

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
 Data File : VN068312.D
 Acq On : 25 Aug 2021 20:34
 Operator : JC/MD
 Sample : M3529-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31117

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: VN068312.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.466	2385	2415	2457	rBV3	75586209	181808861	69.23%	13.457%
2	10.446	3136	3153	3161	rBV	1640939	3011797	1.15%	0.223%
3	10.513	3161	3178	3204	rVV3	85033763	176394545	67.17%	13.056%
4	11.148	3399	3415	3430	rBV2	2469638	4840733	1.84%	0.358%
5	11.226	3430	3444	3462	rVB	3962623	7410905	2.82%	0.549%
6	11.747	3621	3638	3645	rBV	1884680	3568628	1.36%	0.264%
7	11.789	3646	3654	3664	rVV	3082079	5226110	1.99%	0.387%
8	11.848	3664	3676	3690	rVV	13867574	22696056	8.64%	1.680%
9	11.953	3690	3715	3744	rVB3	77282521	150683330	57.38%	11.153%
10	12.090	3746	3766	3778	rBV4	1779397	3590648	1.37%	0.266%
11	12.286	3825	3839	3868	rVB5	86241266	159585876	60.77%	11.812%
12	12.522	3915	3927	3939	rVV	3443215	6417401	2.44%	0.475%
13	12.734	3992	4006	4016	rBV	1722609	2993557	1.14%	0.222%
14	12.921	4064	4076	4087	rBV	2418020	4116743	1.57%	0.305%
15	12.986	4087	4100	4108	rBV	11353952	19699402	7.50%	1.458%
16	13.061	4119	4128	4141	rVB	12645067	19810101	7.54%	1.466%
17	13.224	4174	4189	4207	rBV	8402191	16023639	6.10%	1.186%
18	13.372	4225	4244	4256	rBV2	44016691	73131230	27.85%	5.413%
19	13.420	4256	4262	4273	rVV	3316779	4785308	1.82%	0.354%
20	13.594	4318	4327	4347	rVB	2241336	4830108	1.84%	0.358%
21	13.707	4347	4369	4380	rBV	18760778	34585215	13.17%	2.560%
22	13.879	4421	4433	4458	rVB2	7806744	14878209	5.67%	1.101%
23	14.061	4486	4501	4517	rVB2	56320780	99790276	38.00%	7.386%
24	14.423	4624	4636	4660	rBV2	2299937	4754295	1.81%	0.352%
25	14.581	4687	4695	4724	rVB2	1388431	3325729	1.27%	0.246%
26	14.922	4808	4822	4837	rBV3	1749783	4198225	1.60%	0.311%
27	14.997	4840	4850	4866	rVB	2492845	4334054	1.65%	0.321%
28	15.086	4869	4883	4903	rVB2	3412012	6167898	2.35%	0.457%
29	15.515	5017	5043	5061	rBV5	121816220	262607780	100.00%	19.438%
30	15.609	5062	5078	5096	rVB	6139812	12494180	4.76%	0.925%
31	16.620	5438	5455	5481	rVB	14838022	33260054	12.67%	2.462%

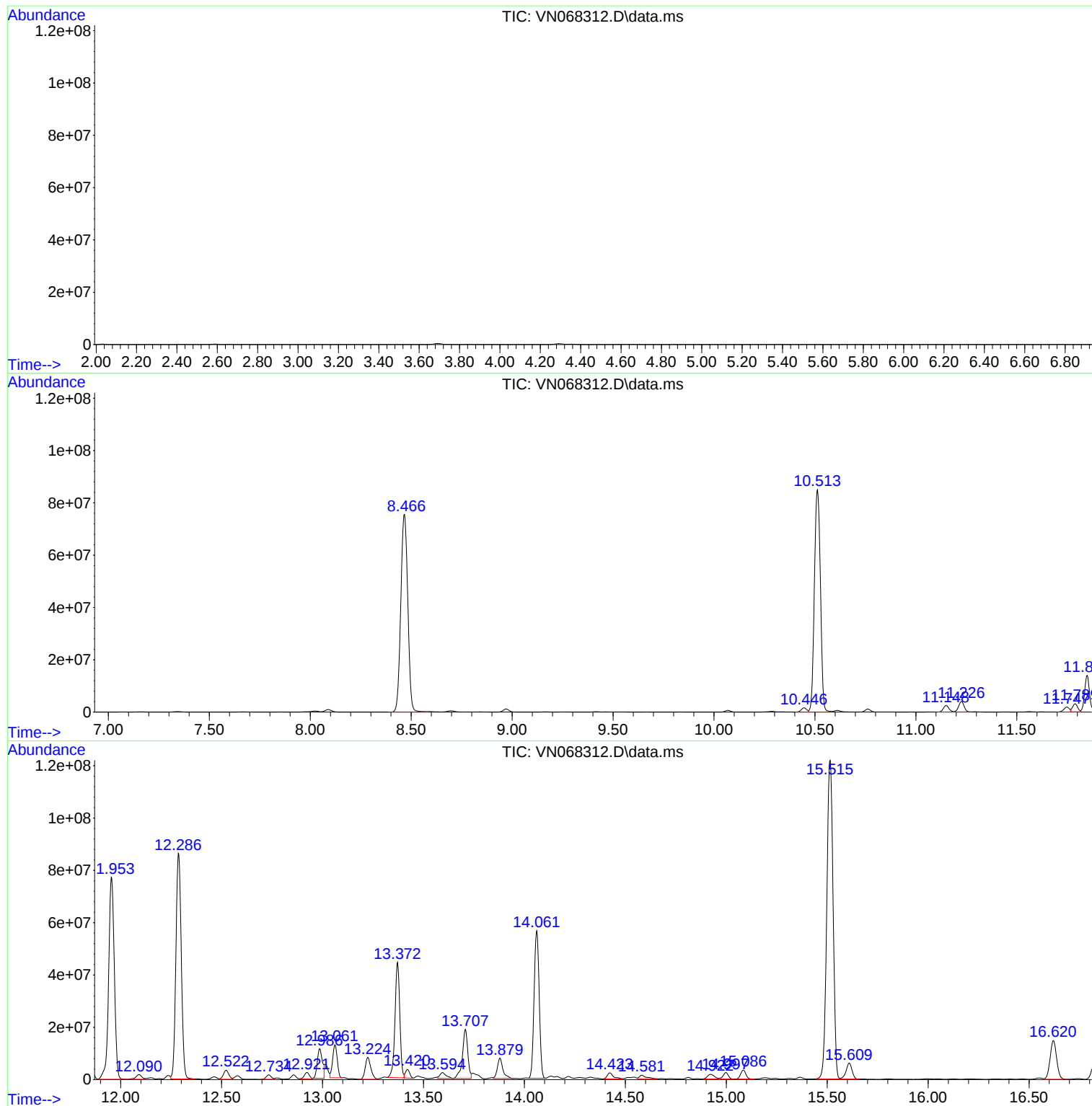
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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



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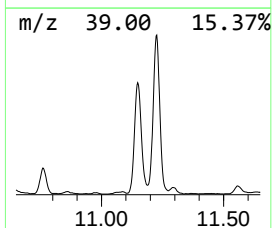
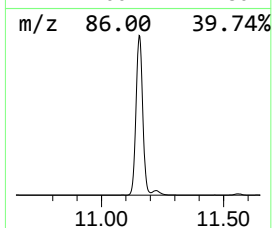
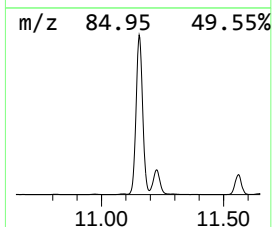
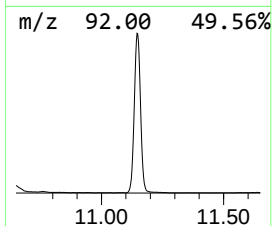
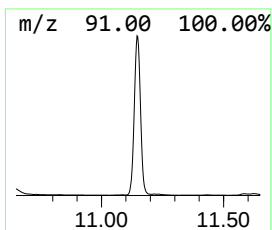
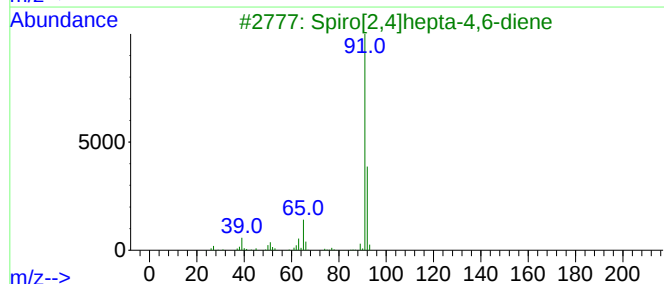
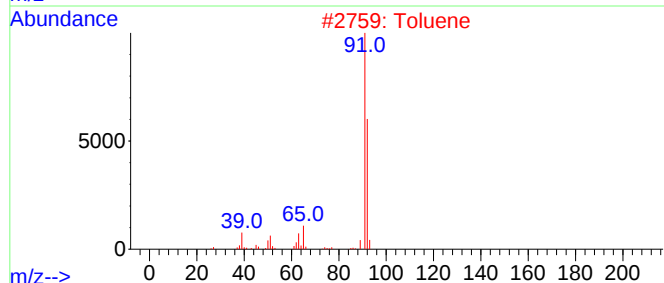
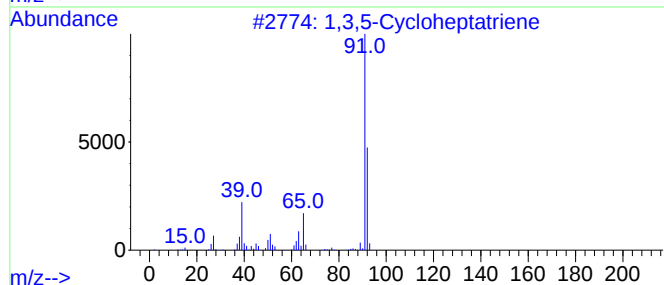
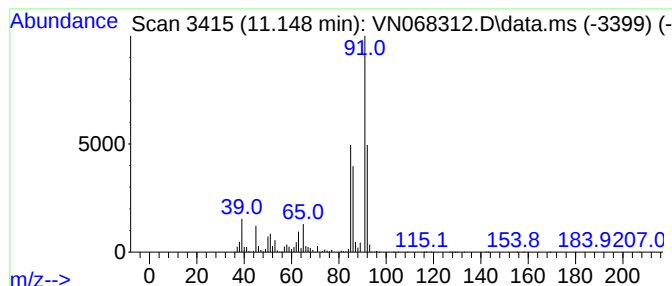
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Quant Title : SW846 8260

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

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.149	67.82 ug/l	4840730	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	86
2			Toluene	92	C7H8	000108-88-3	50
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	45
4			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	41
5			Bicyclo[3.2.0]hepta-2,6-diene	92	C7H8	002422-86-8	35



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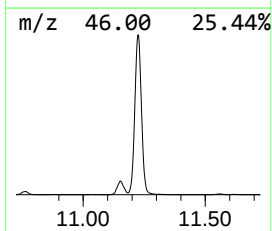
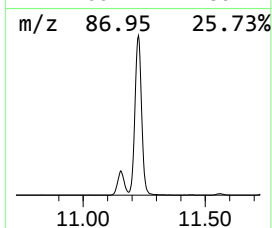
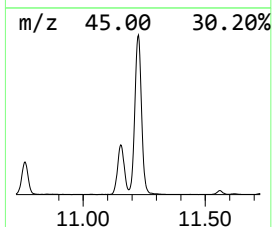
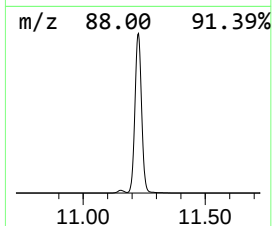
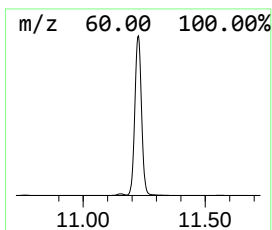
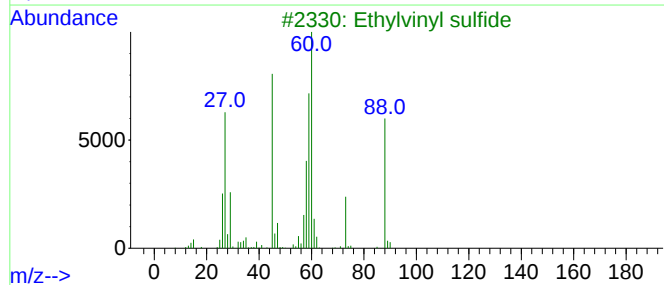
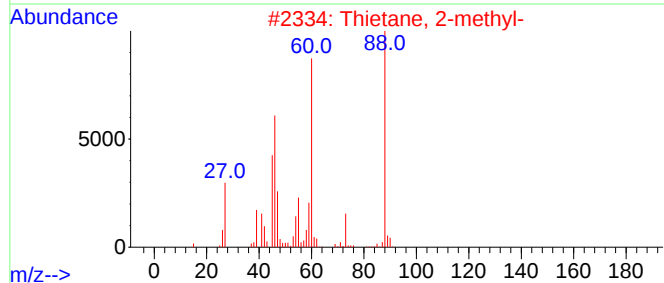
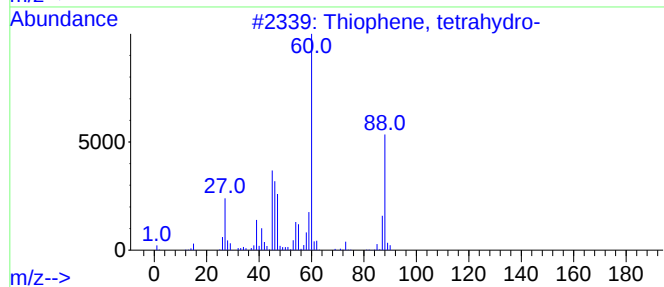
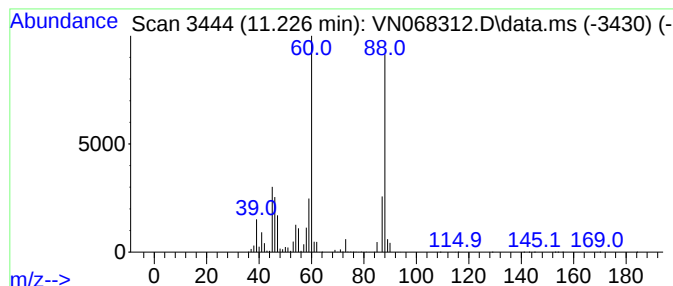
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 2 Thiophene, tetrahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.226	103.83 ug/l	7410910	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	74
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
4			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	40
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	38



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ALS Vial : 25 Sample Multiplier: 1

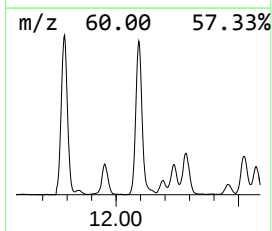
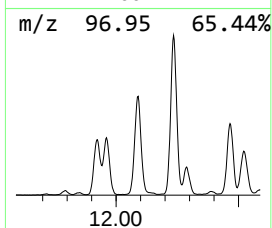
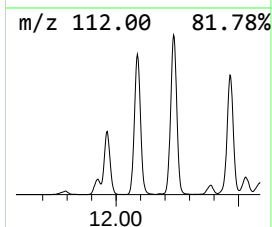
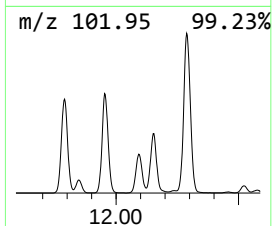
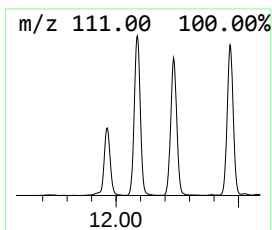
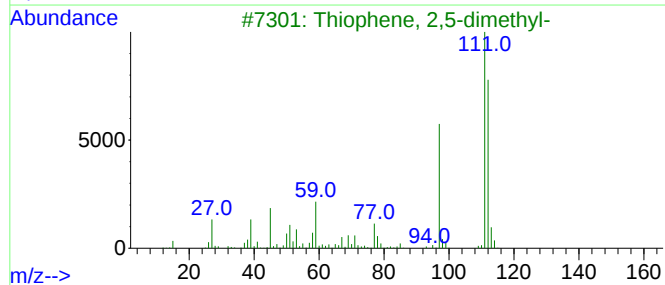
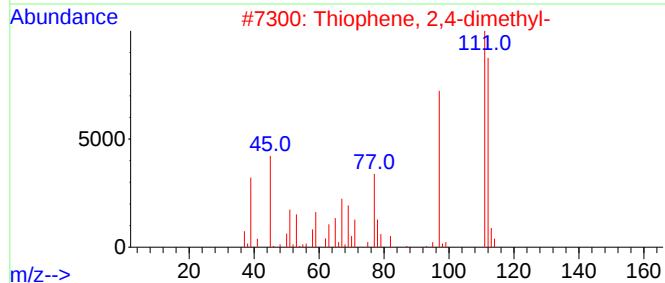
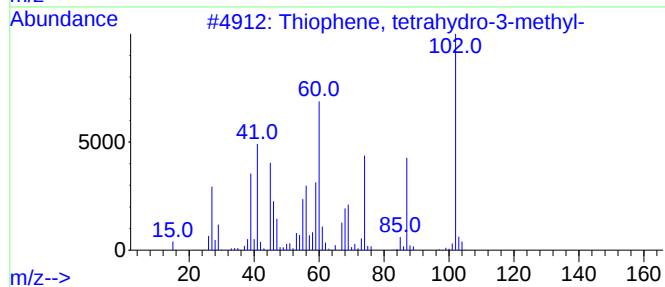
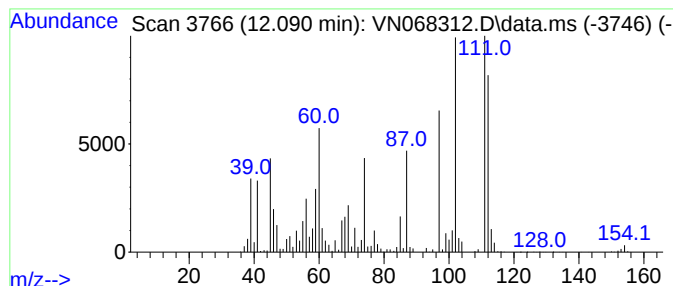
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.090	50.31 ug/l	3590650	Chlorobenzene-d5		11.746	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-		102	C5H10S	004740-00-5	96
2	Thiophene, 2,4-dimethyl-		112	C6H8S	000638-00-6	46
3	Thiophene, 2,5-dimethyl-		112	C6H8S	000638-02-8	45
4	Thiophene, 2,3-dimethyl-		112	C6H8S	000632-16-6	41
5	2-Thiophenecarboxaldehyde		112	C5H4OS	000098-03-3	38



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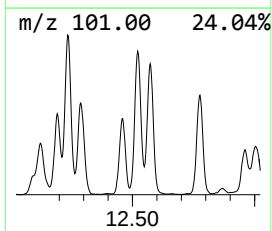
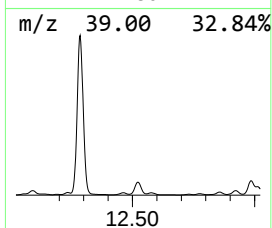
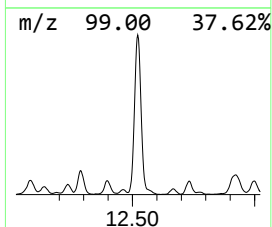
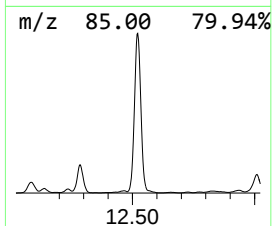
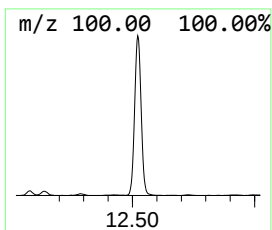
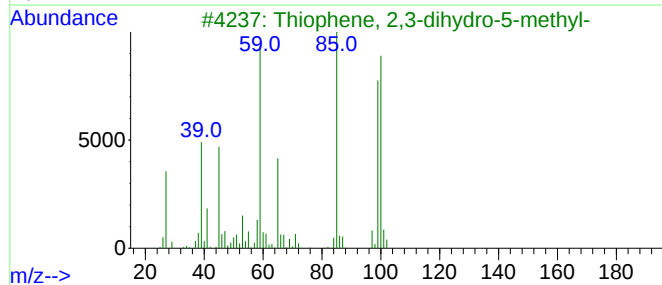
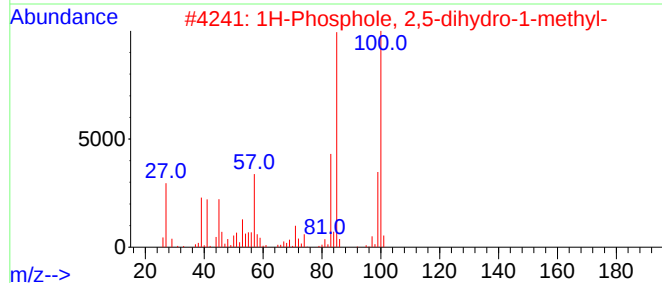
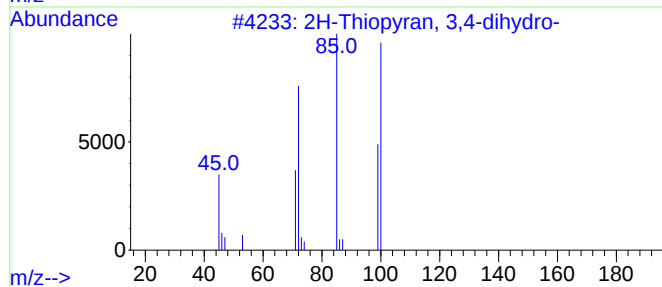
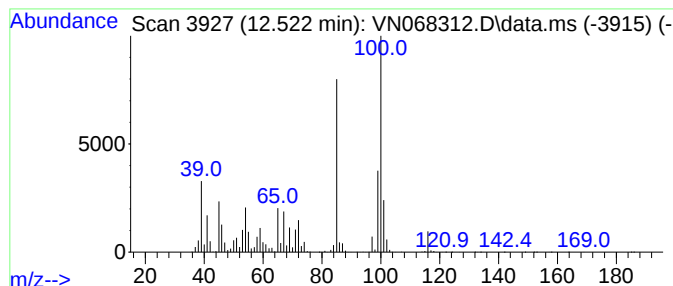
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Peak Number 4 2H-Thiopyran, 3,4-dihydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	89.91 ug/l	6417400	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Thiopyran, 3,4-dihydro-	100	C5H8S	013042-80-3	58
2			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	58
3			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	47
4			2H-Thiopyran, 5,6-dihydro-	100	C5H8S	040697-99-2	45
5			E-4-Methoxy-2-pentene	100	C6H12O	1000279-60-2	40



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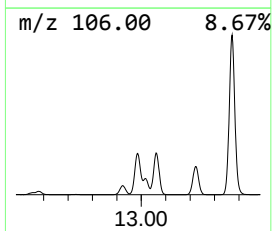
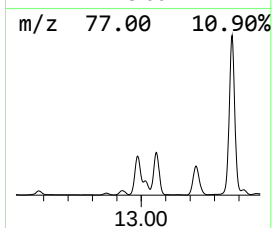
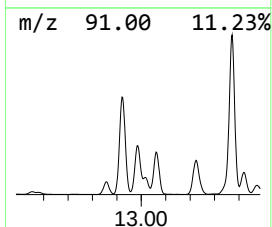
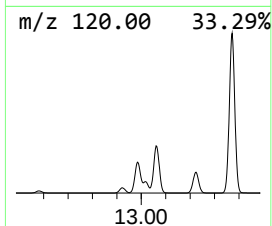
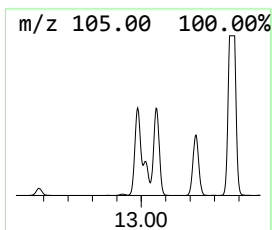
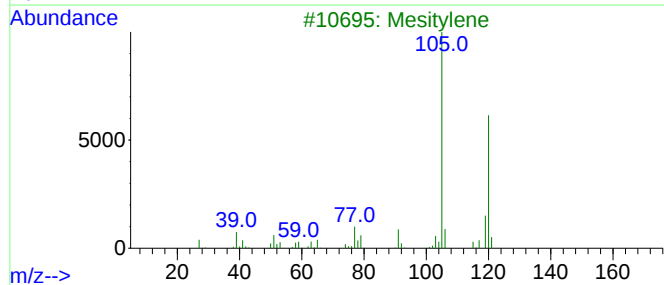
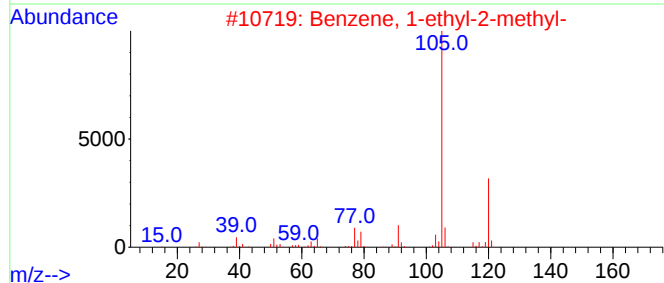
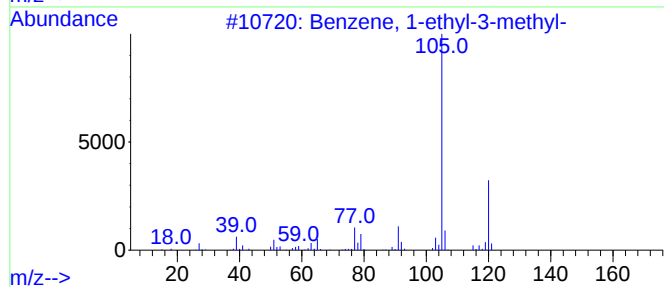
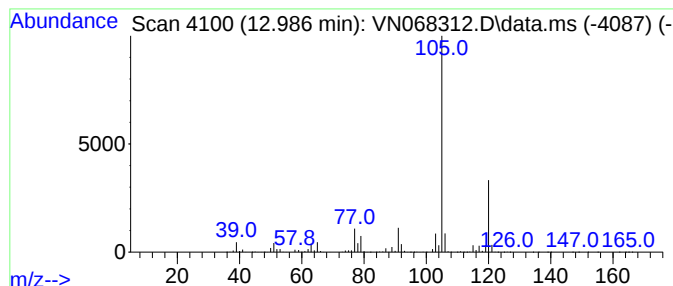
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	28.48 ug/l	19699400	1,4-Dichlorobenzene-d4	13.678

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



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31117

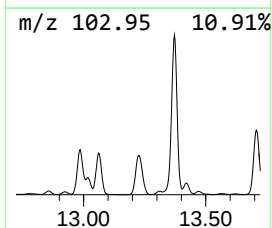
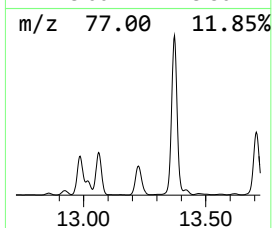
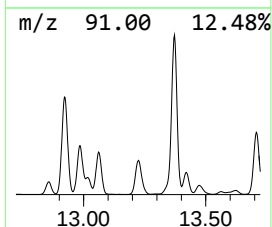
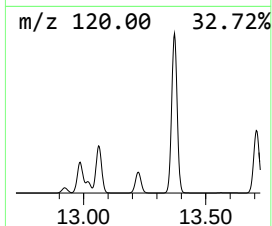
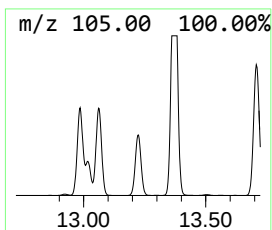
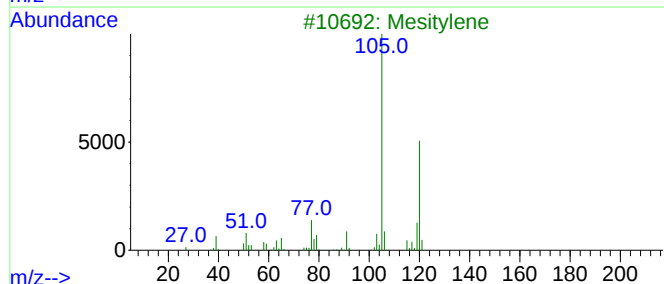
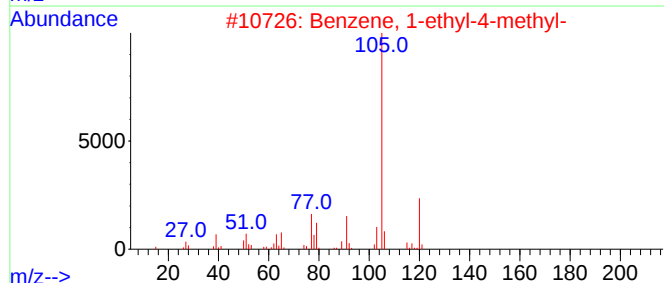
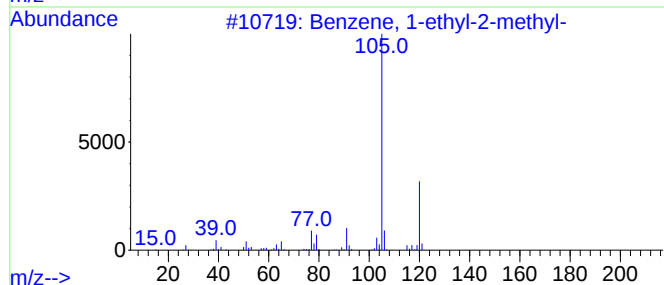
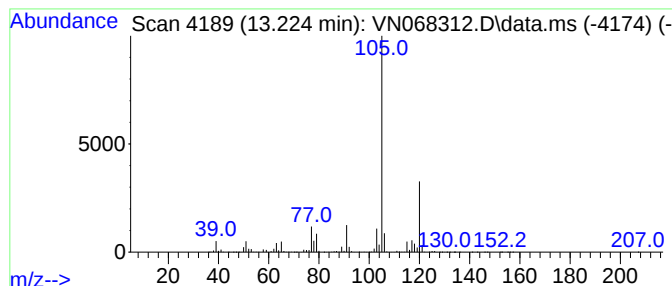
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.224	23.17 ug/l	16023600	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	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	90
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068312.D
Acq On : 25 Aug 2021 20:34
Operator : JC/MD
Sample : M3529-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
31117

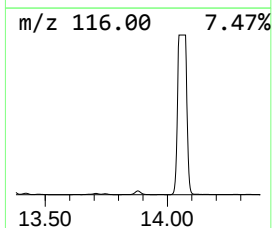
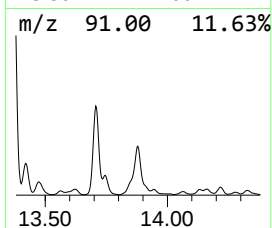
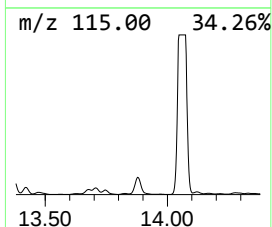
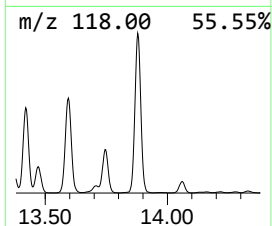
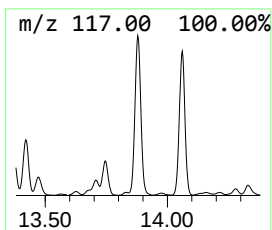
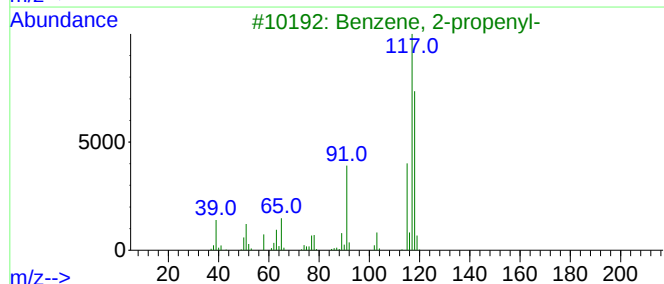
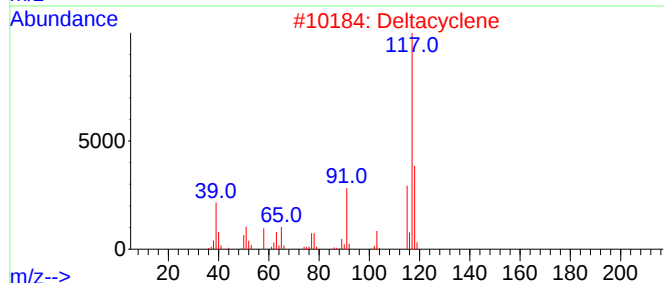
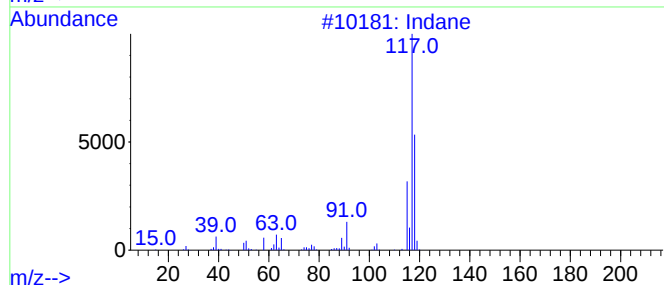
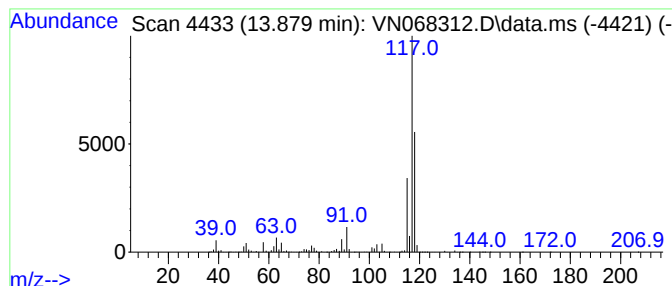
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.879	21.51 ug/l	14878200	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Deltacyclene	118	C9H10	007785-10-6	72
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068312.D
Acq On : 25 Aug 2021 20:34
Operator : JC/MD
Sample : M3529-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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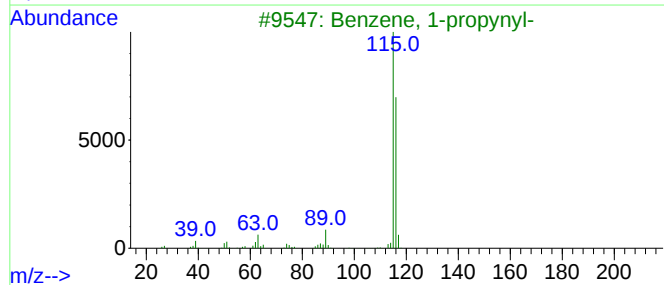
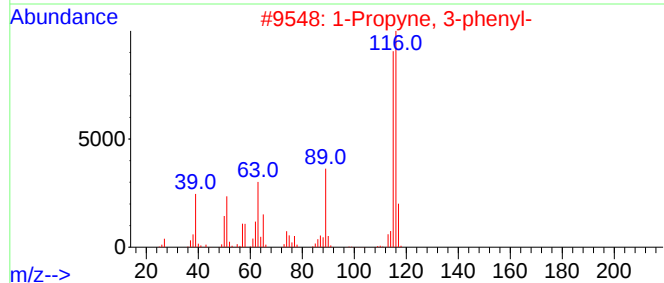
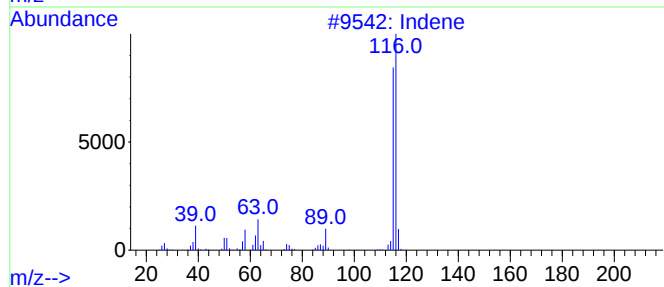
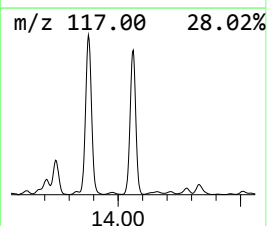
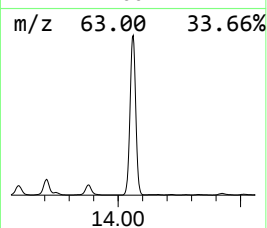
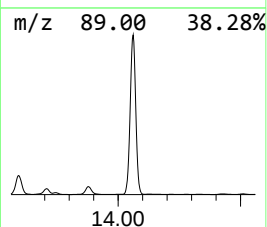
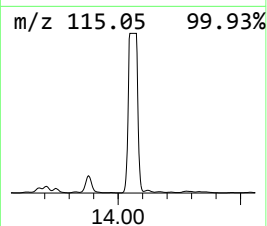
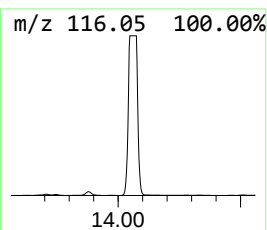
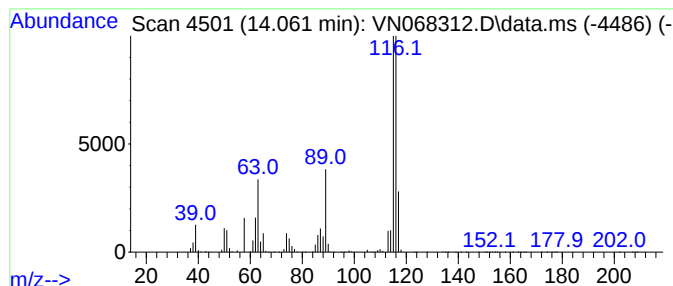
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Quant Title : SW846 8260

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

Peak Number 8 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.061	144.27 ug/l	99790300	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	94
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	87
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	83
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068312.D
Acq On : 25 Aug 2021 20:34
Operator : JC/MD
Sample : M3529-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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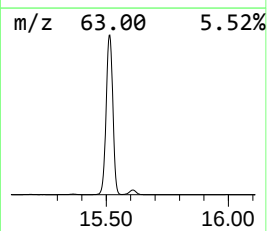
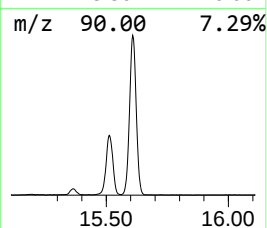
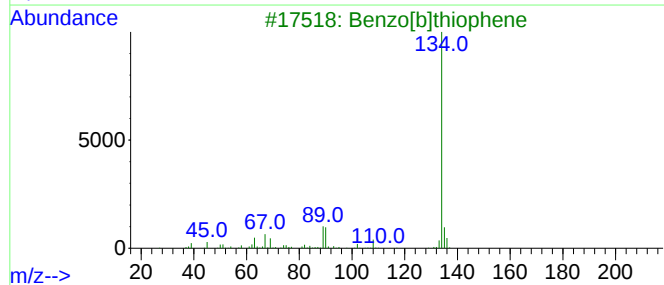
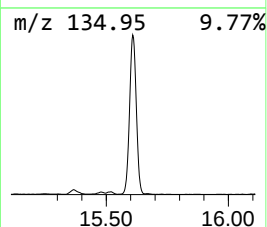
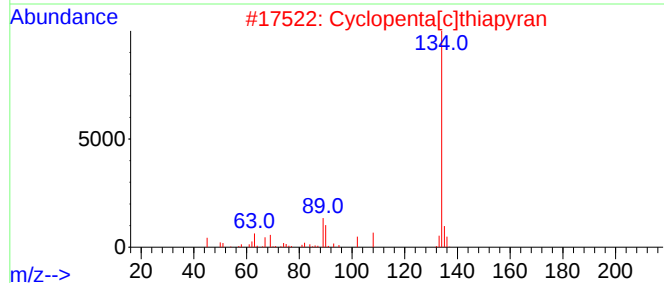
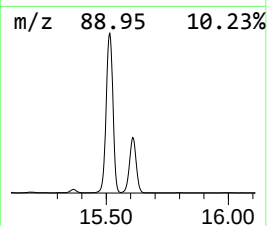
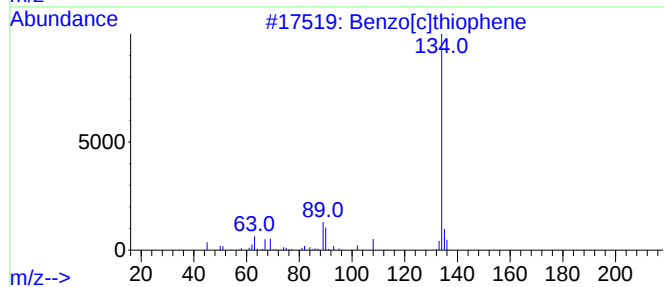
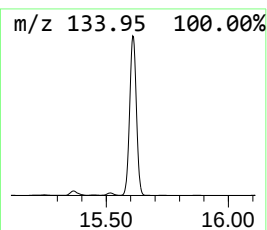
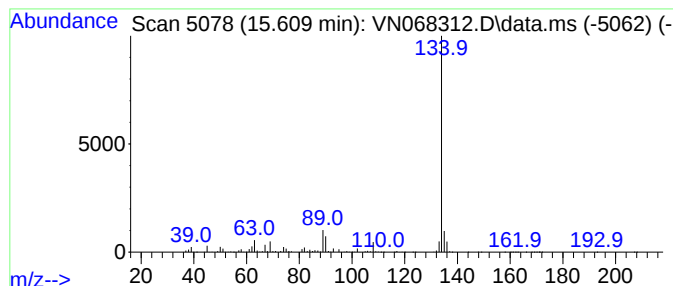
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[c]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	18.06 ug/l	12494200	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
2			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	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			3-Deazaadenine	134	C6H6N4	006811-77-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068312.D
Acq On : 25 Aug 2021 20:34
Operator : JC/MD
Sample : M3529-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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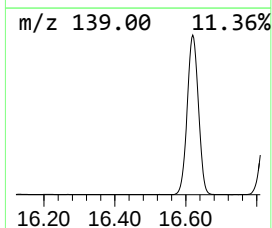
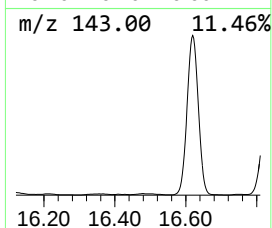
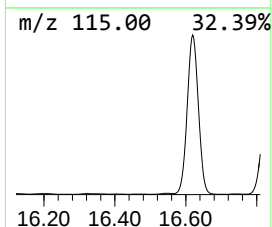
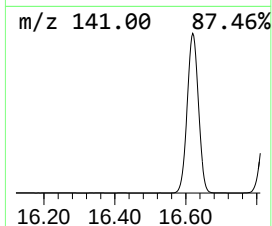
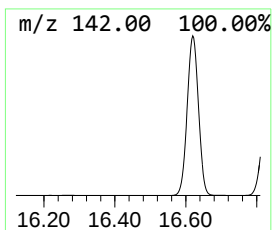
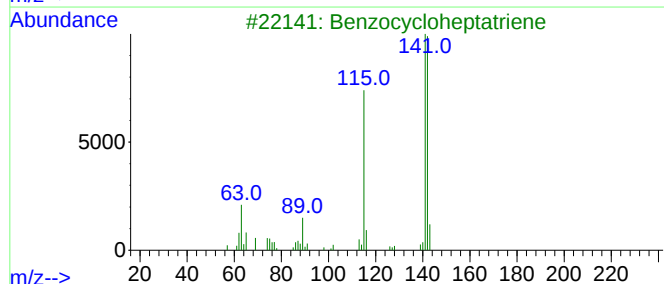
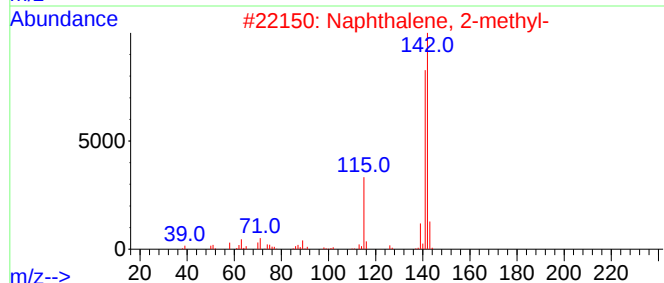
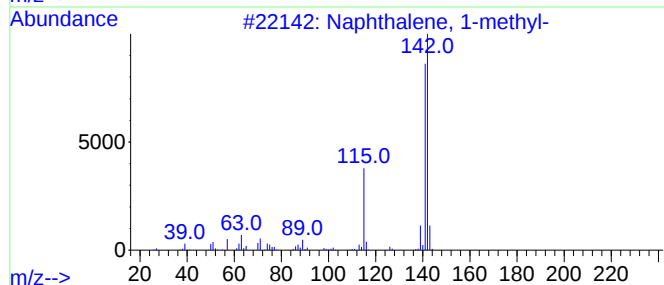
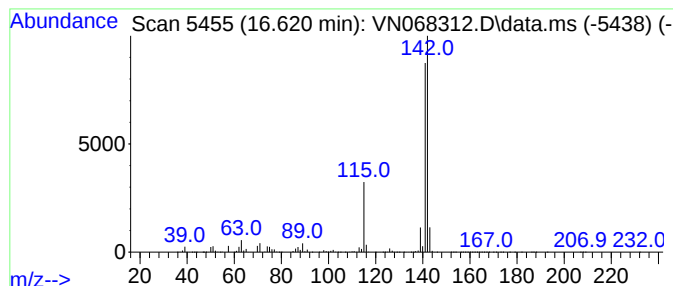
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.620	48.08 ug/l	33260100	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	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 : VN068312.D
Acq On : 25 Aug 2021 20:34
Operator : JC/MD
Sample : M3529-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 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\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3,5-Cyclohept...	11.149	67.8	ug/l	4840730	3	11.746	3568630	50.0
Thiophene, tetr...	11.226	103.8	ug/l	7410910	3	11.746	3568630	50.0
Thiophene, tetr...	12.090	50.3	ug/l	3590650	3	11.746	3568630	50.0
2H-Thiopyran, 3...	12.522	89.9	ug/l	6417400	3	11.746	3568630	50.0
Benzene, 1-ethy...	12.986	28.5	ug/l	19699400	4	13.678	34585200	50.0
Benzene, 1-ethy...	13.224	23.2	ug/l	16023600	4	13.678	34585200	50.0
Indane	13.879	21.5	ug/l	14878200	4	13.678	34585200	50.0
Indene	14.061	144.3	ug/l	99790300	4	13.678	34585200	50.0
Benzo[c]thiophene	15.609	18.1	ug/l	12494200	4	13.678	34585200	50.0
Naphthalene, 1-...	16.620	48.1	ug/l	33260100	4	13.678	34585200	50.0