

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
 Data File : VN068313.D
 Acq On : 25 Aug 2021 20:59
 Operator : JC/MD
 Sample : M3529-06
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41987

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\82N081721W.M
 Title : SW846 8260

Signal : TIC: VN068313.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.692	613	635	676	rBV	449348	1236905	1.78%	0.822%
2	4.291	831	858	901	rBV	792312	2347570	3.38%	1.561%
3	7.340	1973	1995	2019	rBV	338071	915956	1.32%	0.609%
4	8.088	2261	2274	2306	rVB2	889552	2029777	2.93%	1.350%
5	8.458	2383	2412	2436	rBV4	977379	2746639	3.96%	1.826%
6	8.971	2584	2603	2644	rVB	1143253	2410541	3.48%	1.603%
7	10.068	2995	3012	3031	rBV	678815	1271078	1.83%	0.845%
8	10.443	3136	3152	3165	rBV	1607387	3026808	4.36%	2.013%
9	10.507	3165	3176	3204	rVB	1267289	2414582	3.48%	1.605%
10	11.146	3399	3414	3431	rBV2	1615607	3061436	4.41%	2.036%
11	11.223	3432	3443	3459	rVB	648889	1244908	1.79%	0.828%
12	11.746	3619	3638	3649	rBV	1811528	3520554	5.08%	2.341%
13	11.915	3687	3701	3709	rBV	2701937	4967682	7.16%	3.303%
14	12.283	3826	3838	3854	rBV4	1455288	2782414	4.01%	1.850%
15	12.522	3915	3927	3943	rBV3	769186	1419291	2.05%	0.944%
16	12.733	3992	4006	4035	rBV	1447811	2666697	3.84%	1.773%
17	12.924	4065	4077	4090	rBV	450378	842714	1.21%	0.560%
18	13.053	4117	4125	4137	rVB2	419896	733584	1.06%	0.488%
19	13.369	4233	4243	4256	rVB	1186524	2024283	2.92%	1.346%
20	13.677	4344	4358	4380	rVV2	2037686	5046423	7.27%	3.355%
21	13.771	4383	4393	4422	rVV2	1114054	2486925	3.59%	1.654%
22	13.879	4424	4433	4457	rVB	591497	1098338	1.58%	0.730%
23	14.058	4486	4500	4521	rVB	7080500	11895609	17.15%	7.910%
24	14.423	4622	4636	4659	rBV	1900303	3453940	4.98%	2.297%
25	14.997	4833	4850	4864	rVB2	479393	1110599	1.60%	0.738%
26	15.083	4870	4882	4900	rVB	538837	975321	1.41%	0.649%
27	15.364	4975	4987	5006	rBV	575334	1065460	1.54%	0.708%
28	15.509	5017	5041	5059	rBV2	35293776	69367937	100.00%	46.124%
29	15.606	5059	5077	5097	rVB	1822949	4283581	6.18%	2.848%
30	16.620	5438	5455	5480	rVB	3517157	7947654	11.46%	5.285%

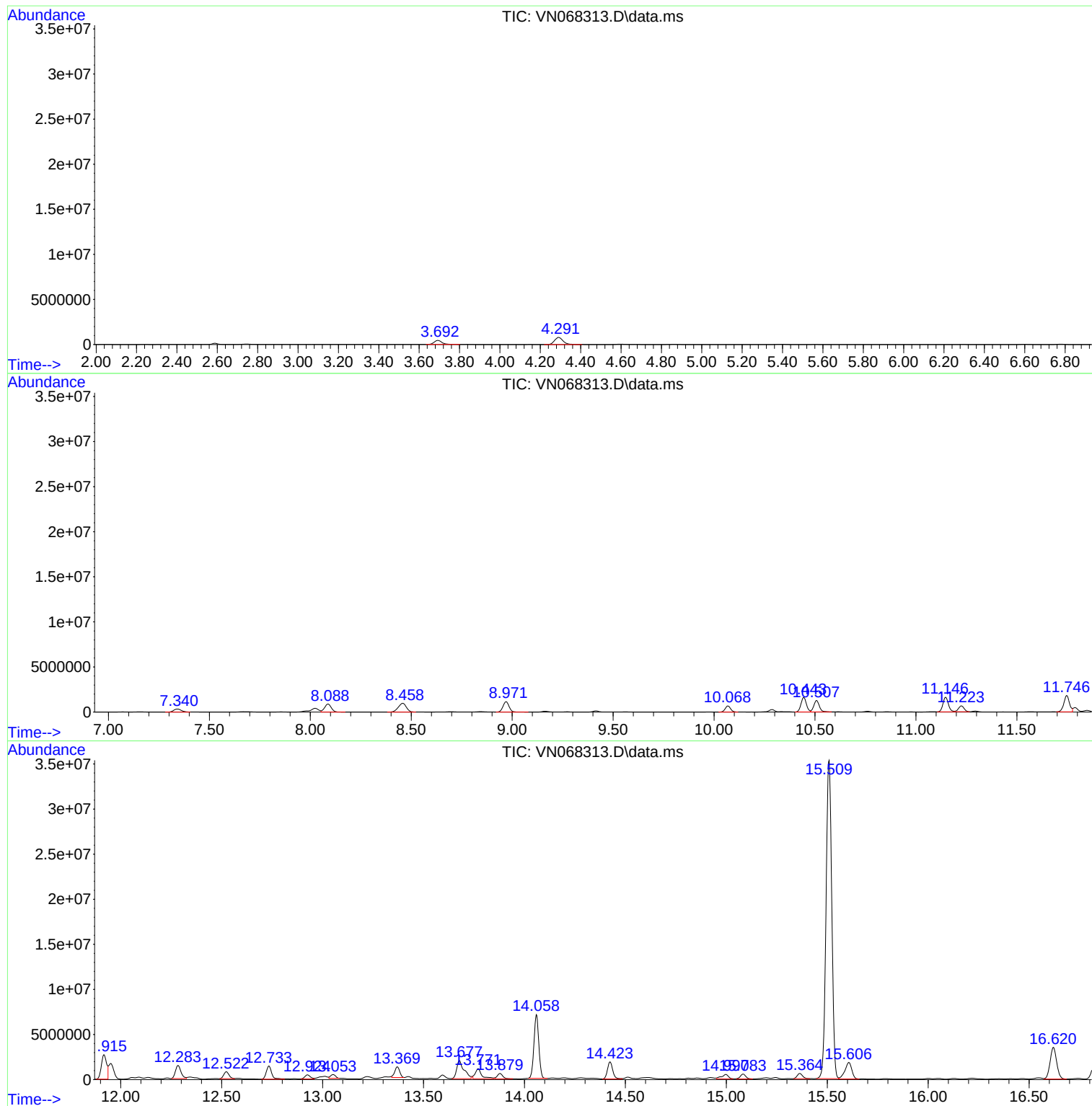
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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



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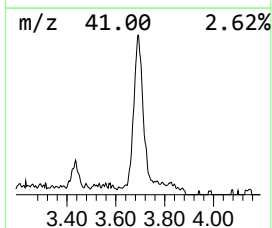
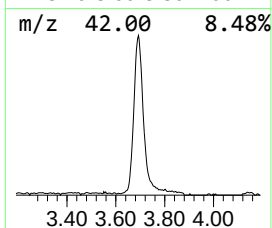
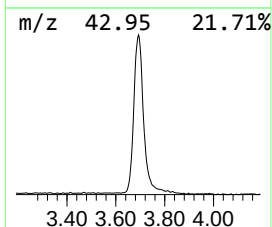
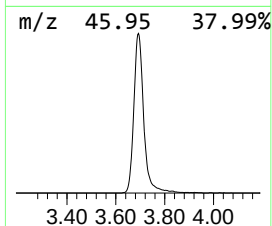
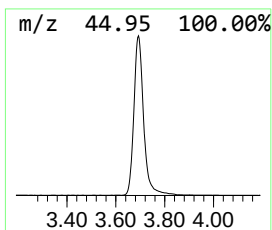
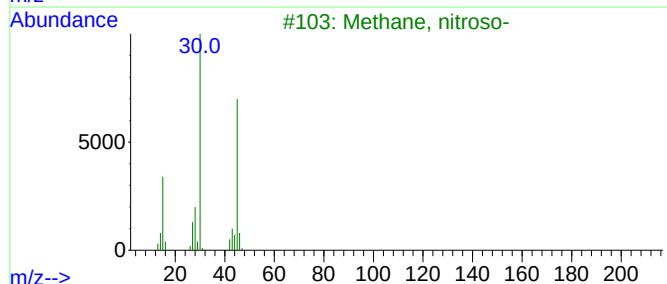
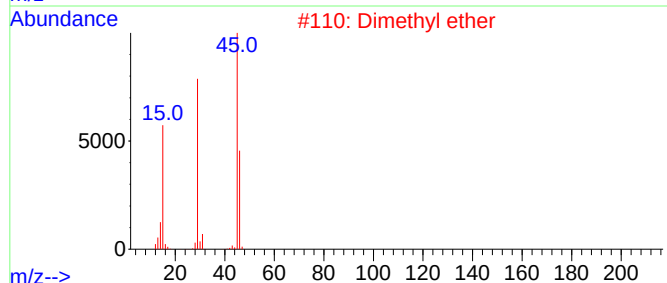
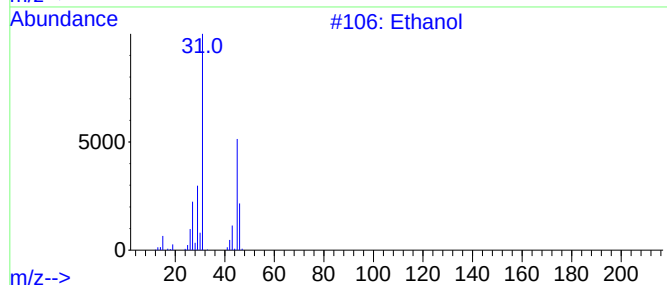
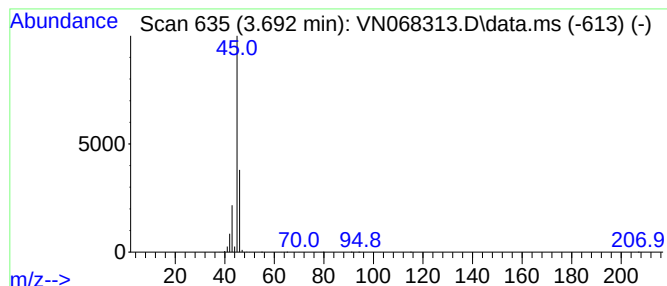
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.692	30.47 ug/l	1236910	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			L-Lactic acid	90	C3H6O3	000079-33-4	2



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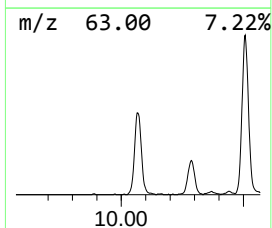
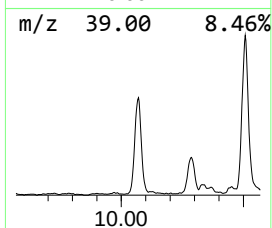
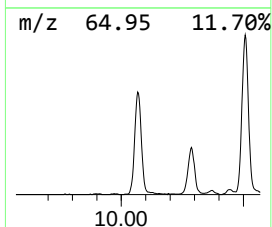
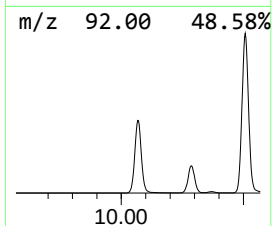
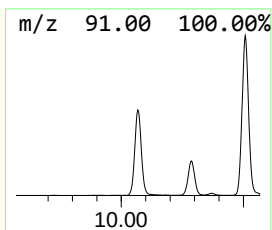
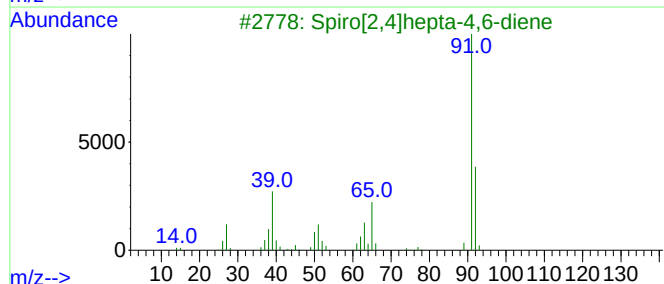
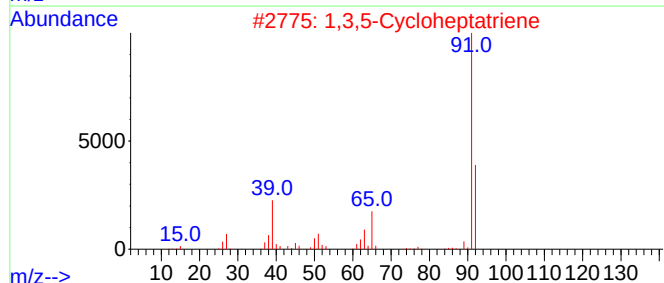
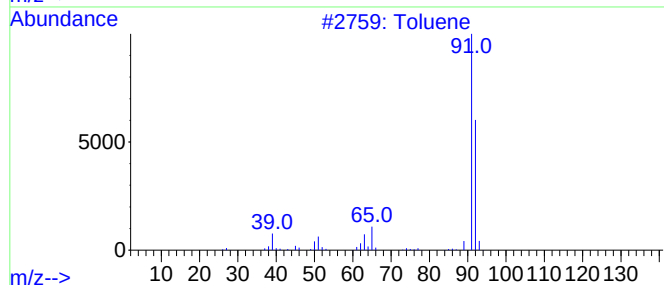
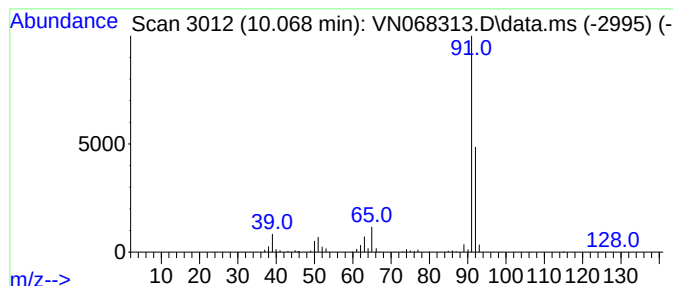
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.068	26.36 ug/l	1271080	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	94
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
4			2,5-Norbornadiene	92	C7H8	000121-46-0	83
5			Molybdenum, di-.mu.-chlorobis[(1... 532	C20H26Cl2Mo2	035625-66-2	72	



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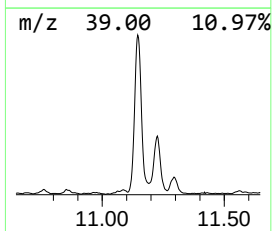
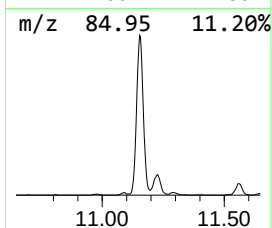
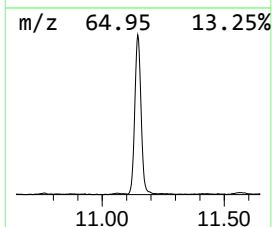
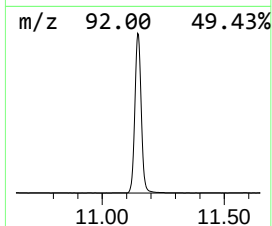
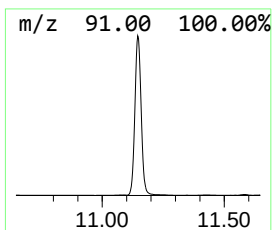
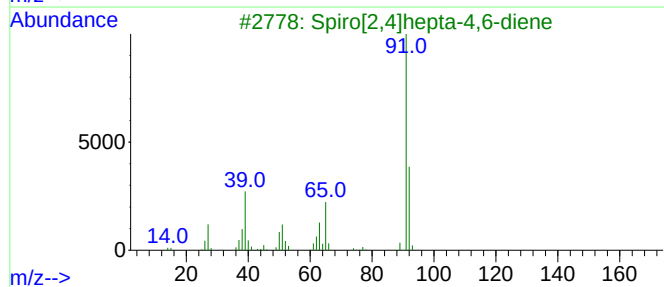
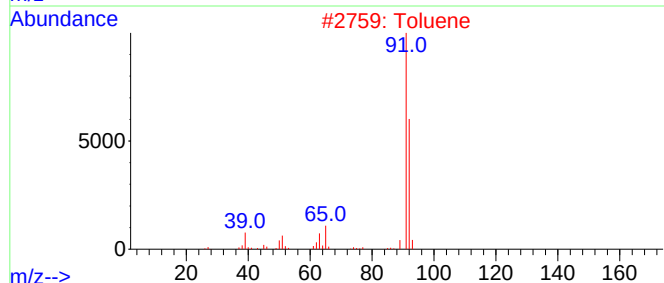
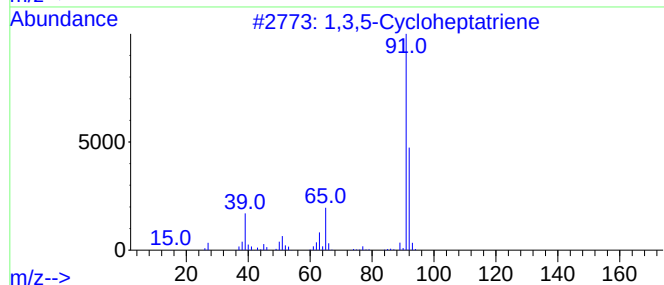
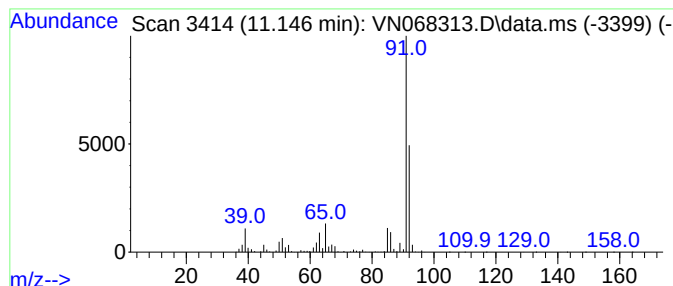
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Quant Title : SW846 8260

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

Peak Number 3 Spiro[2,4]hepta-4,6-diene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.146	43.48 ug/l	3061440	Chlorobenzene-d5	11.746

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	93
2		Toluene	92	C7H8	000108-88-3	81
3		Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	76
4		Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	59
5		1,5-Heptadien-3-yne	92	C7H8	003511-27-1	58



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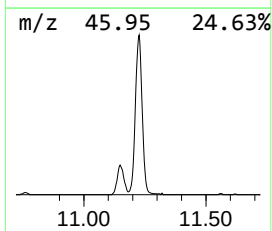
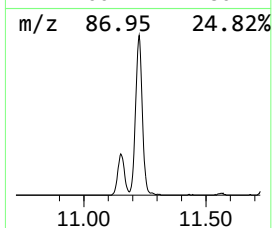
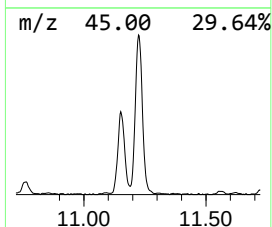
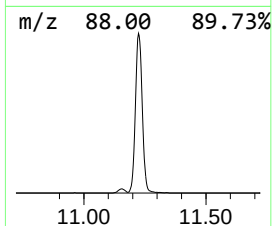
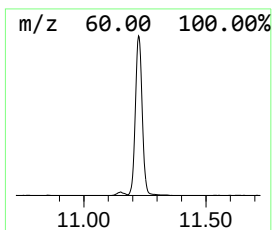
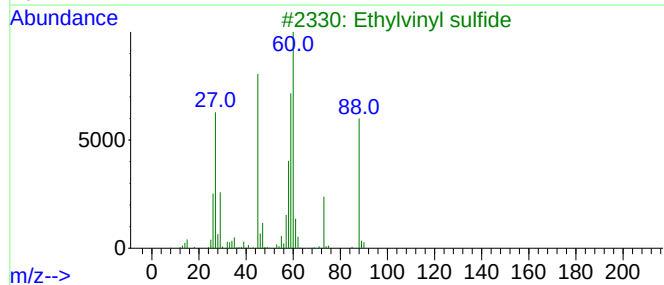
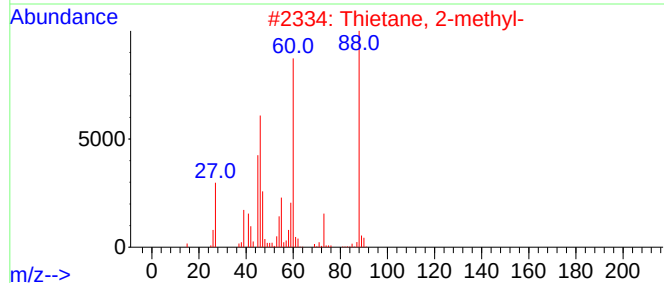
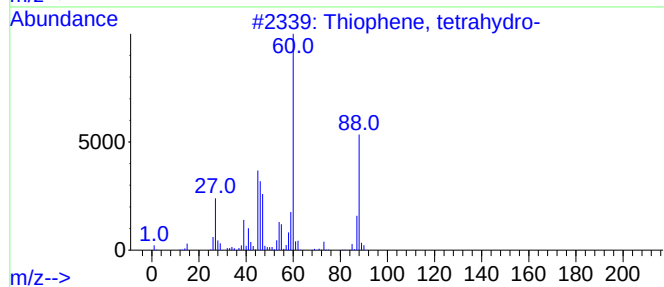
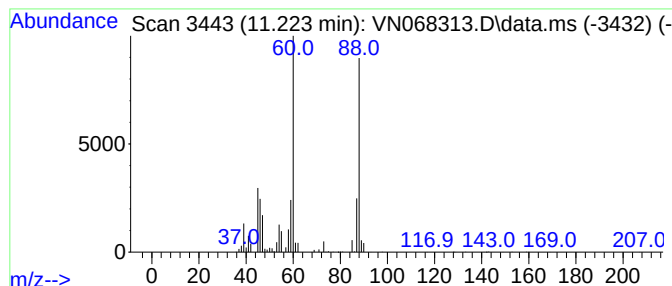
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophene, tetrahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.223	17.68 ug/l	1244910	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	93
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	32



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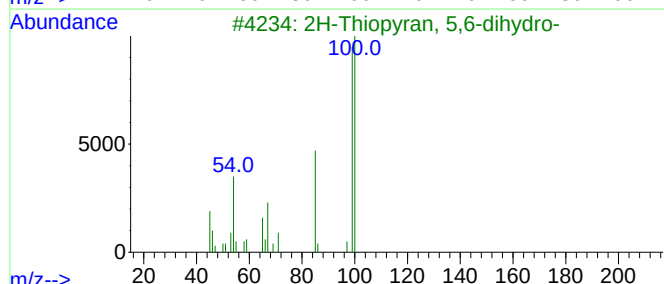
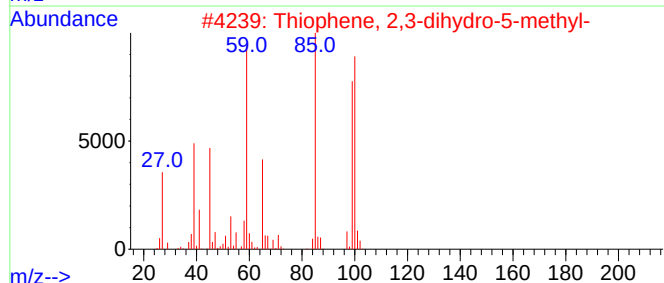
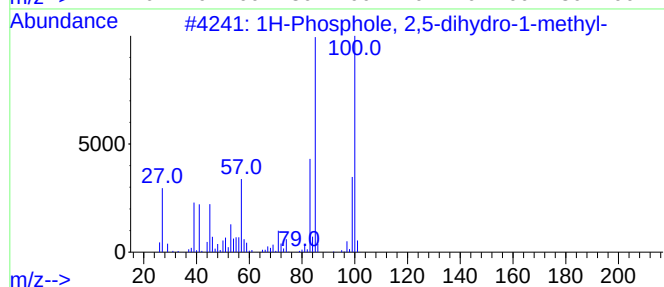
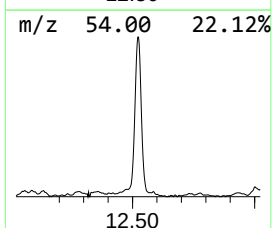
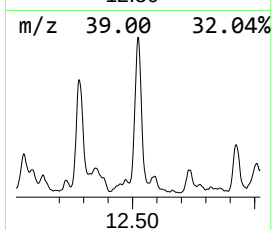
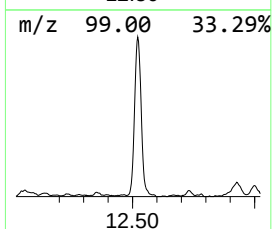
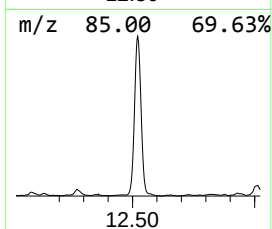
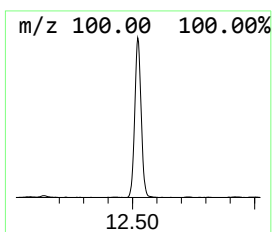
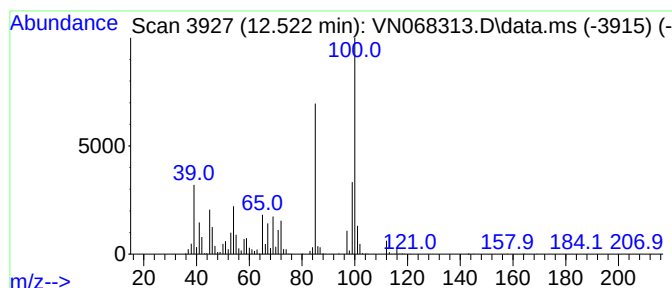
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 5 1H-Phosphole, 2,5-dihydro-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	20.16 ug/l	1419290	Chlorobenzene-d5	11.746

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P		000872-37-7	64
2	Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S		004610-02-0	62
3	2H-Thiopyran, 5,6-dihydro-	100	C5H8S		040697-99-2	58
4	2H-Thiopyran, 3,4-dihydro-	100	C5H8S		013042-80-3	50
5	3-Methoxy-2-methyl-1-butene	100	C6H12O		1000279-60-1	47



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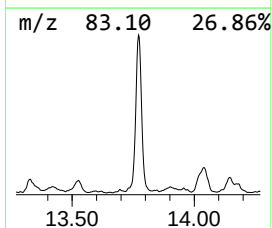
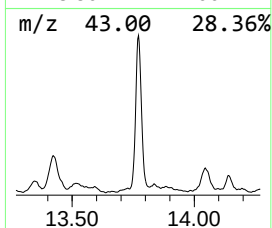
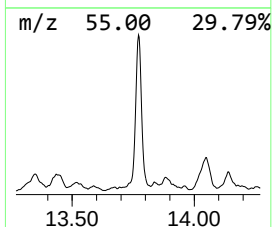
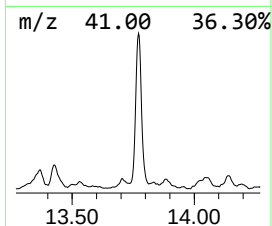
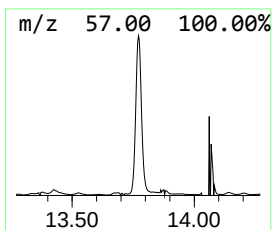
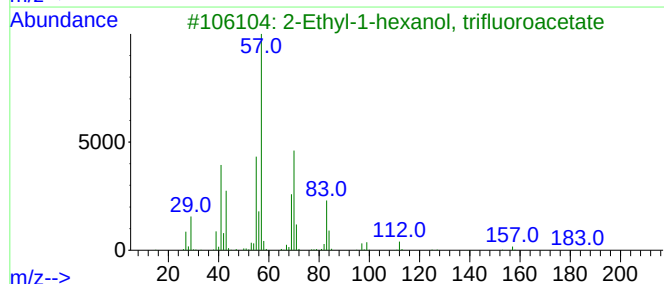
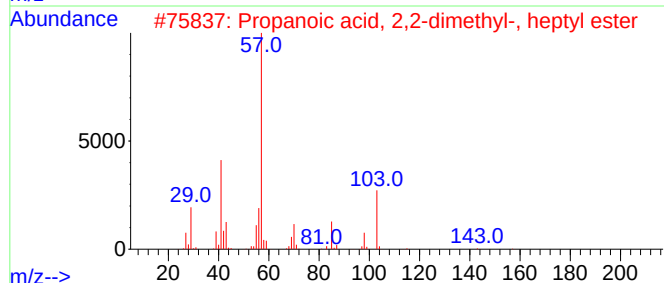
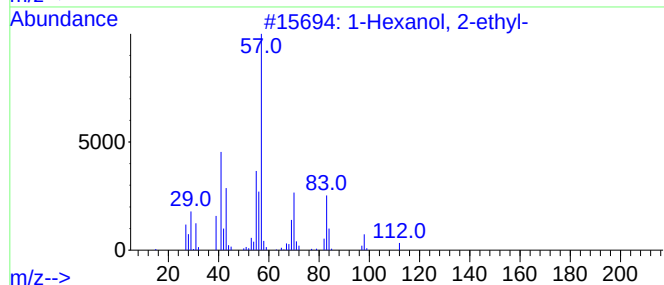
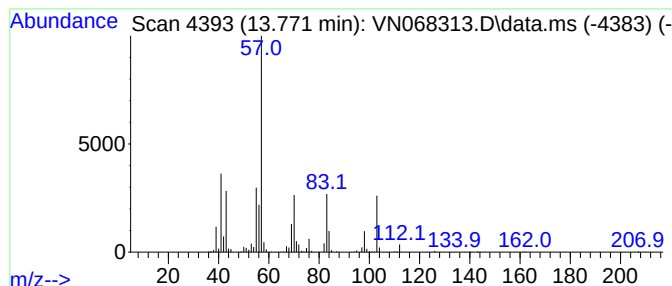
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.771	24.64 ug/l	2486930	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			Propanoic acid, 2,2-dimethyl-, h...	200	C12H24O2	017660-61-6	47
3			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	43
4			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	43
5			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068313.D
Acq On : 25 Aug 2021 20:59
Operator : JC/MD
Sample : M3529-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41987

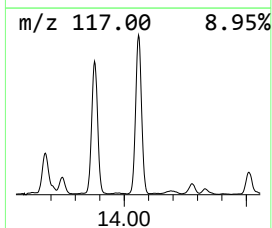
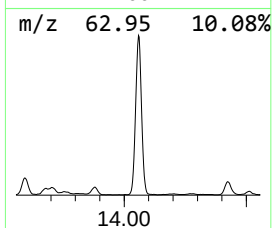
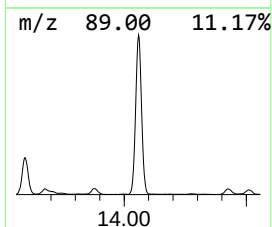
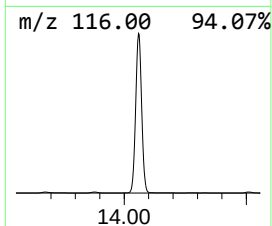
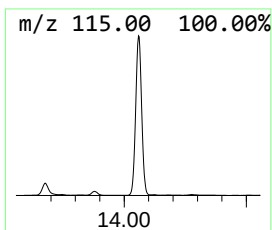
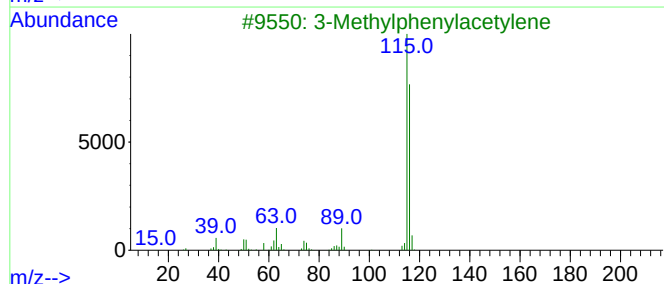
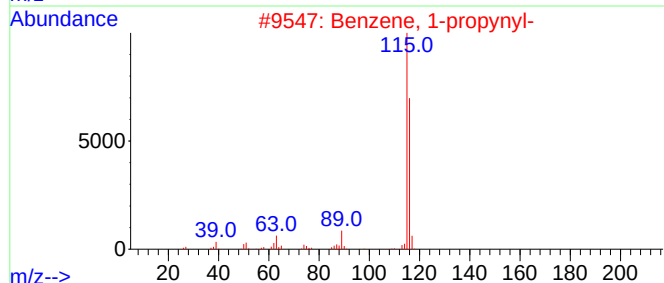
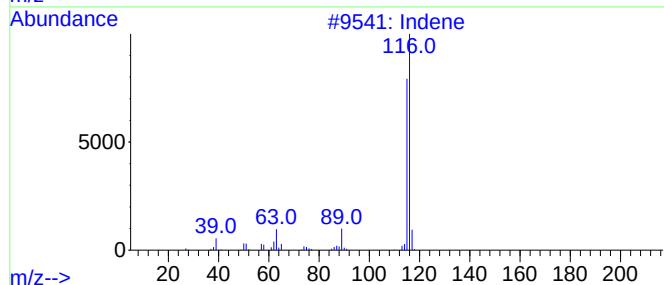
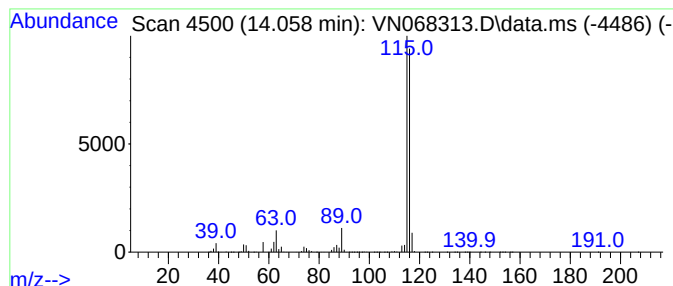
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Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.058	117.86 ug/l	11895600	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068313.D
Acq On : 25 Aug 2021 20:59
Operator : JC/MD
Sample : M3529-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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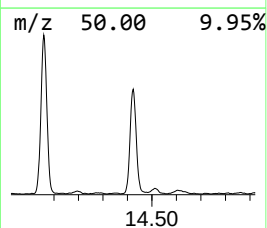
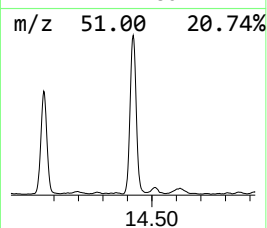
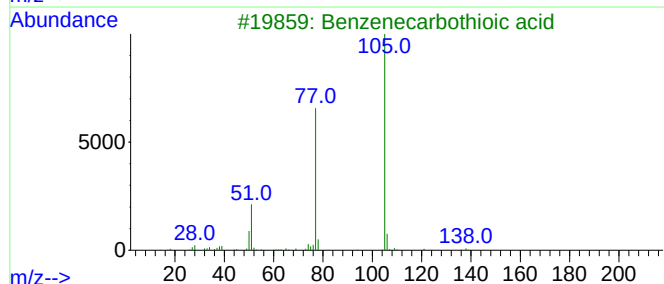
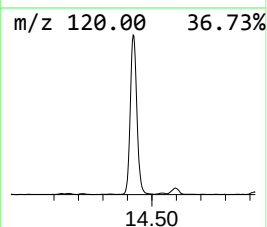
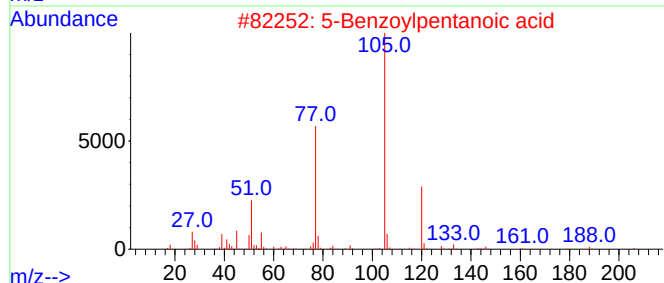
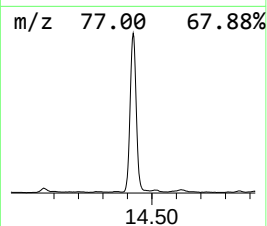
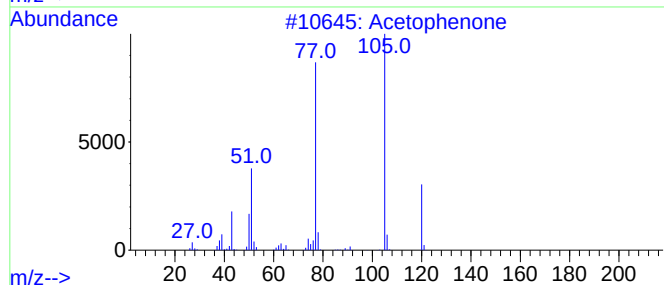
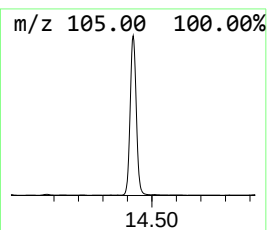
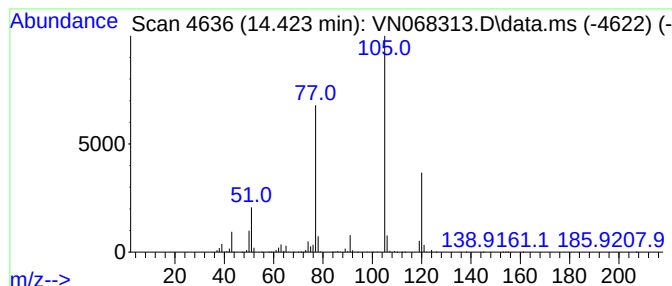
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Quant Title : SW846 8260

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

Peak Number 8 Acetophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.423	34.22 ug/l	3453940	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetophenone	120	C8H8O	000098-86-2	94
2			5-Benzoylpentanoic acid	206	C12H14O3	004144-62-1	83
3			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	64
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	64
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068313.D
Acq On : 25 Aug 2021 20:59
Operator : JC/MD
Sample : M3529-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41987

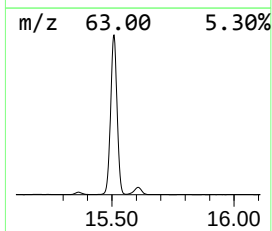
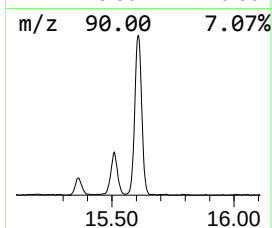
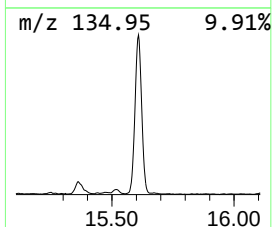
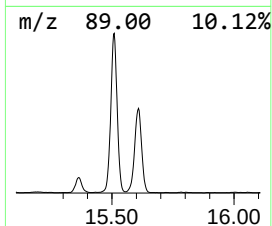
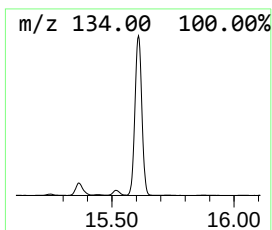
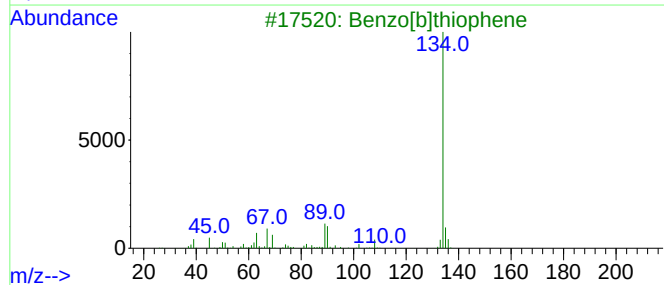
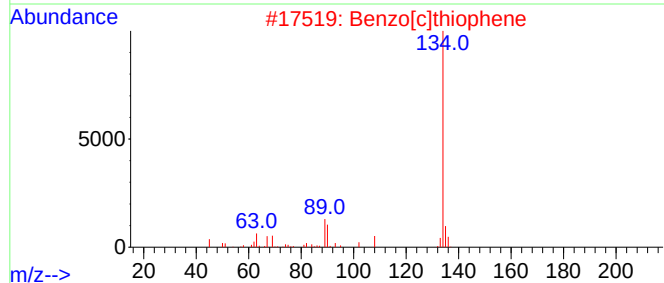
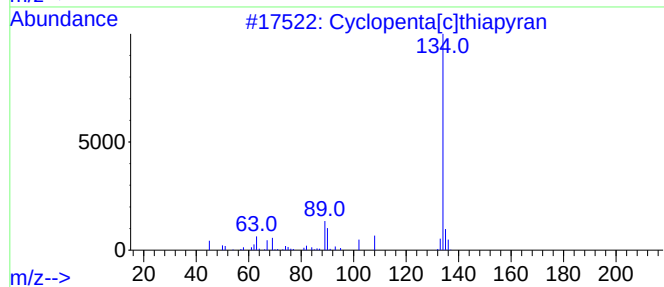
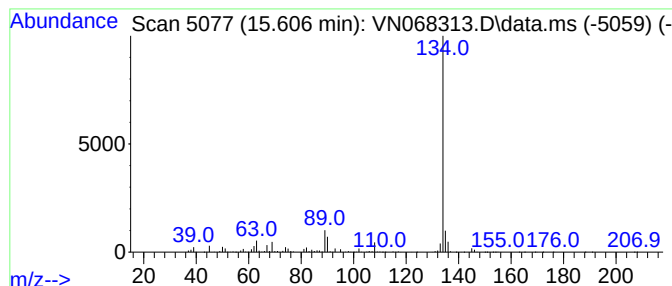
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopenta[c]thiapyran Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.606	42.44 ug/l	4283580	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
3			Benzo[b]thiophene	134	C8H6S	000095-15-8	91
4			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5			5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068313.D
Acq On : 25 Aug 2021 20:59
Operator : JC/MD
Sample : M3529-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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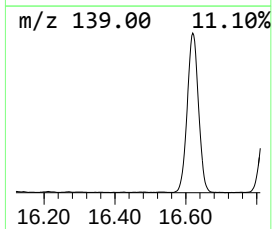
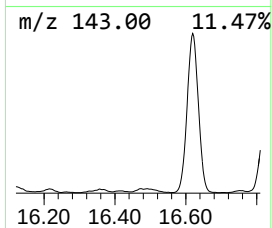
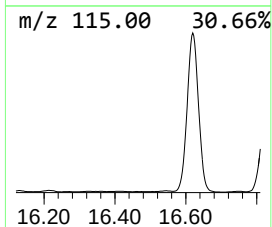
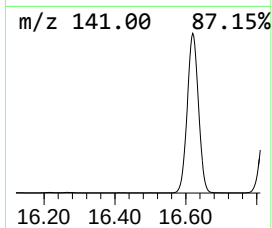
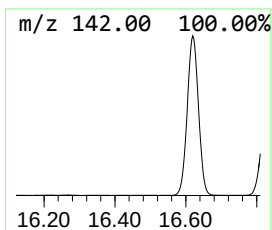
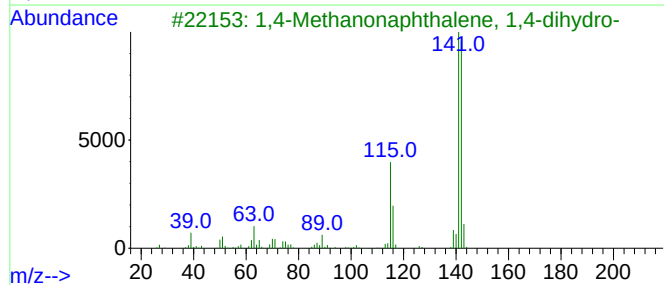
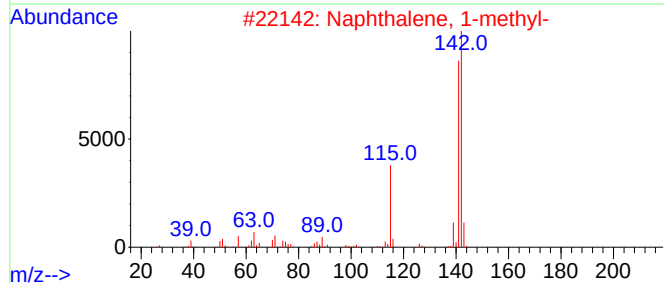
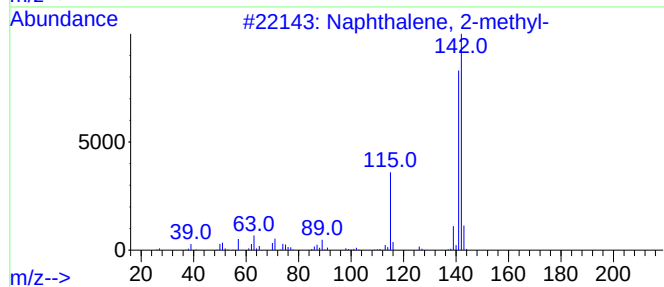
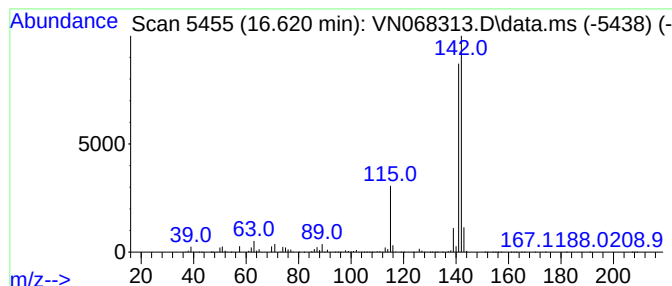
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.620	78.75 ug/l	7947650	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068313.D
Acq On : 25 Aug 2021 20:59
Operator : JC/MD
Sample : M3529-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.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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1,3,5-Cyclohept...	10.068	26.4	ug/l	1271080	2	8.971	2410540	50.0
Spiro[2,4]hepta...	11.146	43.5	ug/l	3061440	3	11.746	3520550	50.0
Thiophene, tetr...	11.223	17.7	ug/l	1244910	3	11.746	3520550	50.0
1H-Phosphole, 2...	12.522	20.2	ug/l	1419290	3	11.746	3520550	50.0
1-Hexanol, 2-et...	13.771	24.6	ug/l	2486930	4	13.677	5046420	50.0
Indene	14.058	117.9	ug/l	11895600	4	13.677	5046420	50.0
Acetophenone	14.423	34.2	ug/l	3453940	4	13.677	5046420	50.0
Cyclopenta[c]th...	15.606	42.4	ug/l	4283580	4	13.677	5046420	50.0
Naphthalene, 1-...	16.620	78.8	ug/l	7947650	4	13.677	5046420	50.0