

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
 Data File : VN067294.D
 Acq On : 11 Jun 2021 17:31
 Operator : JC/MD
 Sample : M2674-04 5X
 Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TMR-DS-04-060921

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\82N061021W.M
 Title : SW846 8260

Signal : TIC: VN067294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.859	1049	1070	1093	rBV	40933	125175	2.84%	0.345%
2	8.021	2236	2249	2260	rBV2	290017	654290	14.85%	1.804%
3	8.086	2261	2273	2293	rVB2	592522	1318466	29.92%	3.635%
4	8.437	2393	2404	2423	rVB2	395024	865091	19.63%	2.385%
5	8.968	2589	2602	2625	rVB	859796	1751255	39.74%	4.828%
6	10.443	3144	3152	3165	rVB	1341228	2354100	53.42%	6.490%
7	11.747	3629	3638	3653	rVB	1251199	2162976	49.08%	5.963%
8	11.950	3705	3714	3730	rVB2	1879740	3549880	80.55%	9.787%
9	12.731	3997	4005	4024	rVB	1199762	2070092	46.97%	5.707%
10	12.986	4092	4100	4107	rBV	744095	1190430	27.01%	3.282%
11	13.222	4182	4188	4203	rVB	567765	939134	21.31%	2.589%
12	13.369	4234	4243	4255	rVB	1402152	2156054	48.92%	5.944%
13	13.592	4320	4326	4345	rVB2	699827	1272180	28.87%	3.507%
14	13.675	4347	4357	4364	rBV	1239138	2190414	49.70%	6.039%
15	14.217	4551	4559	4569	rVB2	401344	600438	13.62%	1.655%
16	14.329	4593	4601	4625	rVB4	397081	794305	18.02%	2.190%
17	14.514	4660	4670	4688	rBV3	755160	1600776	36.32%	4.413%
18	14.817	4772	4783	4788	rBV2	743450	1280787	29.06%	3.531%
19	14.930	4812	4825	4839	rBV4	635835	1692080	38.40%	4.665%
20	14.997	4843	4850	4870	rVB	1011956	1695651	38.48%	4.675%
21	15.086	4873	4883	4899	rBV	893213	1600473	36.32%	4.413%
22	15.587	5059	5070	5084	rBV	2556805	4406907	100.00%	12.150%

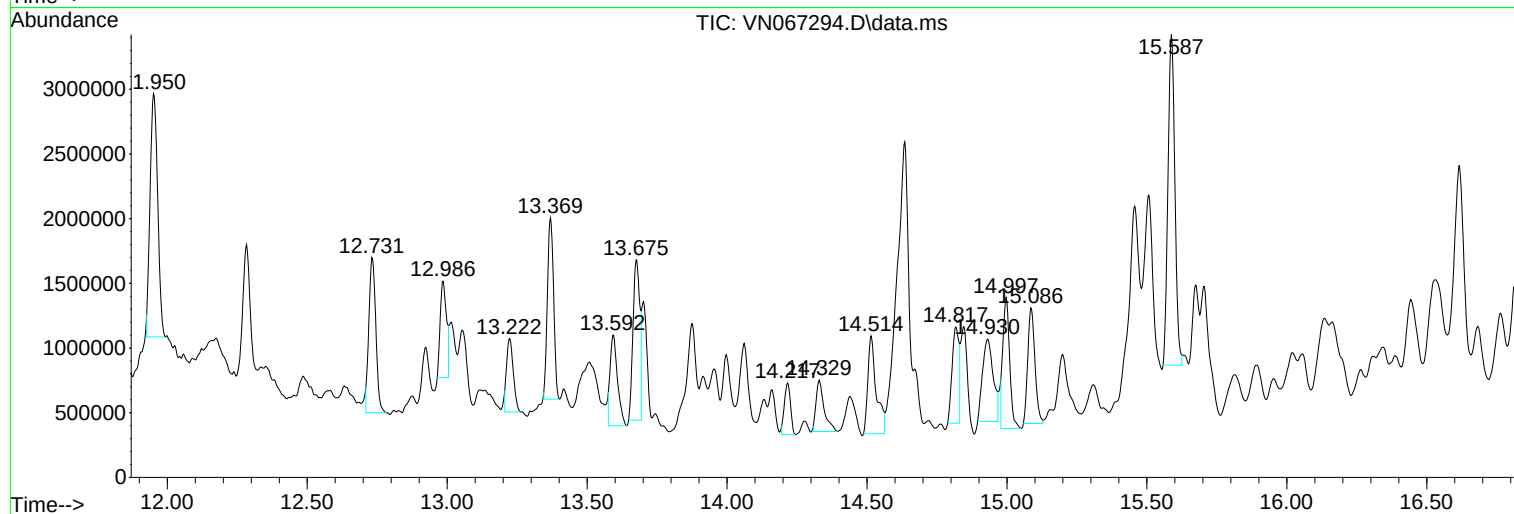
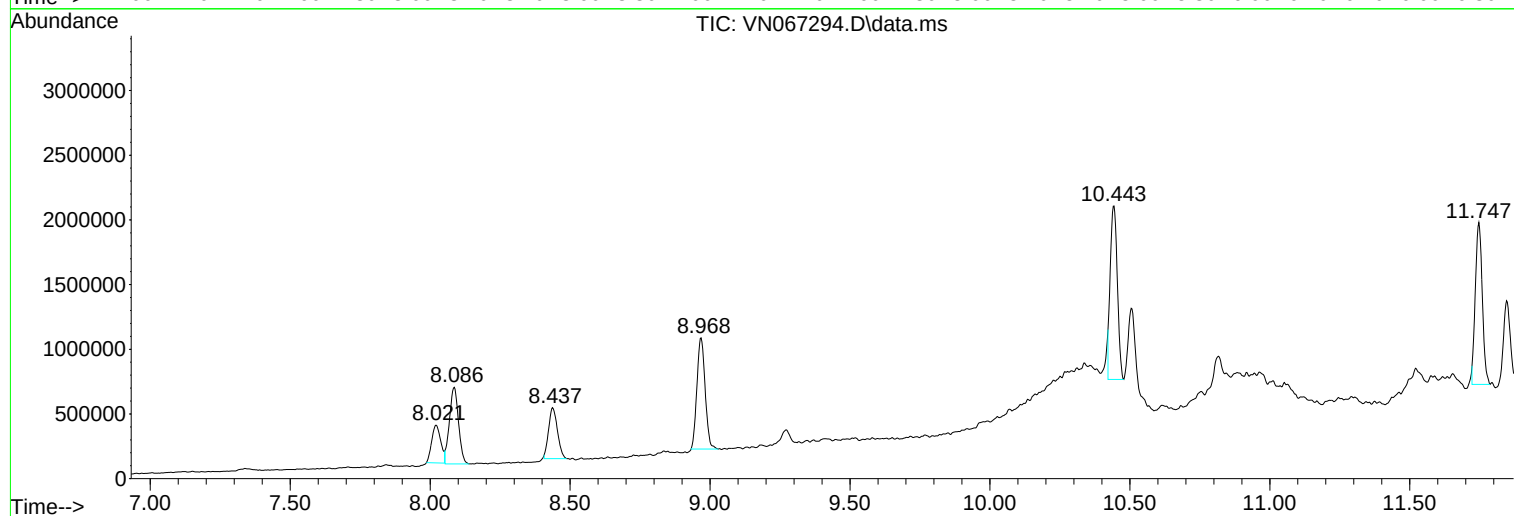
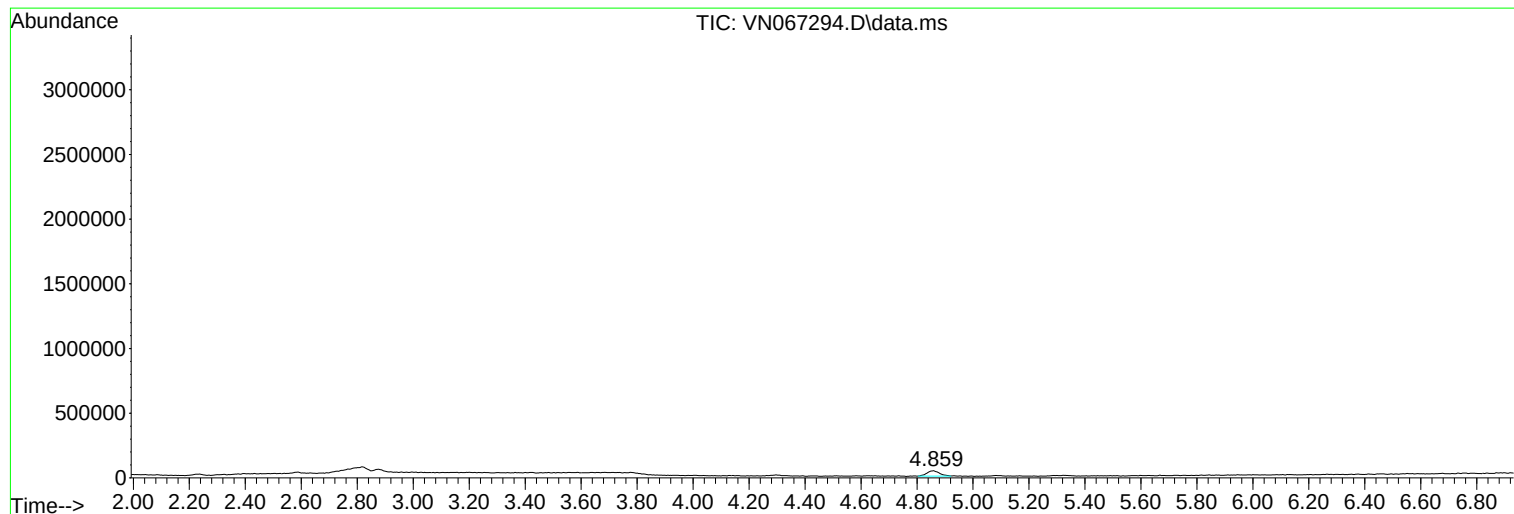
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Instrument :
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ClientSampleId :
TMR-DS-04-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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



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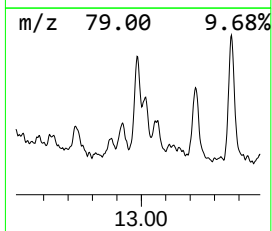
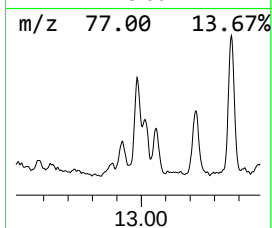
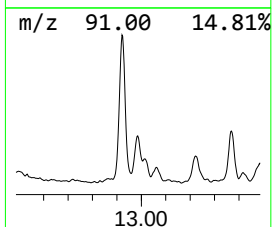
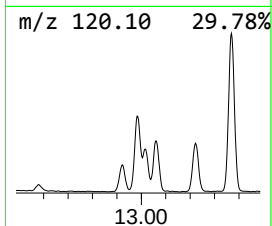
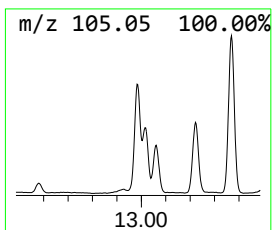
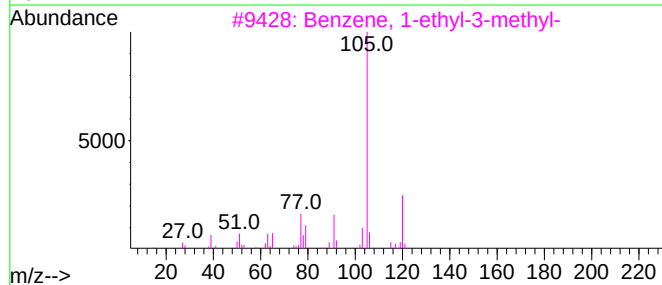
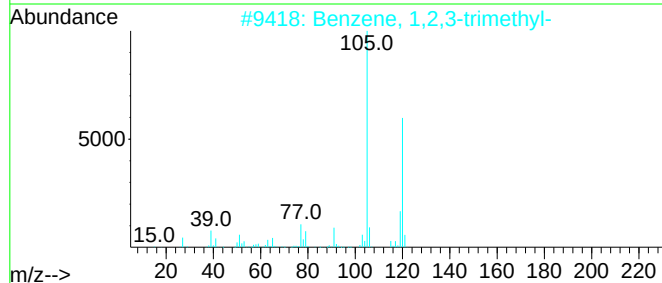
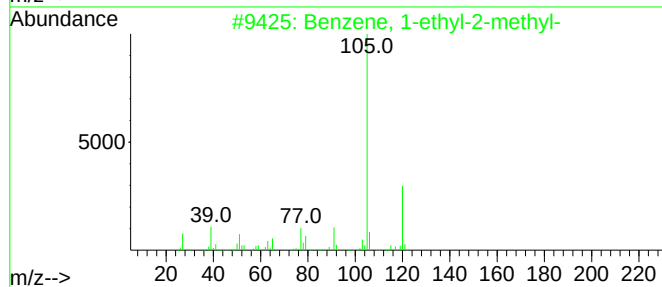
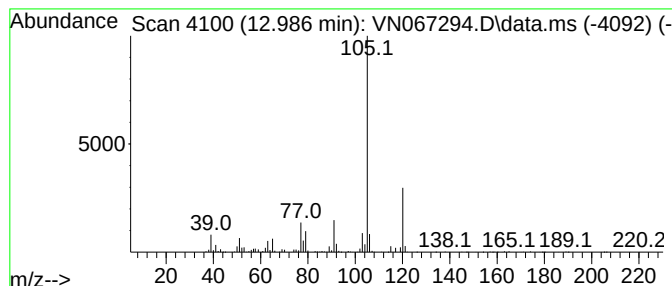
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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	27.17 ug/l	1190430	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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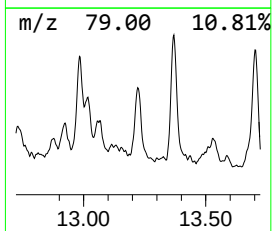
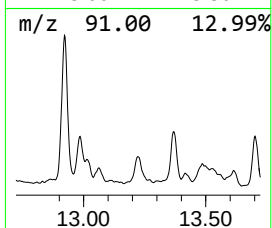
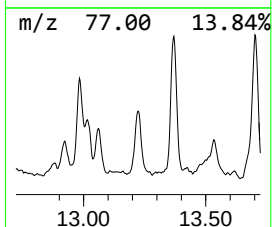
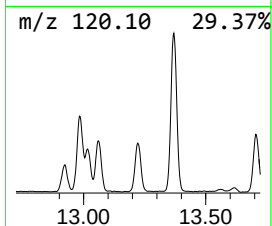
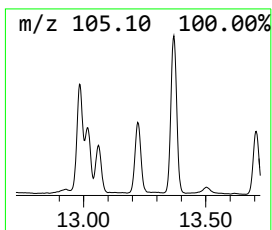
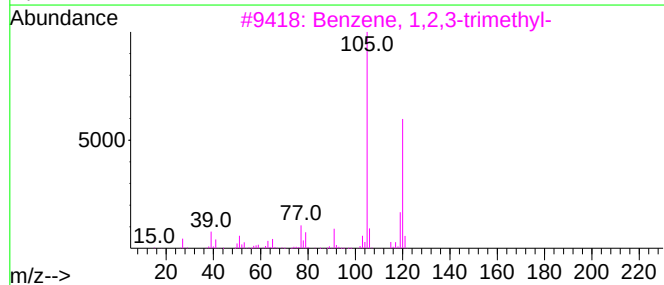
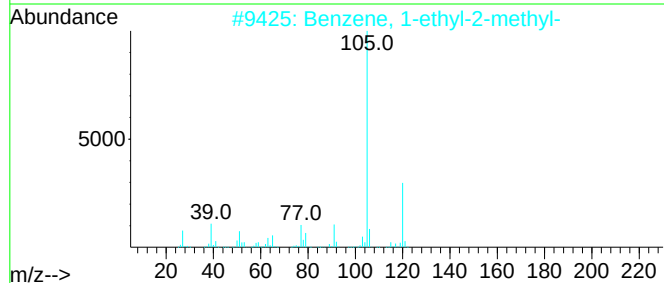
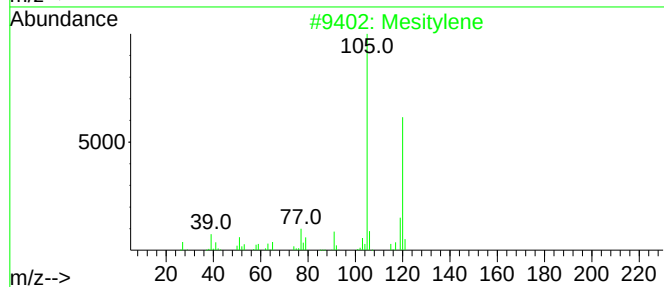
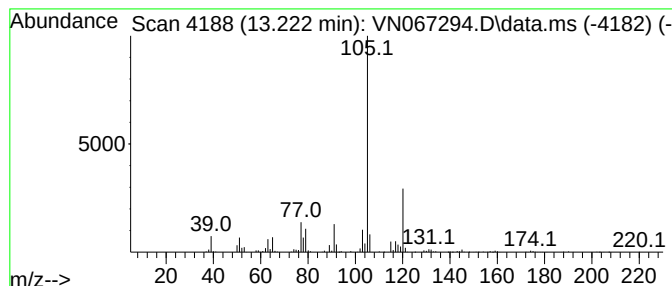
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	21.44 ug/l	939134	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	90
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	86



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Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

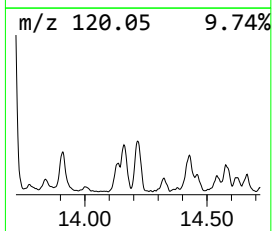
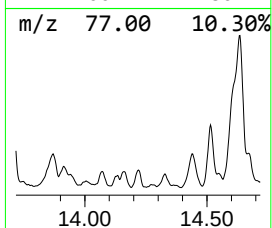
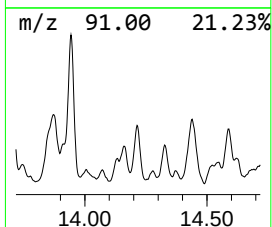
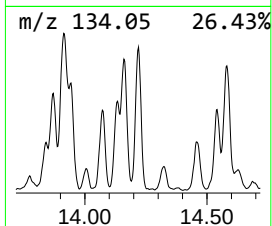
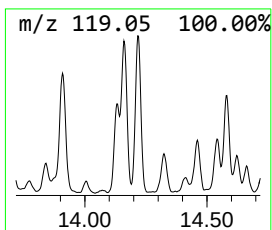
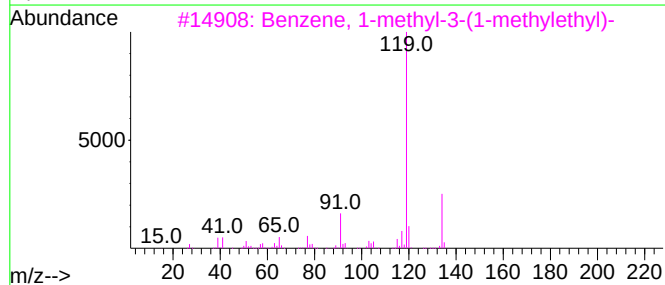
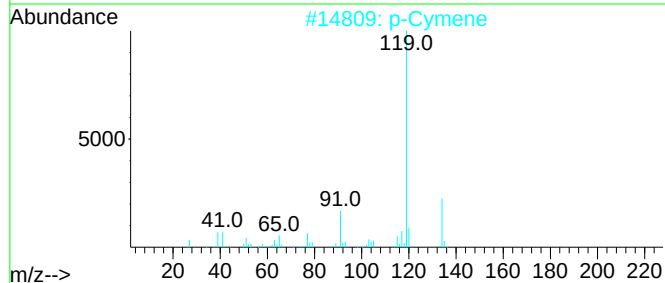
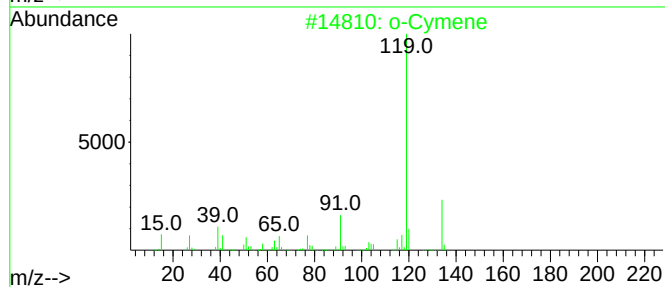
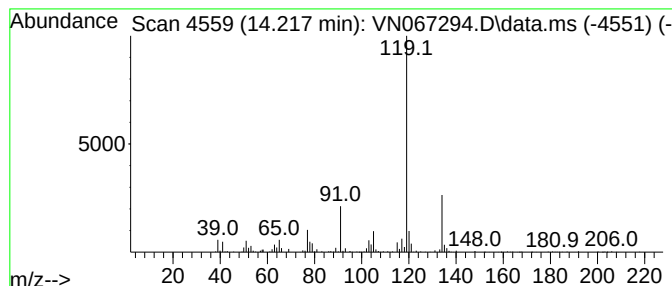
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 3 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	13.71 ug/l	600438	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	94
2			p-Cymene	134	C10H14	000099-87-6	93
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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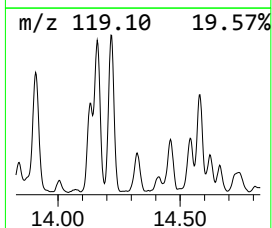
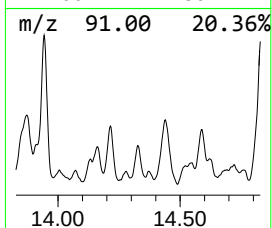
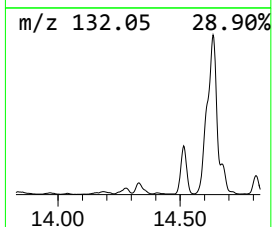
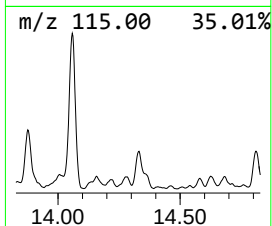
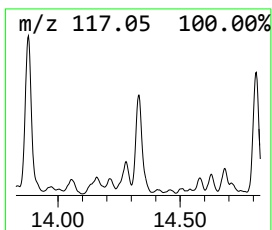
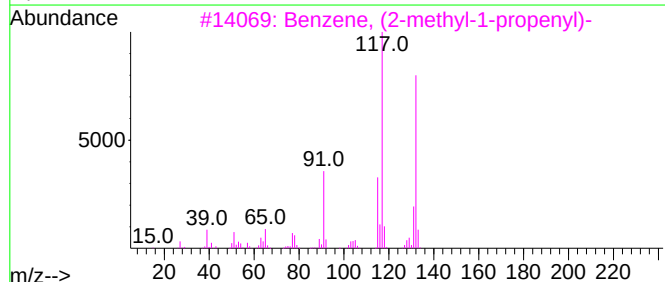
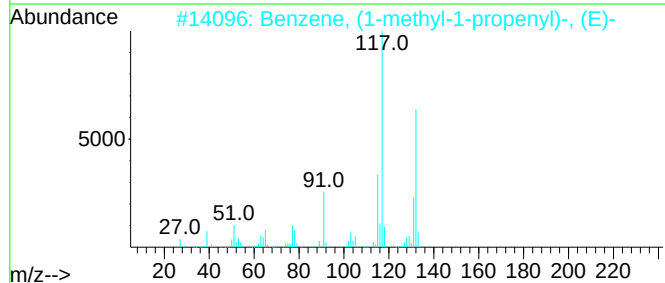
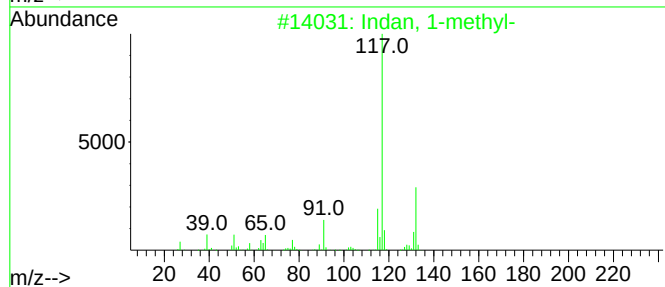
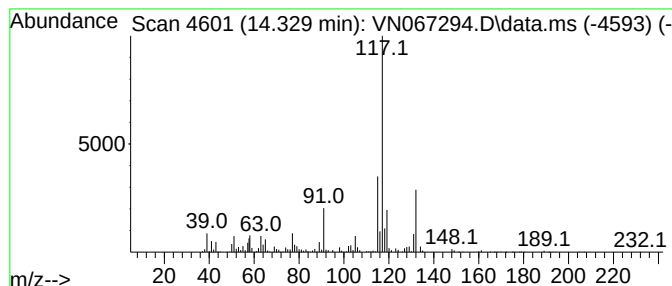
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Quant Title : SW846 8260

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

Peak Number 4 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	18.13 ug/l	794305	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	81
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74



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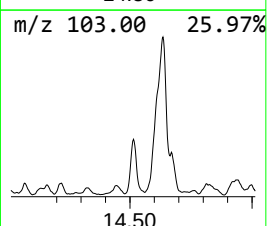
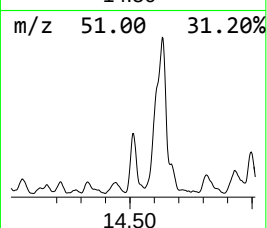
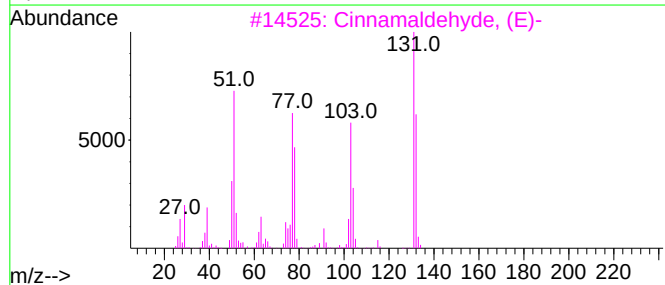
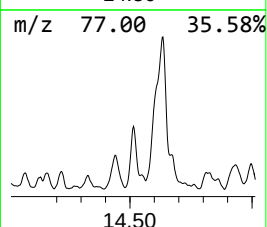
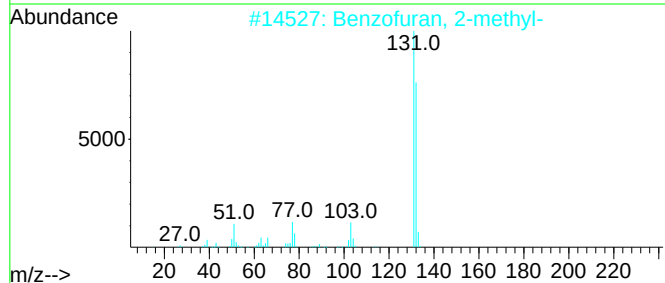
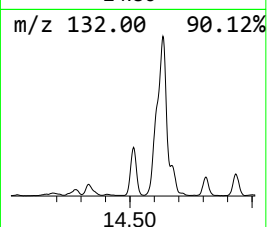
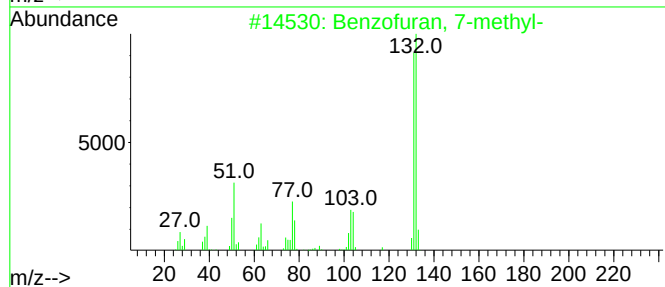
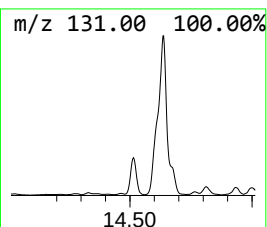
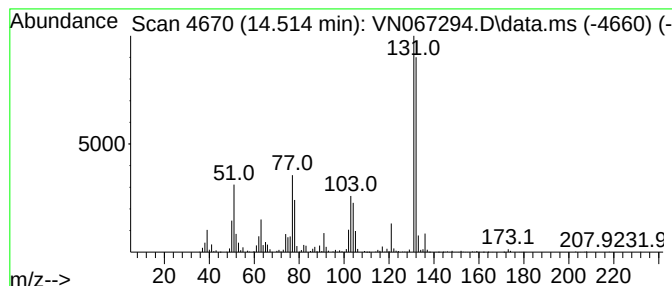
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzofuran, 7-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.514	36.54 ug/l	1600780	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	94
2			Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	93
3			Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	91
4			2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	91
5			3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91



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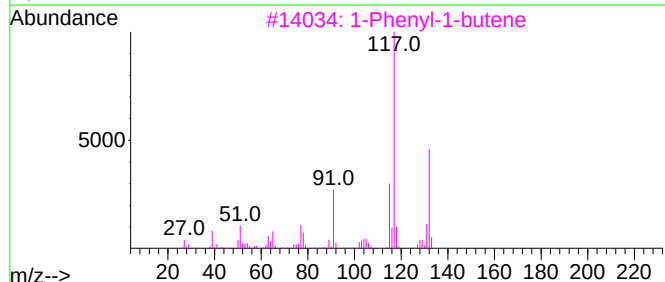
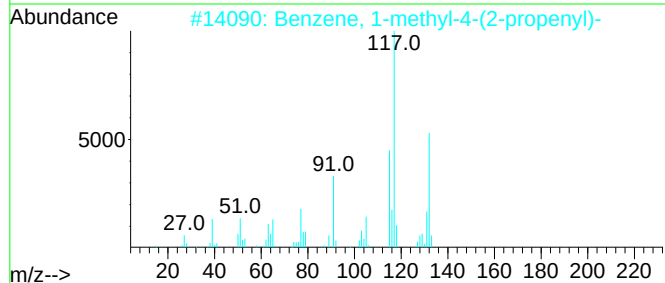
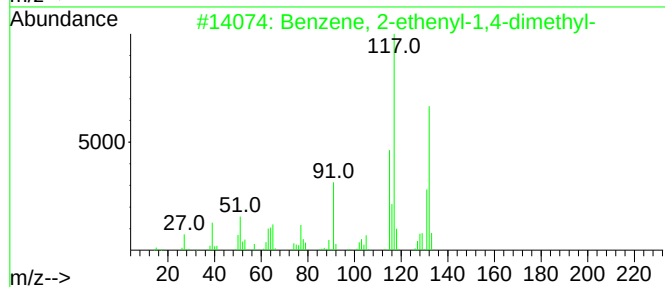
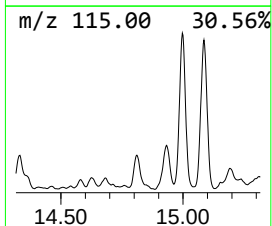
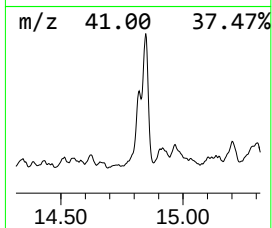
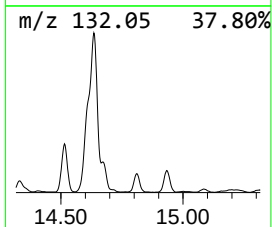
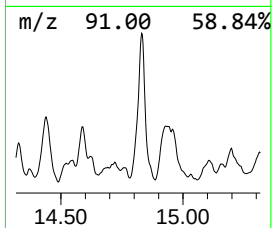
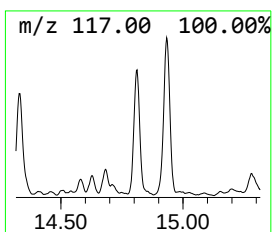
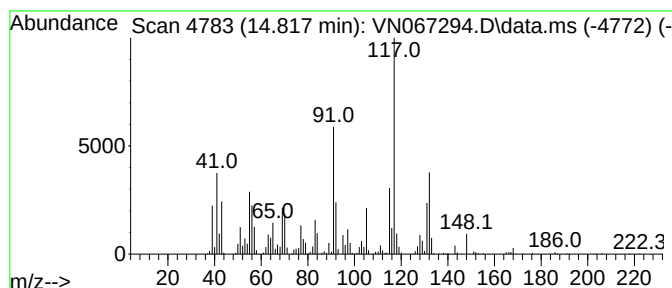
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.817	29.24 ug/l	1280790	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	93
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	92
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067294.D
Acq On : 11 Jun 2021 17:31
Operator : JC/MD
Sample : M2674-04 5X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

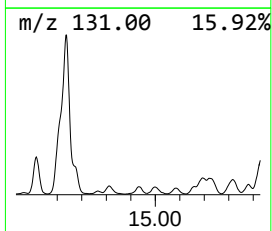
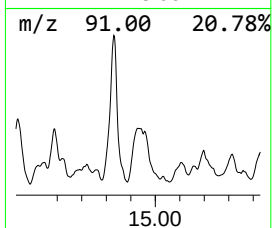
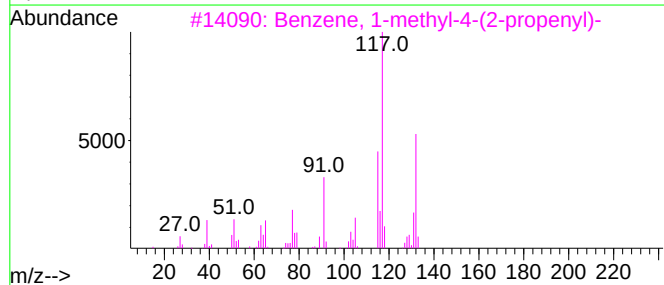
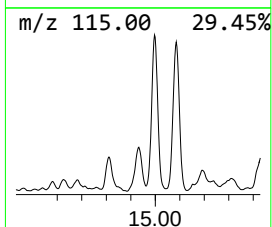
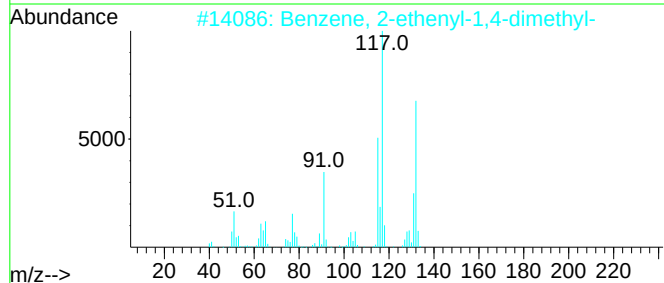
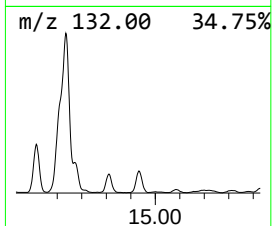
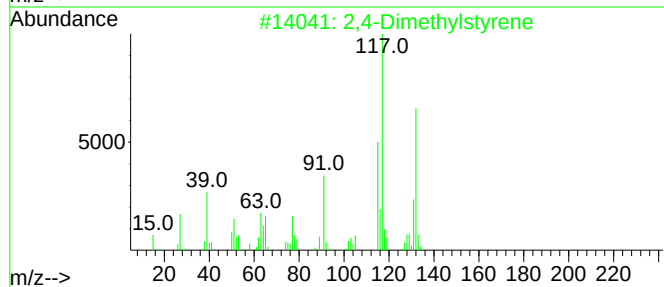
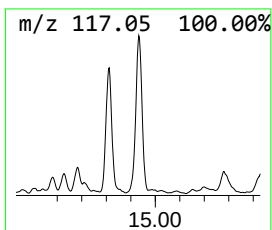
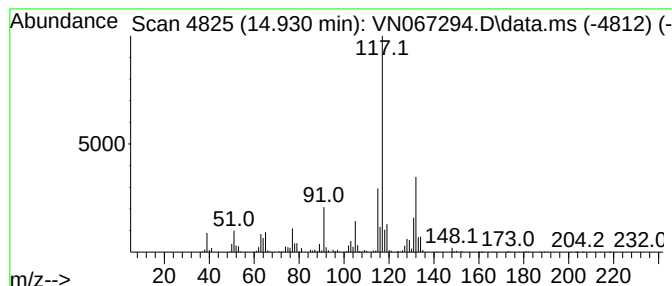
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Quant Title : SW846 8260

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

Peak Number 7 2,4-Dimethylstyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	38.62 ug/l	1692080	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	96
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	92
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	90
5			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067294.D
Acq On : 11 Jun 2021 17:31
Operator : JC/MD
Sample : M2674-04 5X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

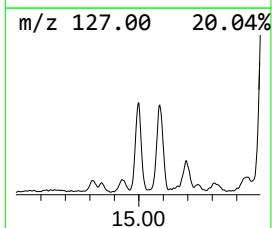
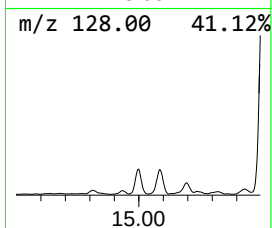
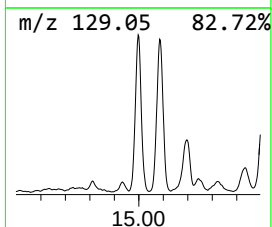
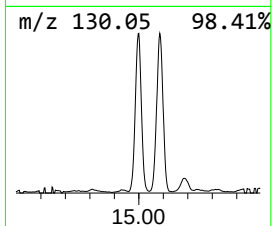
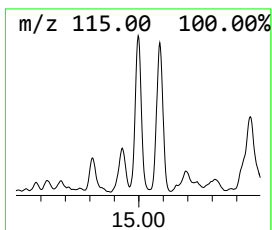
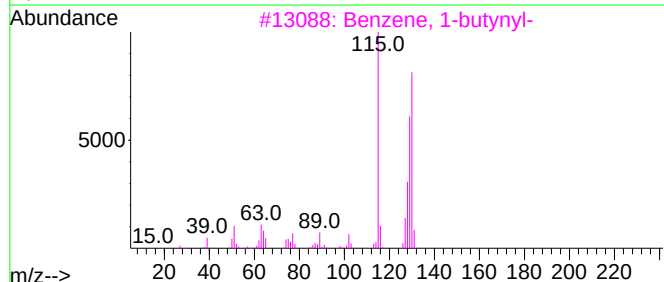
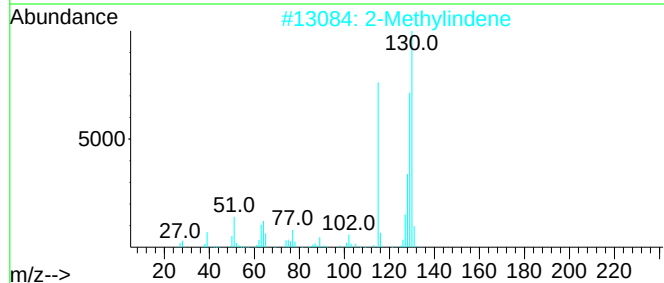
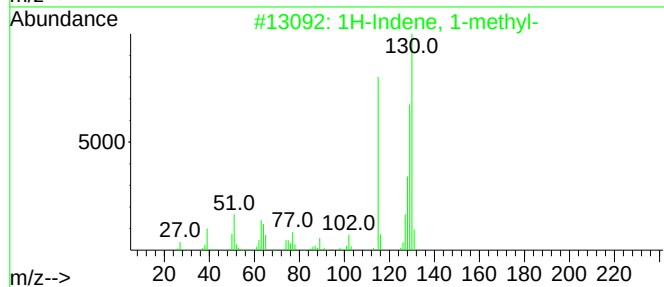
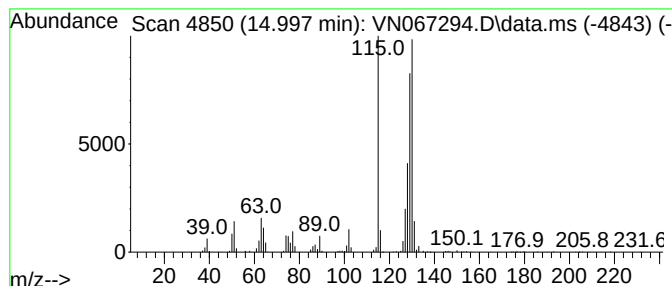
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	38.71 ug/l	1695650	1,4-Dichlorobenzene-d4	13.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2		2-Methylindene	130	C10H10	002177-47-1	95
3		Benzene, 1-butyryl-	130	C10H10	000622-76-4	95
4		Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5		Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067294.D
Acq On : 11 Jun 2021 17:31
Operator : JC/MD
Sample : M2674-04 5X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

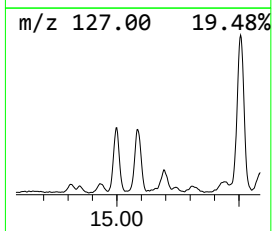
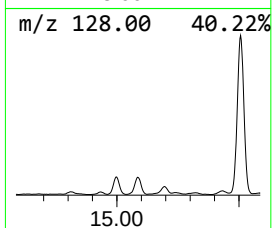
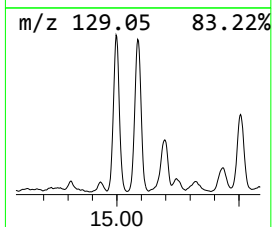
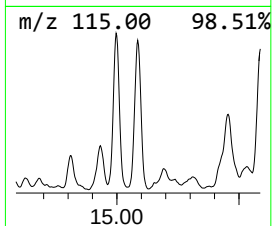
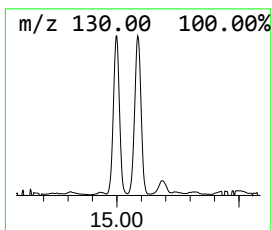
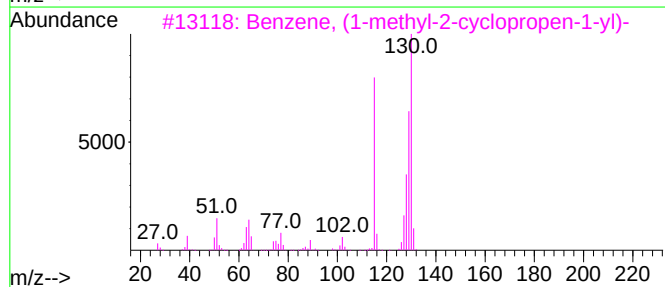
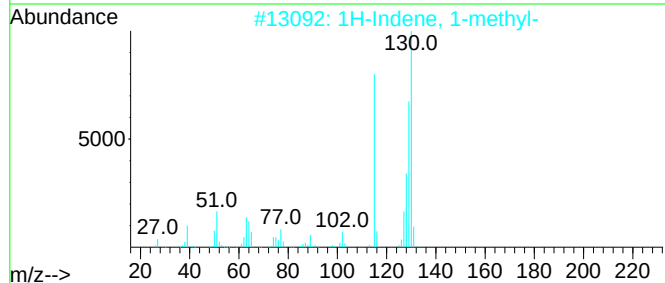
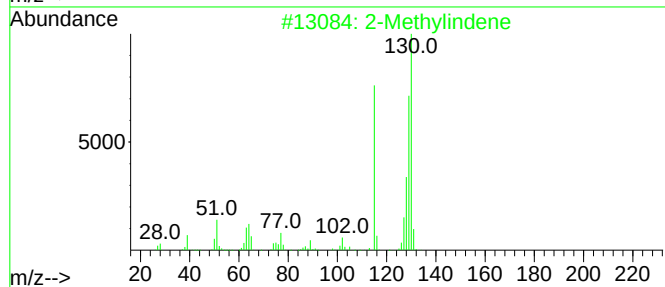
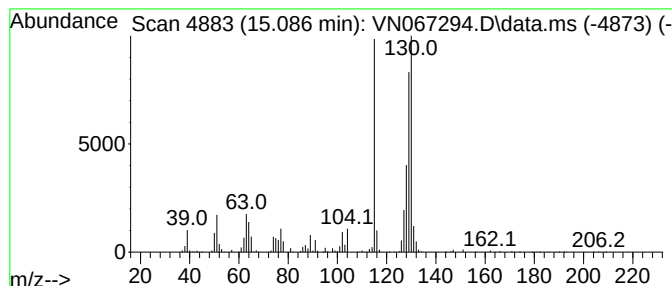
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 9 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	36.53 ug/l	1600470	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	96
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	96
4			Benzene, 1-butynyl-	130	C10H10	000622-76-4	96
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067294.D
Acq On : 11 Jun 2021 17:31
Operator : JC/MD
Sample : M2674-04 5X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

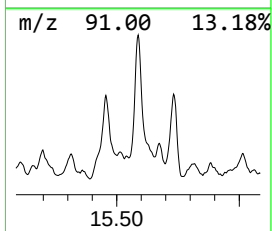
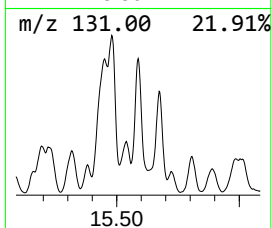
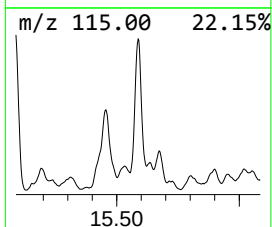
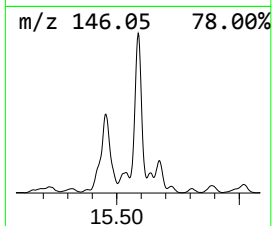
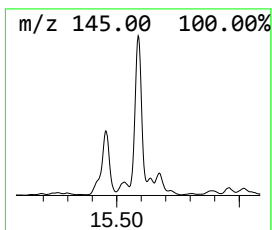
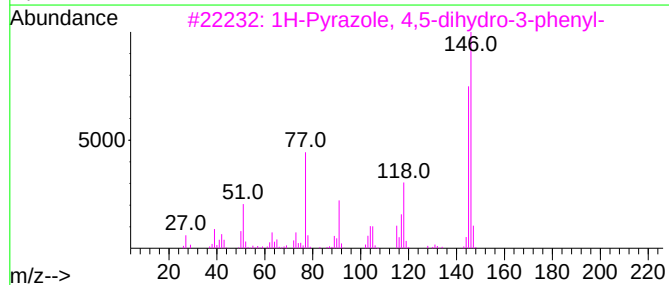
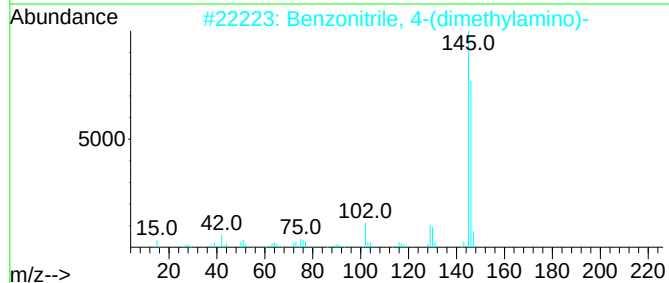
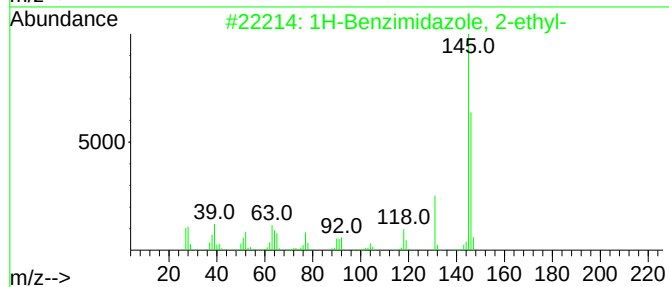
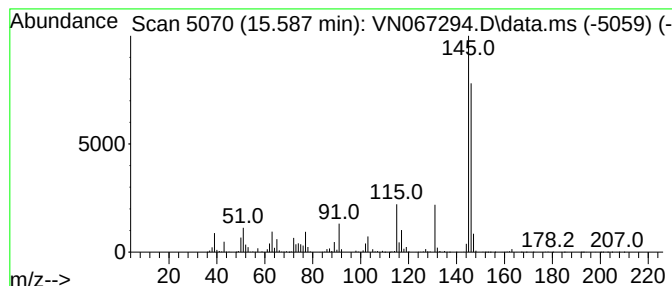
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 10 1H-Benzimidazole, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	100.60 ug/l	4406910	1,4-Dichlorobenzene-d4	13.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	72
2		Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
3		1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	52
4		Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	50
5		1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067294.D
Acq On : 11 Jun 2021 17:31
Operator : JC/MD
Sample : M2674-04 5X
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-04-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.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, 1,2,3-...	13.222	21.4	ug/l	939134	4	13.675	2190410	50.0
o-Cymene	14.217	13.7	ug/l	600438	4	13.675	2190410	50.0
Indan, 1-methyl-	14.329	18.1	ug/l	794305	4	13.675	2190410	50.0
Benzofuran, 7-m...	14.514	36.5	ug/l	1600780	4	13.675	2190410	50.0
Benzene, 2-ethe...	14.817	29.2	ug/l	1280790	4	13.675	2190410	50.0
2,4-Dimethylsty...	14.930	38.6	ug/l	1692080	4	13.675	2190410	50.0
1H-Indene, 1-me...	14.997	38.7	ug/l	1695650	4	13.675	2190410	50.0
2-Methylindene	15.086	36.5	ug/l	1600470	4	13.675	2190410	50.0
1H-Benzimidazol...	15.587	100.6	ug/l	4406910	4	13.675	2190410	50.0