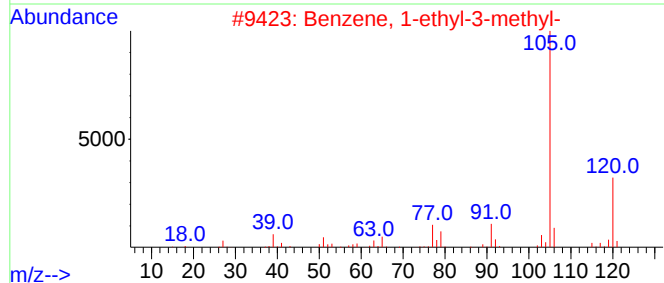
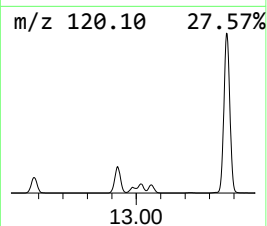
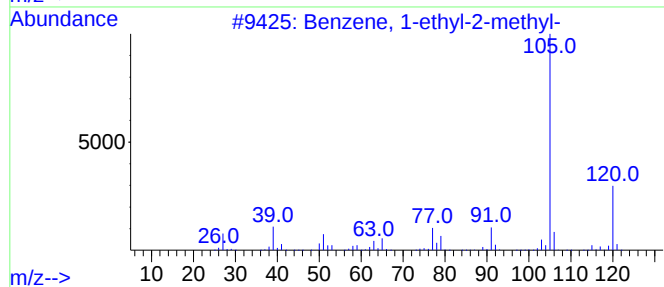
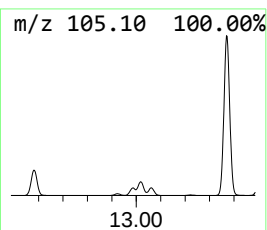
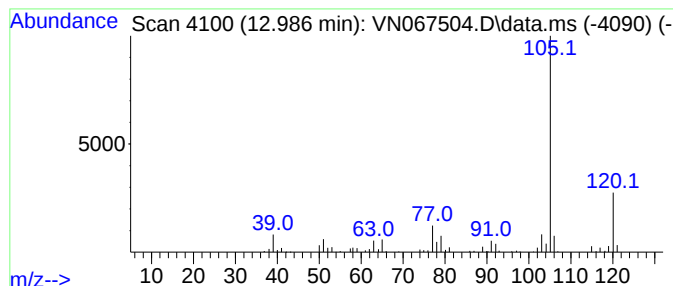
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	13.41 ug/l	281392	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-3-methyl-	120	C9H12	000620-14-4	91
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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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
MW-2

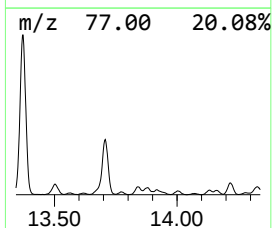
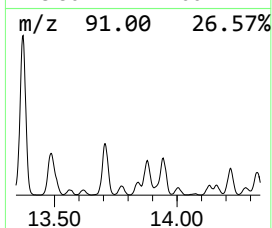
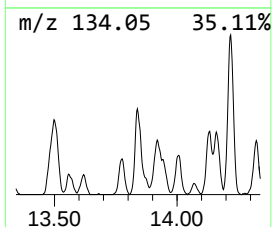
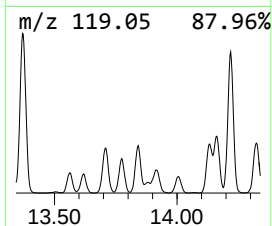
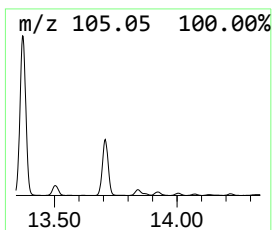
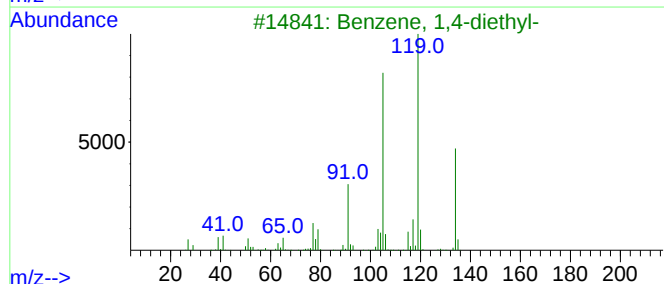
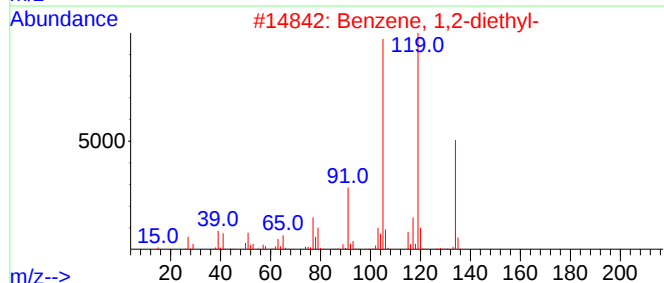
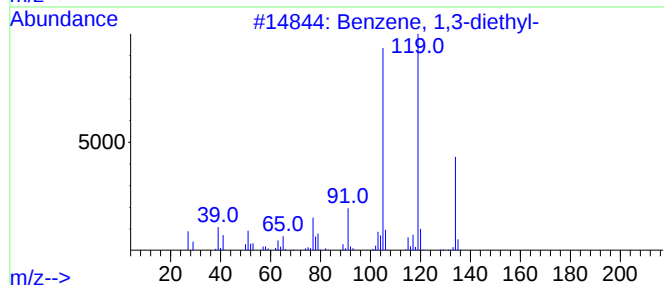
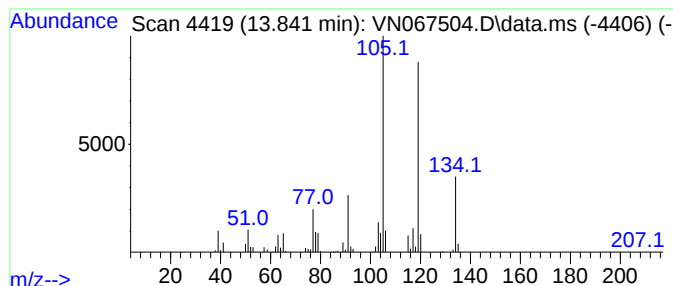
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,3-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	17.14 ug/l	359598	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

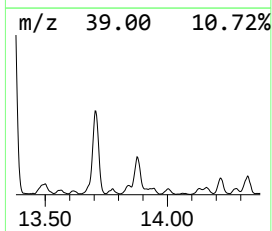
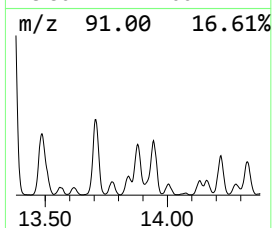
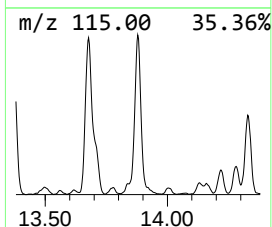
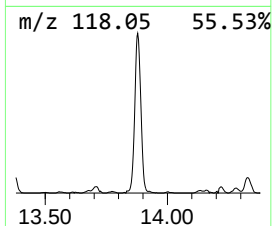
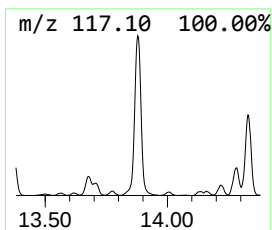
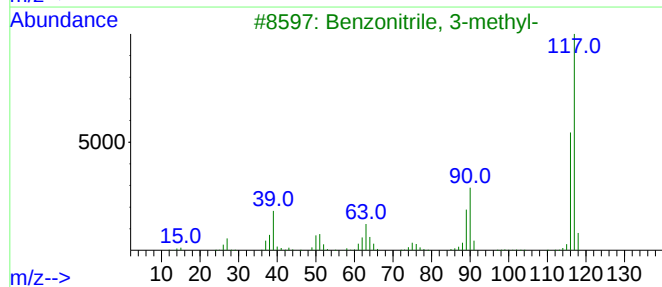
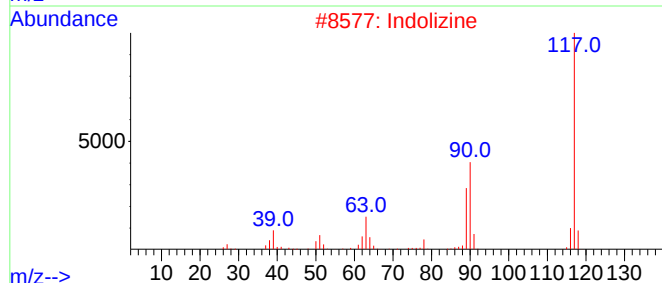
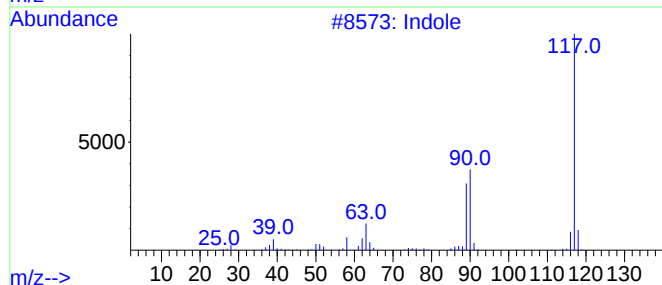
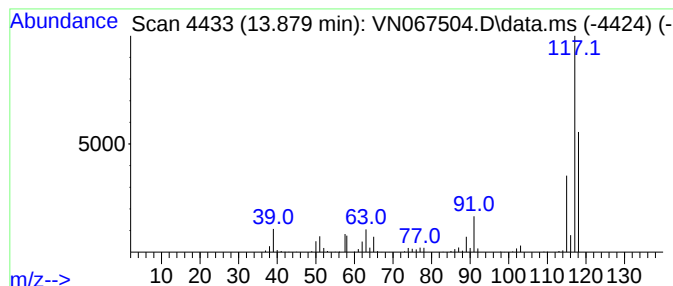
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.879 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.879	40.43 ug/l	848368	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	49
2			Indolizine	117	C8H7N	000274-40-8	47
3			Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	43
4			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42
5			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	40



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Instrument :
MSVOA_N
ClientSampleId :
MW-2

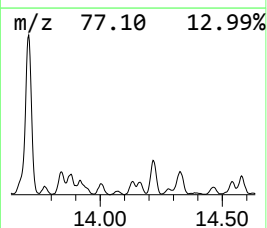
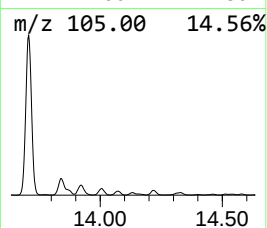
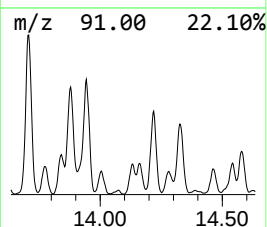
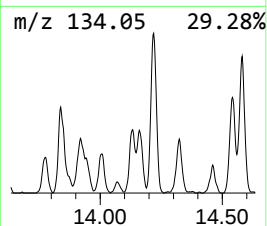
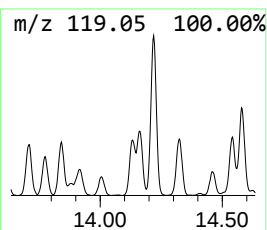
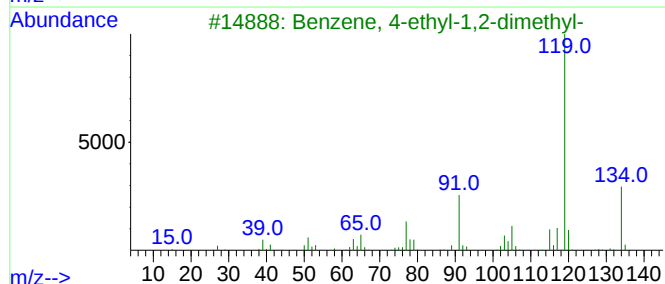
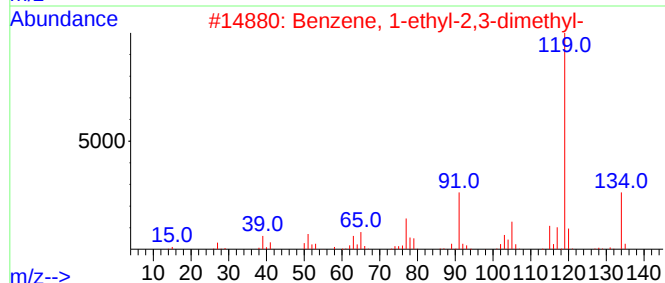
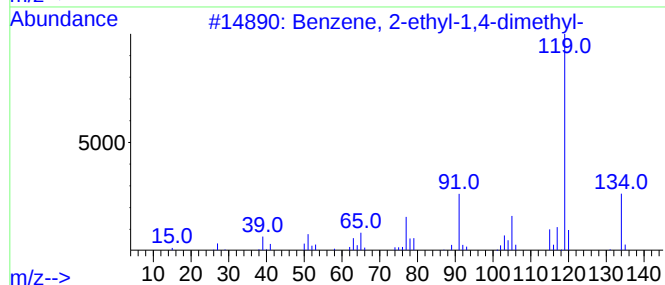
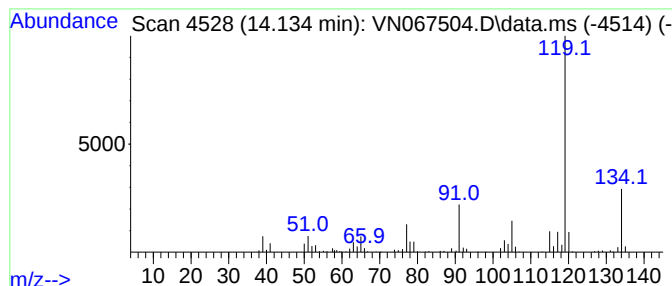
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.134	11.54 ug/l	242109	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



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Instrument :
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ClientSampleId :
MW-2

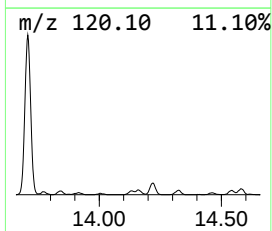
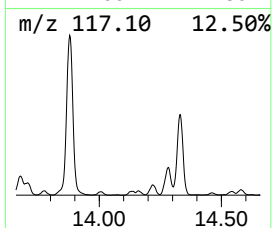
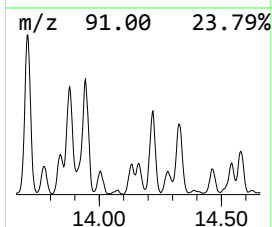
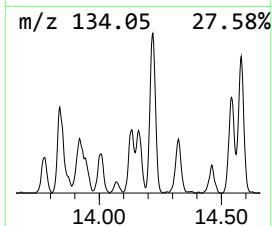
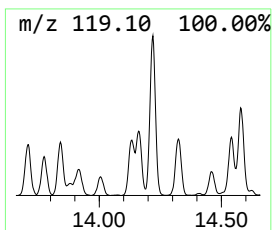
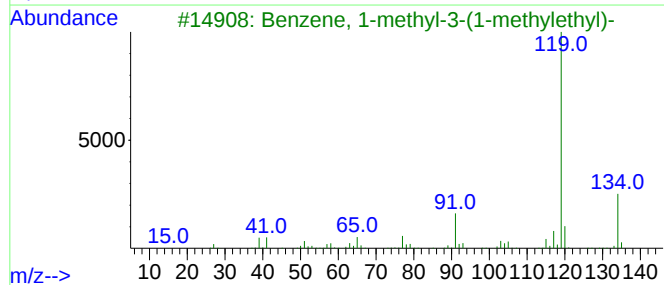
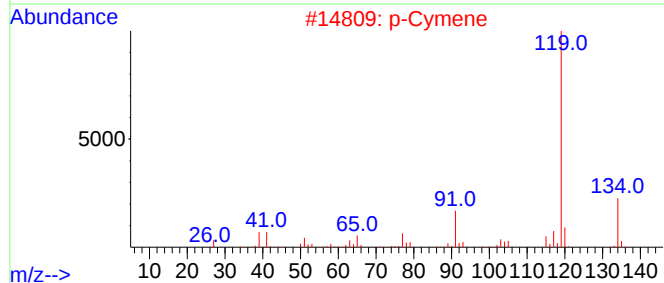
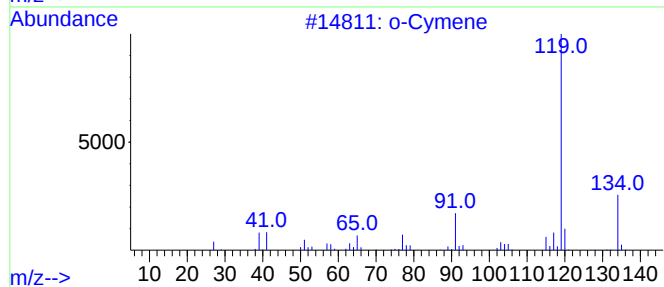
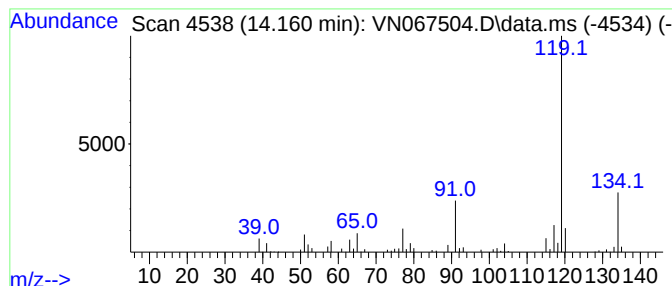
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.160	9.73 ug/l	204147	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	91
2			p-Cymene	134	C10H14	000099-87-6	91
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	91
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	90
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067504.D
Acq On : 25 Jun 2021 15:06
Operator : JC/MD
Sample : M2806-02 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

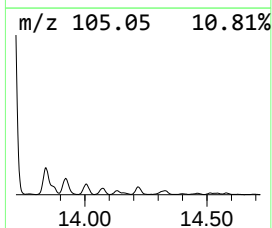
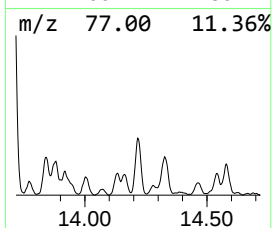
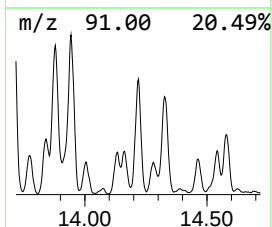
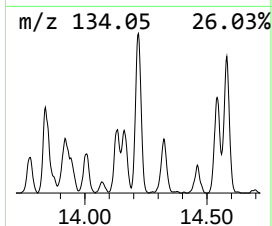
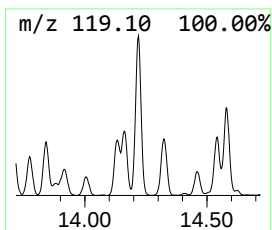
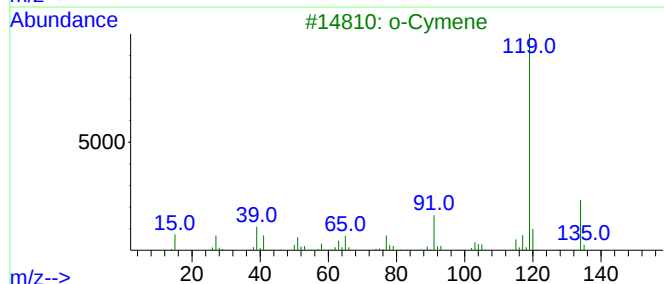
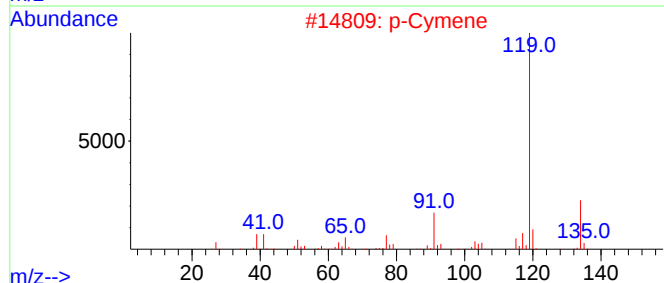
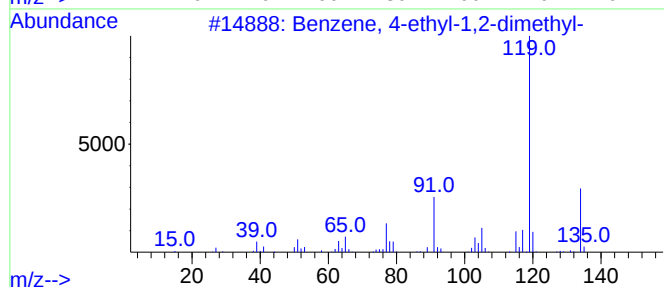
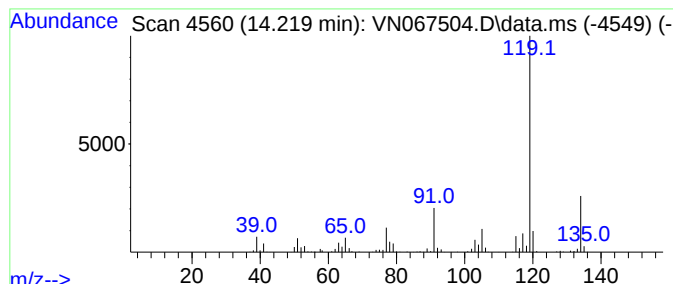
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	28.92 ug/l	606810	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			p-Cymene	134	C10H14	000099-87-6	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067504.D
Acq On : 25 Jun 2021 15:06
Operator : JC/MD
Sample : M2806-02 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

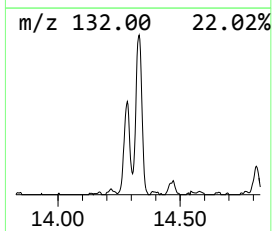
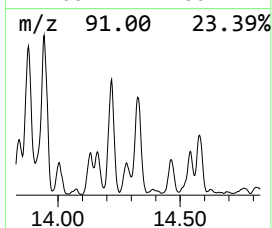
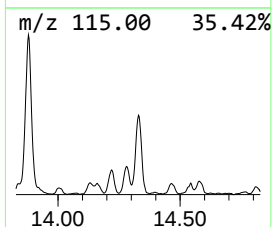
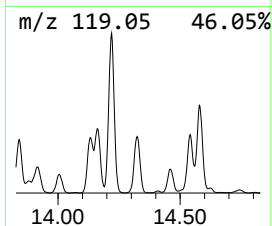
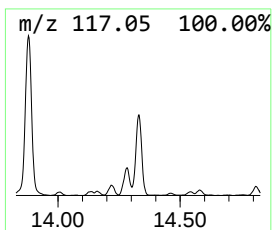
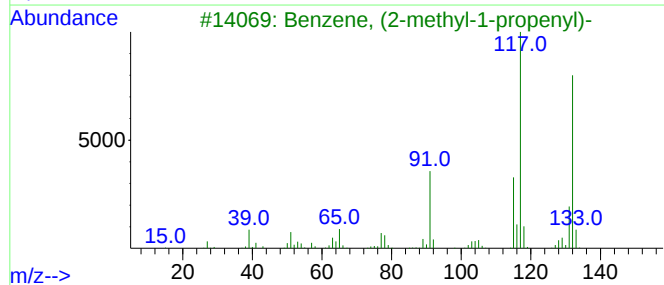
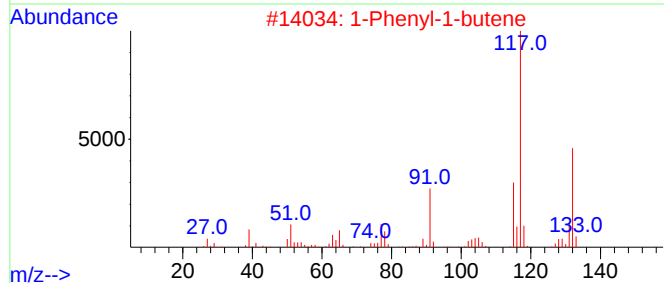
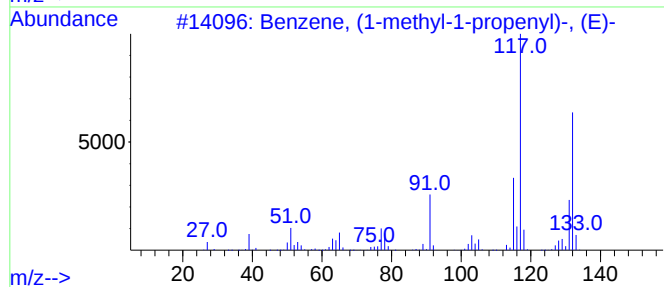
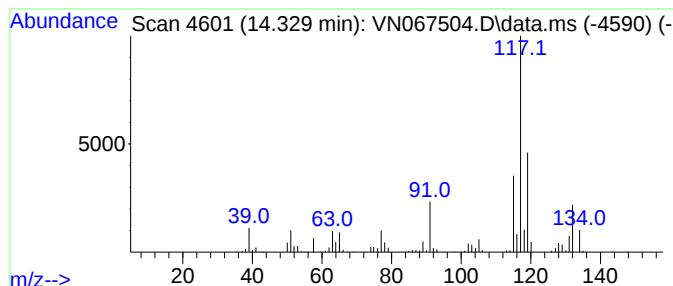
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, (1-methyl-1-propen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	32.70 ug/l	686192	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	70
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
5			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067504.D
Acq On : 25 Jun 2021 15:06
Operator : JC/MD
Sample : M2806-02 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

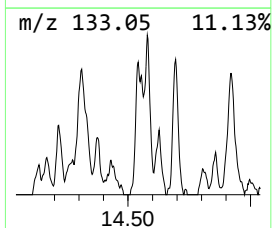
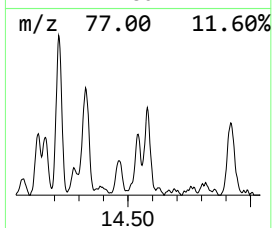
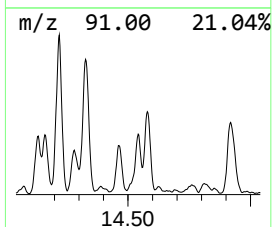
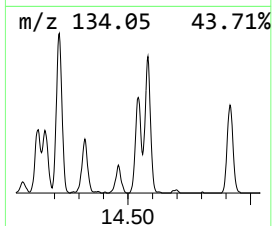
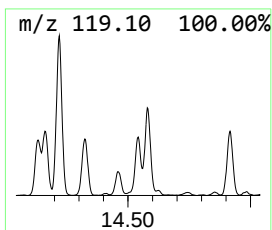
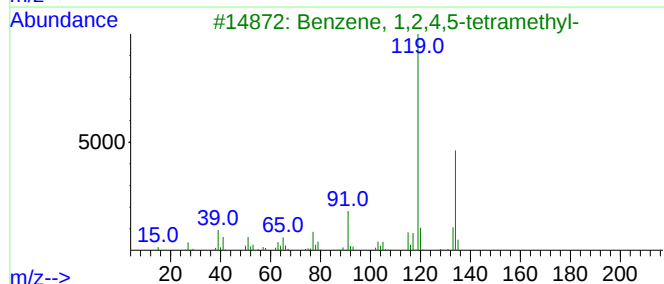
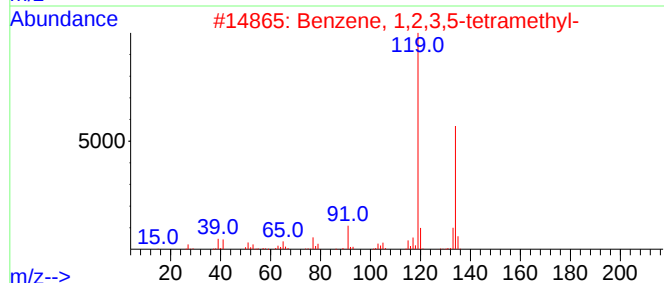
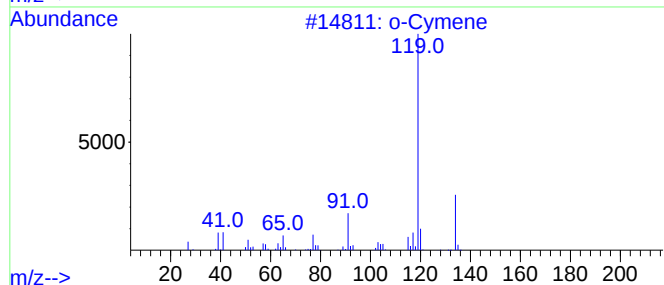
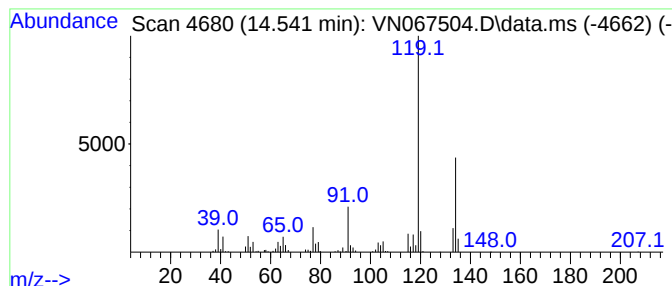
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	12.64 ug/l	265251	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	96
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
4			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	95
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067504.D
Acq On : 25 Jun 2021 15:06
Operator : JC/MD
Sample : M2806-02 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

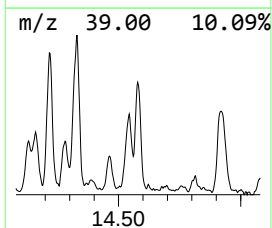
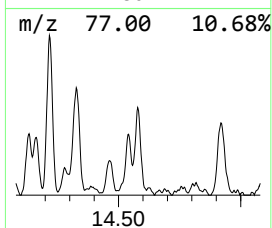
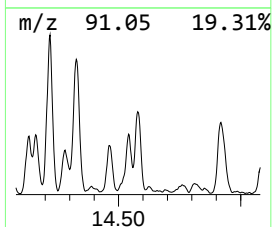
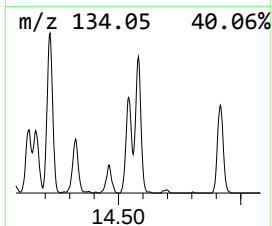
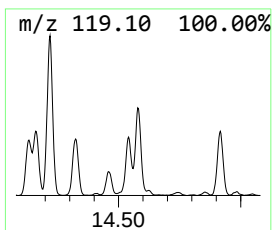
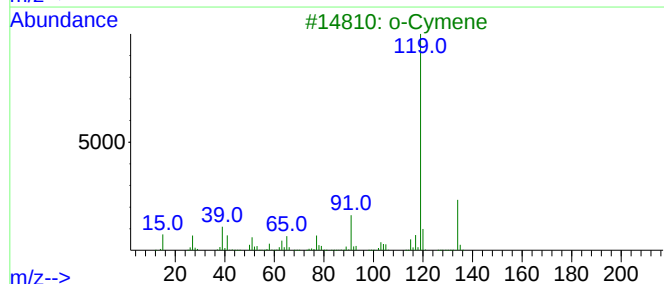
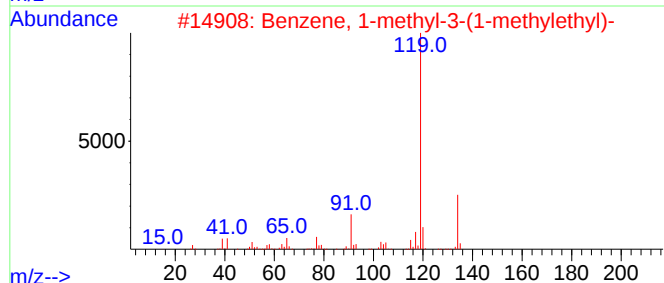
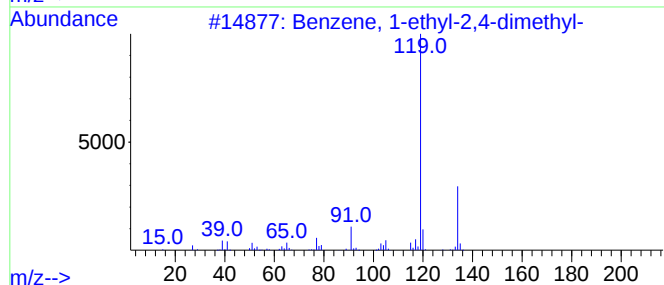
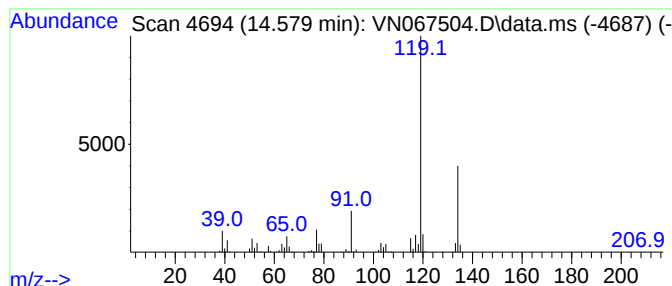
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.579	15.57 ug/l	326787	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	91
3			o-Cymene	134	C10H14	000527-84-4	91
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067504.D
Acq On : 25 Jun 2021 15:06
Operator : JC/MD
Sample : M2806-02 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

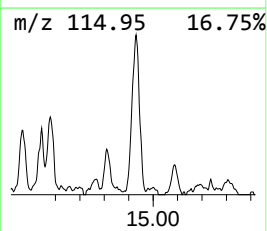
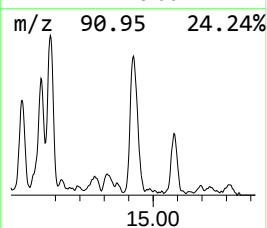
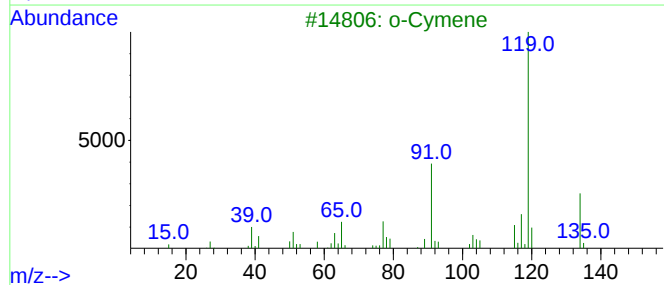
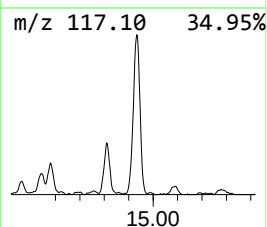
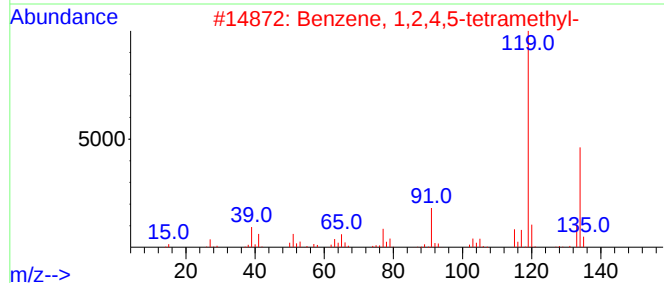
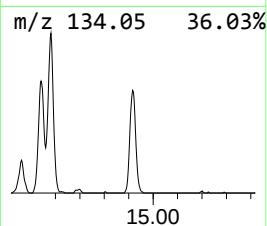
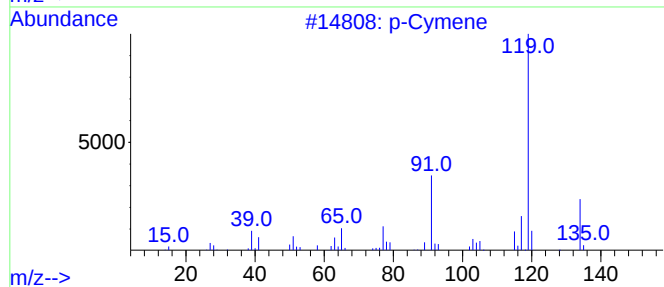
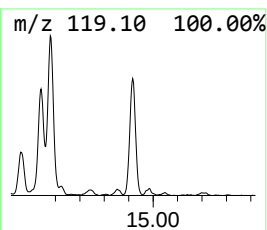
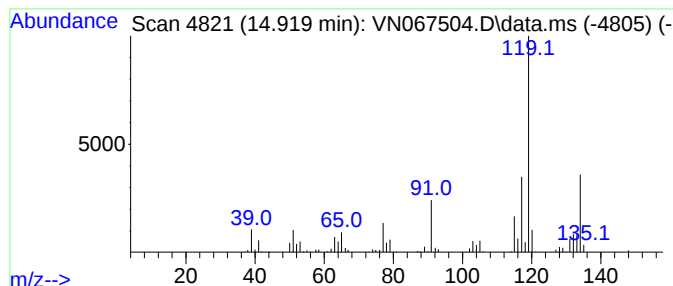
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 p-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.919	21.95 ug/l	460609	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	81
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
3			o-Cymene	134	C10H14	000527-84-4	81
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067504.D
Acq On : 25 Jun 2021 15:06
Operator : JC/MD
Sample : M2806-02 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1,3-di...	13.841	17.1	ug/l	359598	4	13.678	1049110	50.0
unknown13.879	13.879	40.4	ug/l	848368	4	13.678	1049110	50.0
Benzene, 2-ethy...	14.134	11.5	ug/l	242109	4	13.678	1049110	50.0
o-Cymene	14.160	9.7	ug/l	204147	4	13.678	1049110	50.0
Benzene, 4-ethy...	14.219	28.9	ug/l	606810	4	13.678	1049110	50.0
Benzene, (1-met...	14.329	32.7	ug/l	686192	4	13.678	1049110	50.0
Benzene, 1,2,3,...	14.541	12.6	ug/l	265251	4	13.678	1049110	50.0
Benzene, 1-ethy...	14.579	15.6	ug/l	326787	4	13.678	1049110	50.0
p-Cymene	14.919	21.9	ug/l	460609	4	13.678	1049110	50.0