

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
 Data File : VN067289.D
 Acq On : 11 Jun 2021 15:30
 Operator : JC/MD
 Sample : M2674-05 10X
 Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TMR-DS-05-060921

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: VN067289.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.862	1057	1071	1085	rBV2	12990	31830	1.13%	0.151%
2	8.021	2225	2249	2260	rBV2	337334	805512	28.66%	3.832%
3	8.086	2261	2273	2299	rVB	627716	1443456	51.36%	6.867%
4	8.440	2383	2405	2429	rBV2	400351	941926	33.52%	4.481%
5	8.968	2584	2602	2639	rBV	911575	1931547	68.73%	9.189%
6	10.443	3133	3152	3168	rBV	1422301	2726166	97.01%	12.970%
7	11.746	3622	3638	3660	rBV	1360209	2469384	87.87%	11.748%
8	11.846	3668	3675	3688	rVB2	40187	65651	2.34%	0.312%
9	11.953	3703	3715	3733	rVB3	135248	266885	9.50%	1.270%
10	12.280	3827	3837	3850	rVB2	80339	135161	4.81%	0.643%
11	12.731	3992	4005	4027	rVB	1132993	1994301	70.96%	9.488%
12	12.986	4091	4100	4106	rBV	89908	150241	5.35%	0.715%
13	13.222	4179	4188	4201	rBV2	80314	143145	5.09%	0.681%
14	13.369	4235	4243	4257	rVB	215811	368617	13.12%	1.754%
15	13.675	4343	4357	4393	rBV	1356696	2810263	100.00%	13.370%
16	13.997	4471	4477	4489	rVB4	108105	147330	5.24%	0.701%
17	14.133	4520	4528	4531	rBV2	42352	53223	1.89%	0.253%
18	14.217	4554	4559	4568	rVB2	77979	104475	3.72%	0.497%
19	14.514	4660	4670	4686	rBV4	113794	234455	8.34%	1.115%
20	14.817	4772	4783	4790	rBV5	179099	346924	12.34%	1.650%
21	14.935	4809	4827	4838	rBV7	157800	421922	15.01%	2.007%
22	15.086	4875	4883	4895	rVB2	114280	181414	6.46%	0.863%
23	15.453	5001	5020	5030	rBV3	339732	863254	30.72%	4.107%
24	15.587	5059	5070	5091	rBV	557197	1003568	35.71%	4.774%
25	15.673	5095	5102	5119	rVB6	156348	243094	8.65%	1.157%
26	16.443	5379	5389	5404	rVB3	196191	404751	14.40%	1.926%
27	16.520	5407	5418	5431	rBV2	190704	411053	14.63%	1.956%
28	16.762	5497	5508	5518	rBV7	152200	320102	11.39%	1.523%

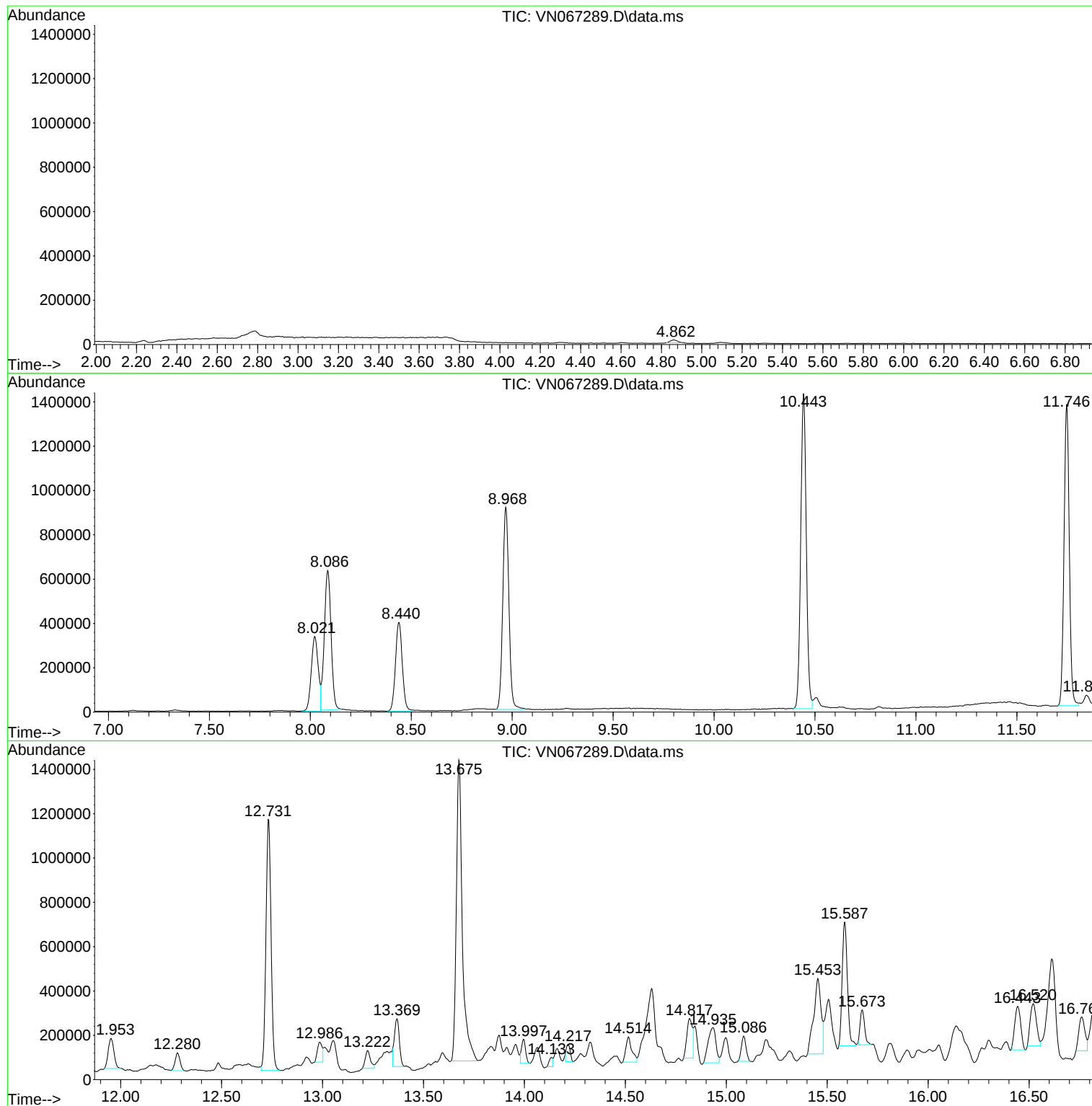
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

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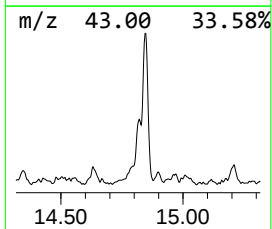
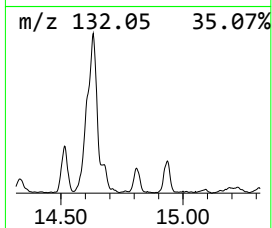
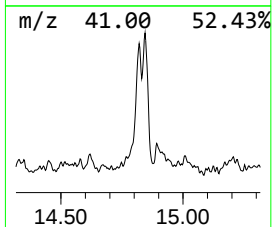
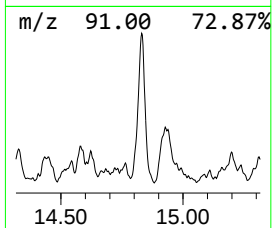
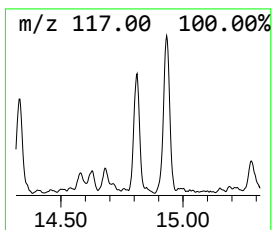
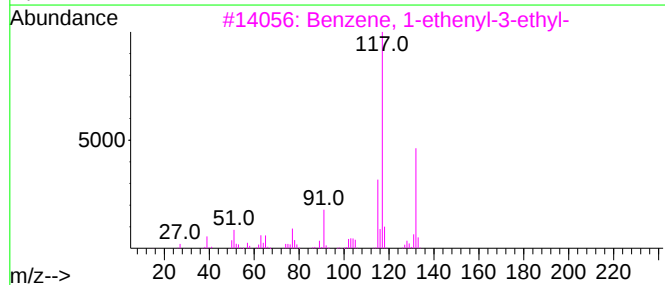
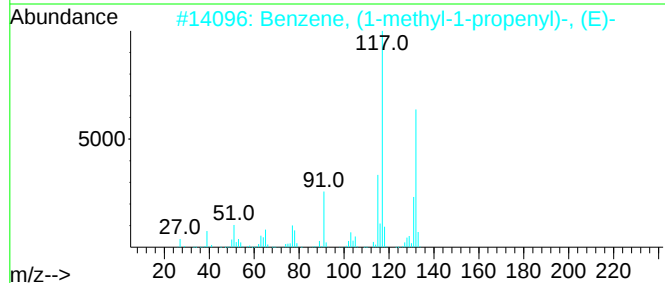
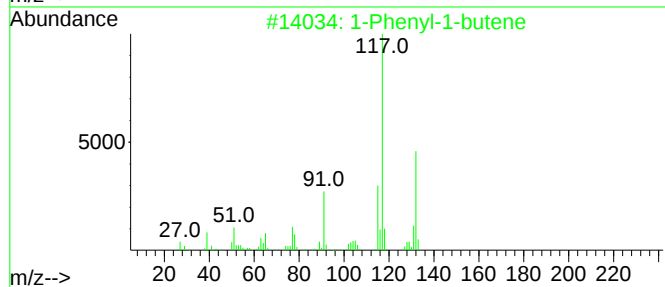
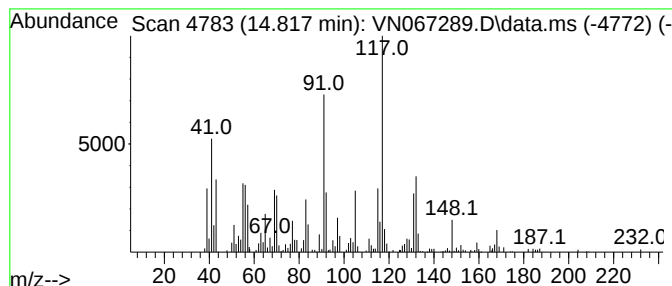
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Phenyl-1-butene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.817	6.17 ug/l	346924	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	64
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	64



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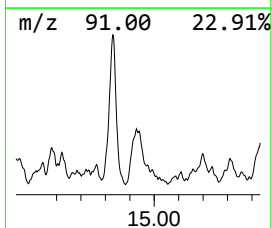
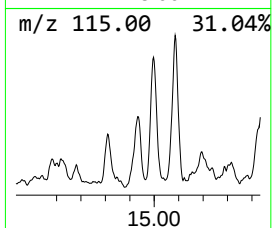
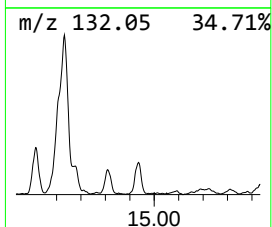
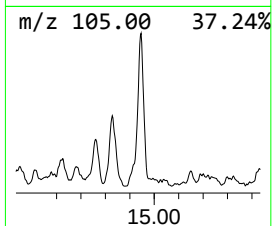
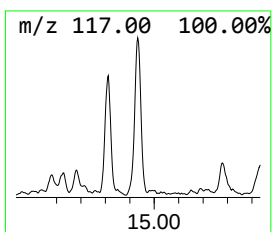
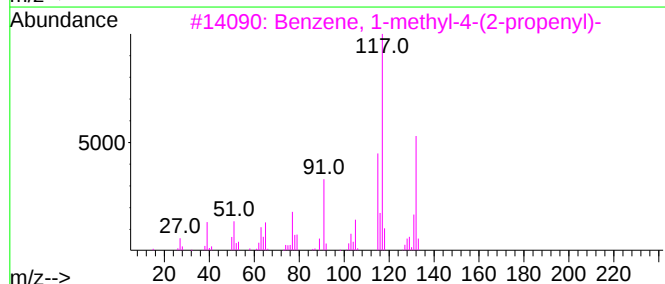
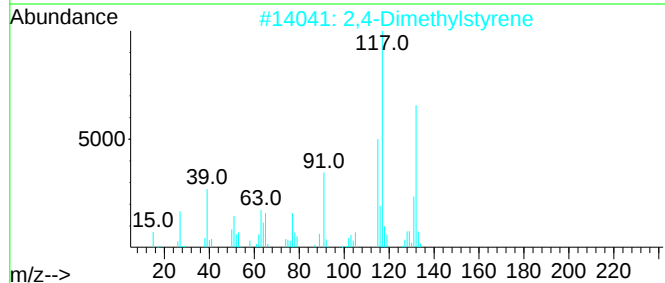
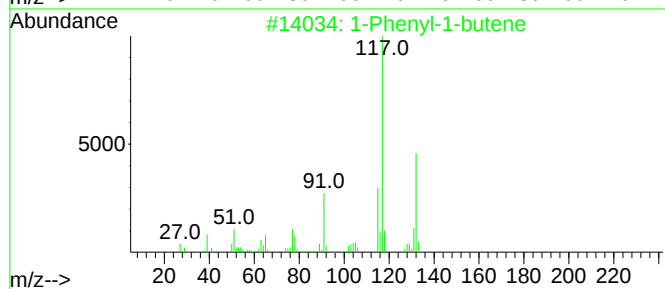
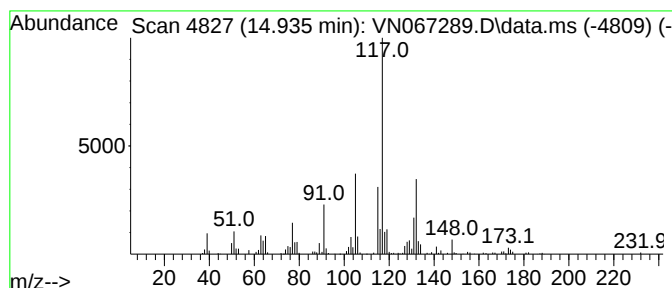
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 2 2,4-Dimethylstyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	7.51 ug/l	421922	1,4-Dichlorobenzene-d4	13.678

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2		2,4-Dimethylstyrene	132	C10H12	002234-20-0	91
3		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	90
4		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
5		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

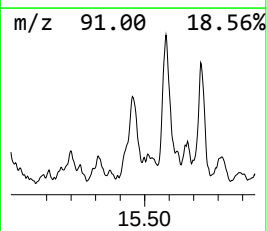
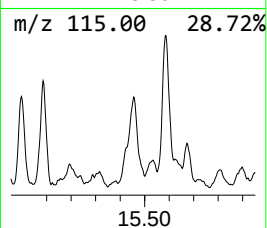
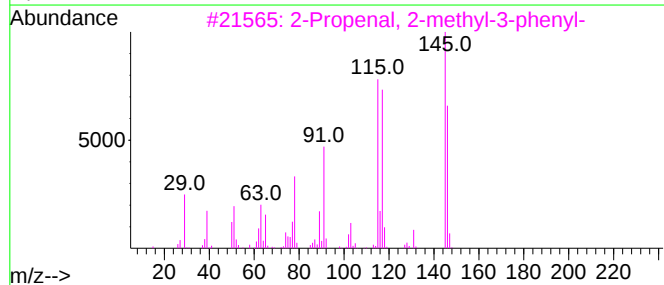
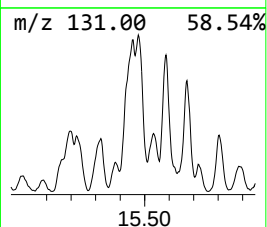
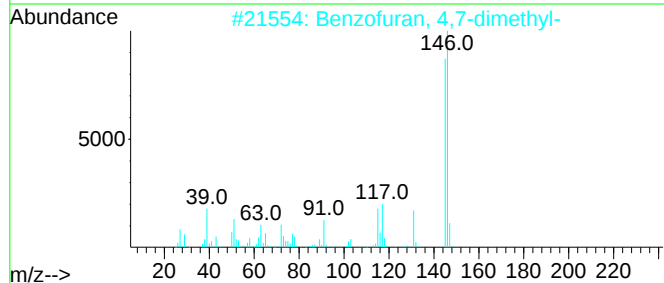
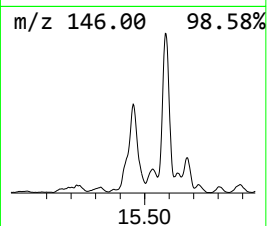
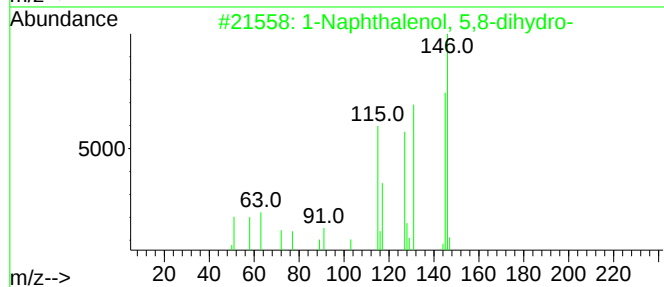
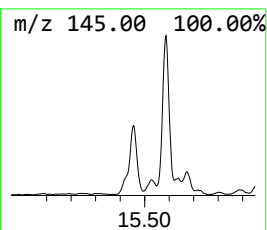
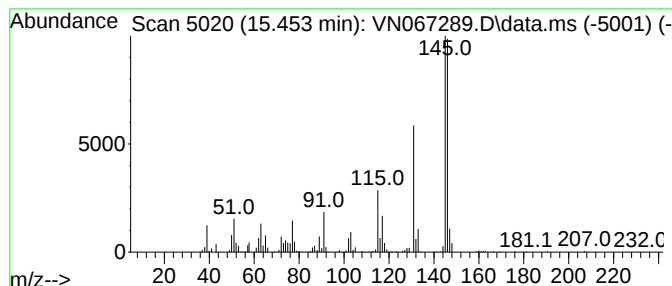
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Naphthalenol, 5,8-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.453	15.36 ug/l	863254	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenol, 5,8-dihydro-	146	C10H10O	027673-48-9	87		
2	Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	60		
3	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	58		
4	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	52		
5	3-Buten-2-one, 4-phenyl-	146	C10H10O	000122-57-6	50		



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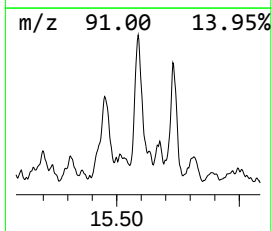
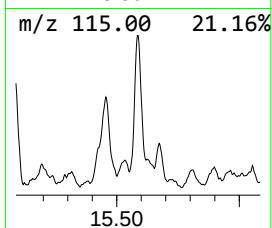
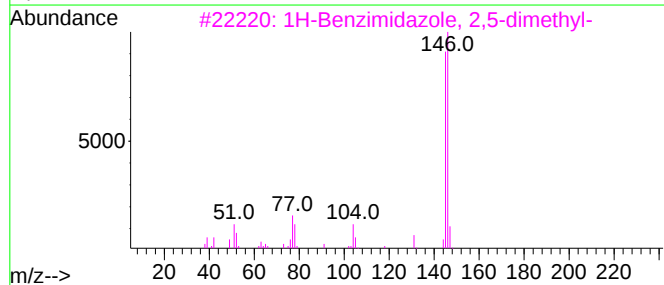
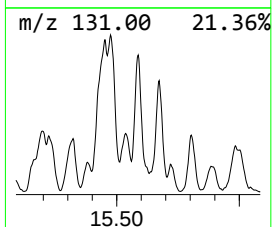
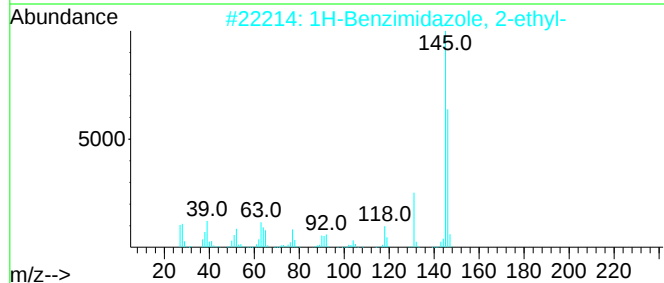
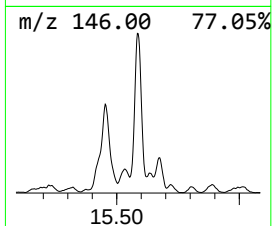
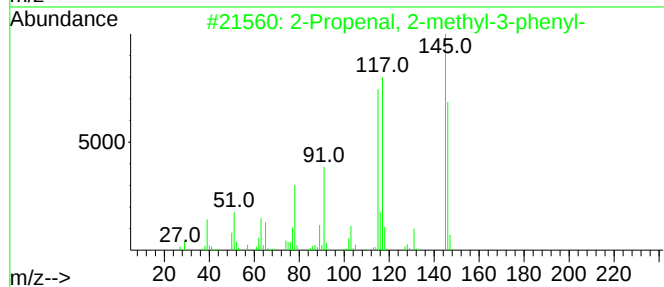
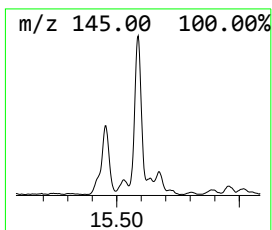
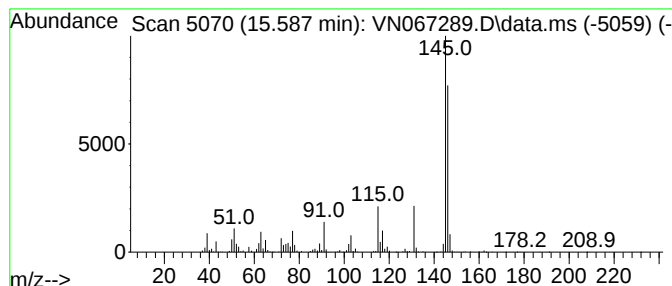
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Propenal, 2-methyl-3-phenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	17.86 ug/l	1003570	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	72
2			1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	64
3			1H-Benzimidazole, 2,5-dimethyl-	146	C9H10N2	001792-41-2	59
4			Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
5			1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	50



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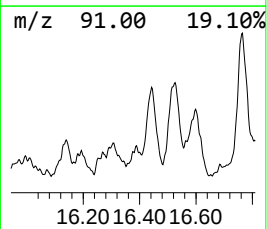
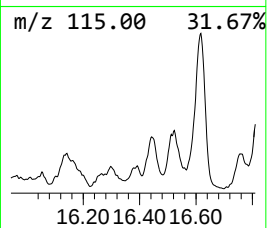
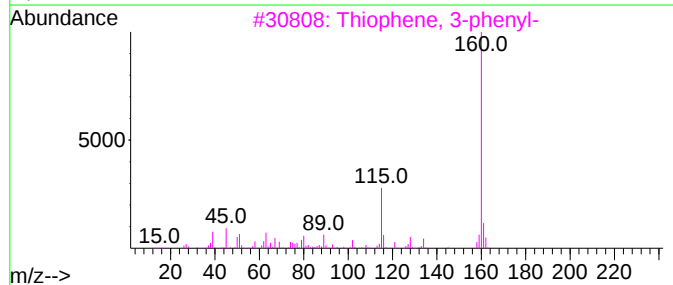
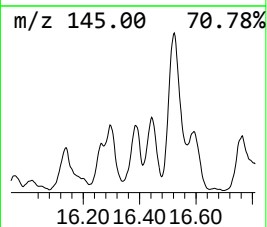
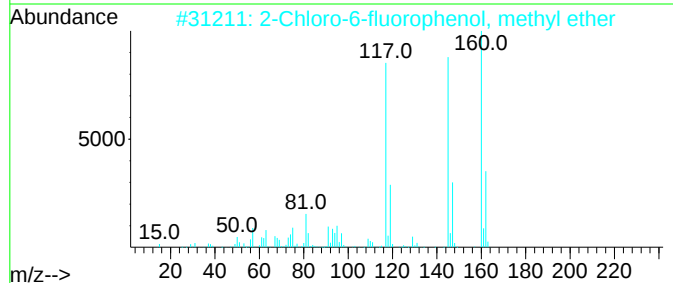
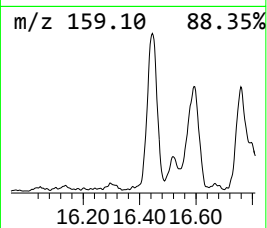
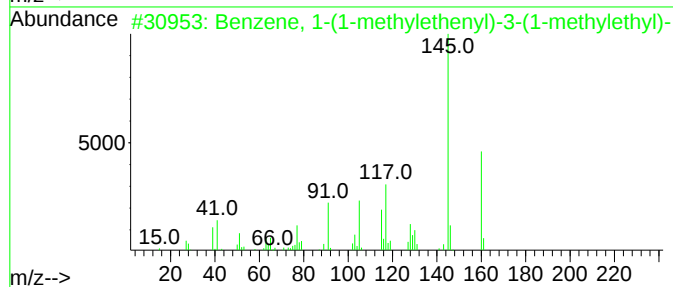
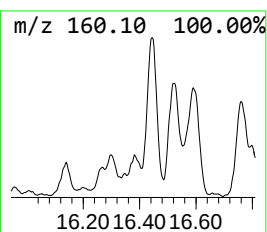
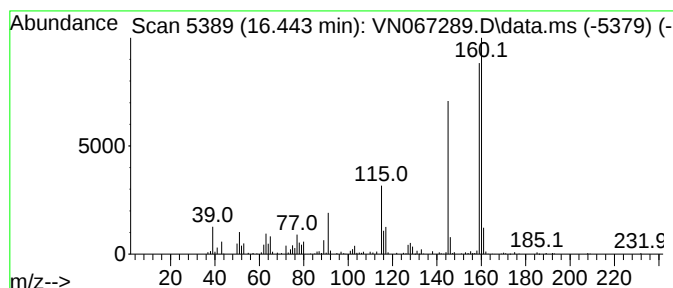
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown16.443 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.443	7.20 ug/l	404751	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	49
2			2-Chloro-6-fluorophenol, methyl ...	160	C7H6ClFO	1000352-53-9	43
3			Thiophene, 3-phenyl-	160	C10H8S	002404-87-7	43
4			1H-Benzimidazole, 1-ethyl-2-methyl-	160	C10H12N2	005805-76-5	38
5			5-Isopropyl-2-methylphenethyl ac...	220	C14H20O2	027913-43-5	38



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ClientSampleId :
TMR-DS-05-060921

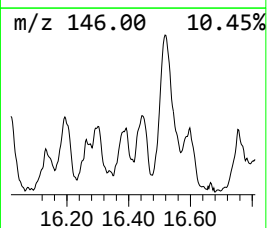
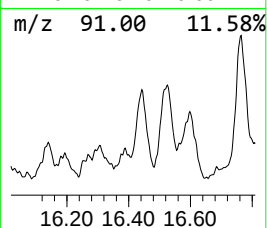
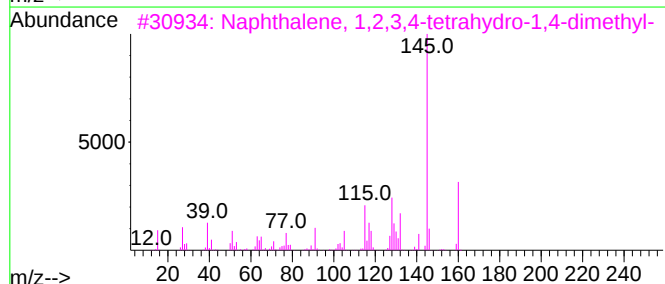
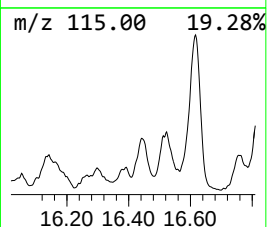
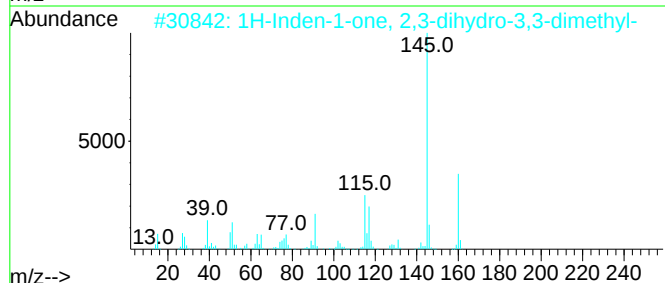
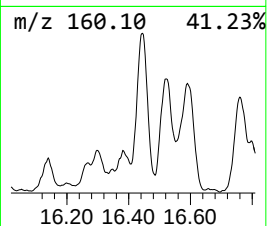
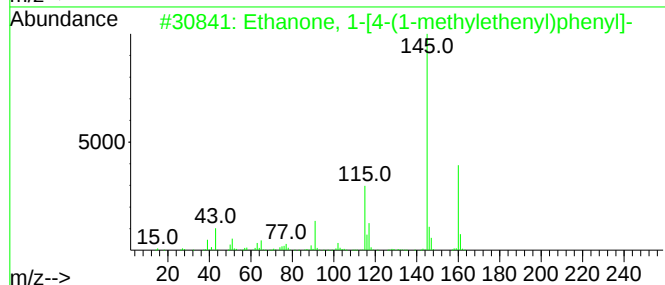
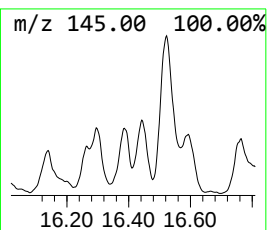
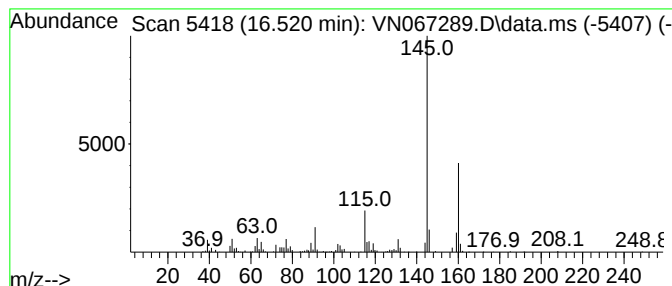
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Quant Title : SW846 8260

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

Peak Number 6 Ethanone, 1-[4-(1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.520	7.31 ug/l	411053	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-[4-(1-methylethenyl)...	160	C11H12O	005359-04-6	74
2			1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	72
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	72
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	64
5			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067289.D
Acq On : 11 Jun 2021 15:30
Operator : JC/MD
Sample : M2674-05 10X
Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

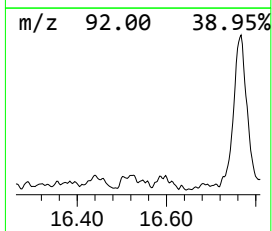
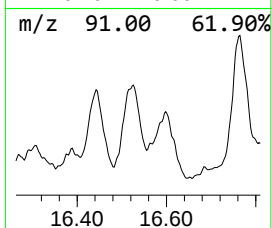
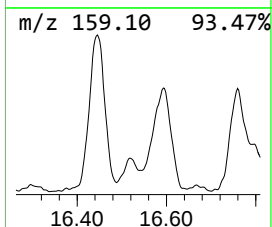
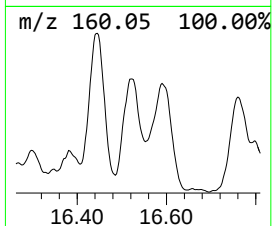
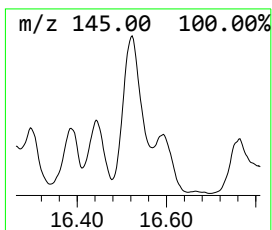
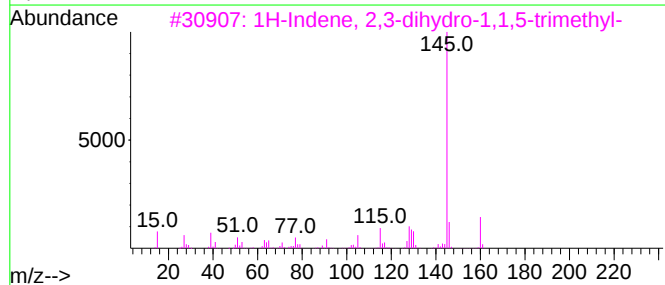
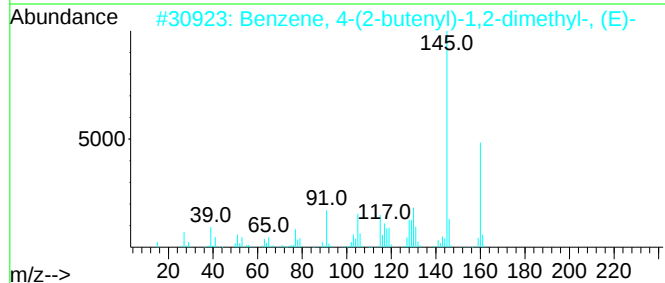
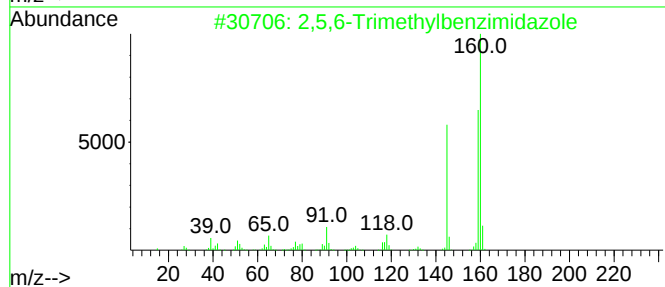
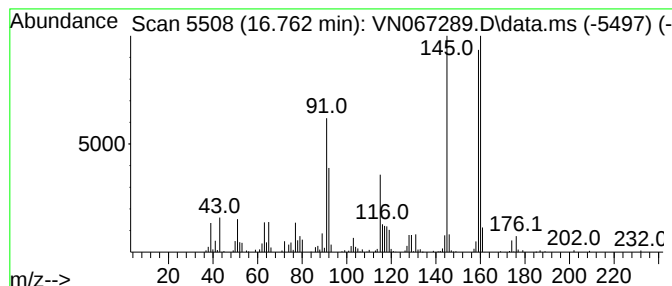
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Quant Title : SW846 8260

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

Peak Number 7 2,5,6-Trimethylbenzimidazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	5.70 ug/l	320102	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5,6-Trimethylbenzimidazole	160	C10H12N2	003363-56-2	58
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	55
3			1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	53
4			1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	49
5			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067289.D
Acq On : 11 Jun 2021 15:30
Operator : JC/MD
Sample : M2674-05 10X
Misc : 5.05g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-05-060921

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
1-Phenyl-1-butene	14.817	6.2	ug/l	346924	4	13.678	2810260	50.0
2,4-Dimethylsty...	14.935	7.5	ug/l	421922	4	13.678	2810260	50.0
1-Naphthalenol,...	15.453	15.4	ug/l	863254	4	13.678	2810260	50.0
2-Propenal, 2-m...	15.587	17.9	ug/l	1003570	4	13.678	2810260	50.0
unknown16.443	16.443	7.2	ug/l	404751	4	13.678	2810260	50.0
Ethanone, 1-[4-...	16.520	7.3	ug/l	411053	4	13.678	2810260	50.0
2,5,6-Trimethyl...	16.762	5.7	ug/l	320102	4	13.678	2810260	50.0