

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
 Data File : VN068311.D
 Acq On : 25 Aug 2021 20:10
 Operator : JC/MD
 Sample : M3529-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31116

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: VN068311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.291	833	858	904	rBV	587766	1786722	1.94%	0.743%
2	8.086	2261	2273	2311	rVB	830019	1907574	2.07%	0.794%
3	8.458	2383	2412	2440	rBV3	984550	2726482	2.96%	1.134%
4	8.968	2584	2602	2628	rBV	1063978	2210127	2.40%	0.919%
5	10.068	2992	3012	3046	rBV	1366732	2553455	2.77%	1.062%
6	10.285	3066	3093	3105	rBV2	668957	1745050	1.89%	0.726%
7	10.443	3136	3152	3164	rBV	1568577	2922627	3.17%	1.216%
8	10.507	3164	3176	3205	rVB	2572184	4852303	5.26%	2.019%
9	11.146	3399	3414	3429	rBV	2708619	4876503	5.29%	2.029%
10	11.226	3429	3444	3459	rVV	2989721	5755363	6.24%	2.394%
11	11.747	3623	3638	3648	rBV	1715529	3152237	3.42%	1.311%
12	11.787	3649	3653	3665	rVV	646275	955405	1.04%	0.397%
13	11.916	3687	3701	3707	rVV2	3013179	5251781	5.70%	2.185%
14	11.950	3709	3714	3735	rVV	3507463	6023726	6.53%	2.506%
15	12.055	3736	3753	3781	rVV	3589484	7097706	7.70%	2.953%
16	12.288	3825	3840	3854	rBV5	3039119	6246418	6.78%	2.599%
17	12.530	3918	3930	3940	rBV	1411505	2511076	2.72%	1.045%
18	12.586	3944	3951	3977	rVB5	736924	1495025	1.62%	0.622%
19	12.734	3992	4006	4017	rBV	1484546	2552780	2.77%	1.062%
20	12.790	4017	4027	4044	rVB	927052	1634170	1.77%	0.680%
21	12.924	4064	4077	4089	rBV	845489	1466453	1.59%	0.610%
22	13.055	4118	4126	4138	rVB3	856166	1530761	1.66%	0.637%
23	13.155	4142	4163	4176	rVB2	1112549	2331460	2.53%	0.970%
24	13.230	4177	4191	4207	rVB4	756209	1570050	1.70%	0.653%
25	13.324	4209	4226	4232	rBV5	714256	1519888	1.65%	0.632%
26	13.369	4233	4243	4253	rVV	2639204	4901764	5.32%	2.039%
27	13.420	4255	4262	4273	rVV	1338358	2175138	2.36%	0.905%
28	13.678	4345	4358	4364	rBV	1976707	3406442	3.70%	1.417%
29	13.879	4422	4433	4467	rVB2	838211	2063187	2.24%	0.858%
30	14.058	4472	4500	4517	rBV	21038850	35564818	38.58%	14.796%
31	14.423	4623	4636	4659	rBV4	1167509	2430018	2.64%	1.011%
32	14.919	4809	4821	4836	rBV4	614796	1364265	1.48%	0.568%
33	14.997	4837	4850	4865	rVV	2354168	3999360	4.34%	1.664%
34	15.083	4867	4882	4901	rVB	3240693	5867030	6.36%	2.441%
35	15.188	4908	4921	4935	rBV4	455810	1002937	1.09%	0.417%
36	15.509	5015	5041	5059	rBV2	45821386	92184979	100.00%	38.352%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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37	15.606	5060	5077	5094	rVB	1666659	3641967	3.95%	1.515%
38	16.620	5438	5455	5477	rVB	2278364	5090357	5.52%	2.118%

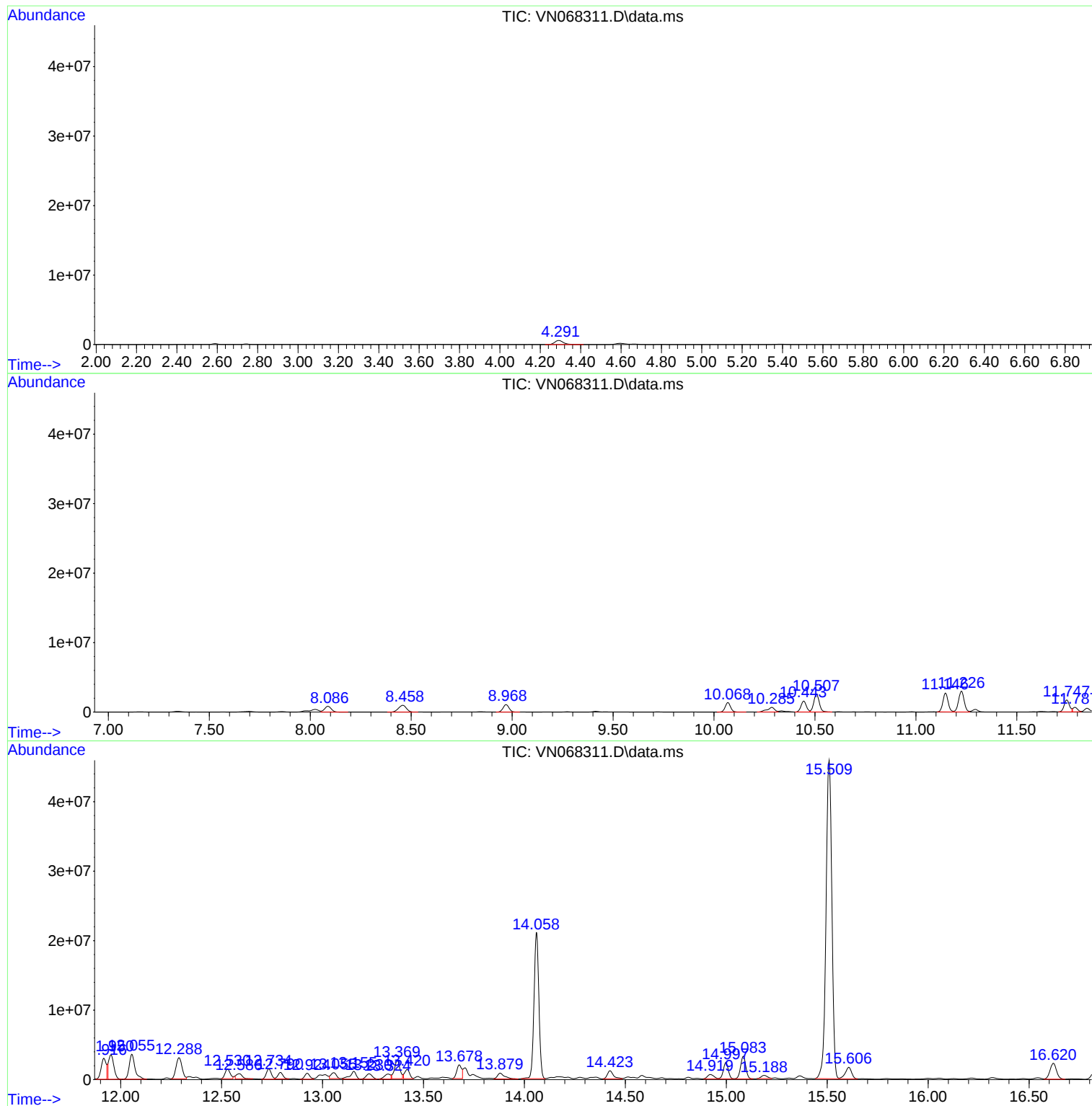
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Quant Title : SW846 8260

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



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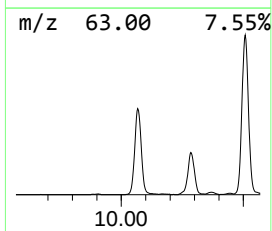
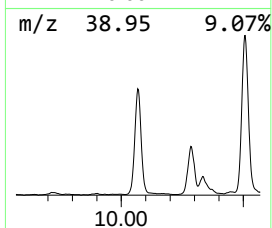
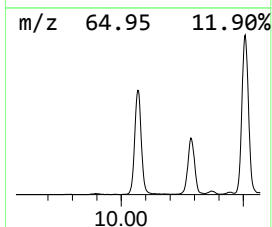
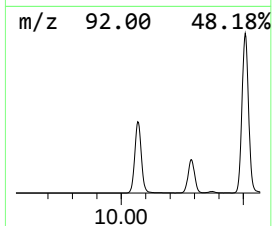
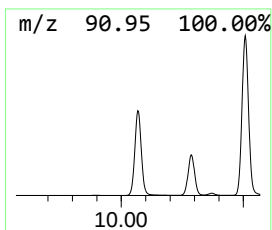
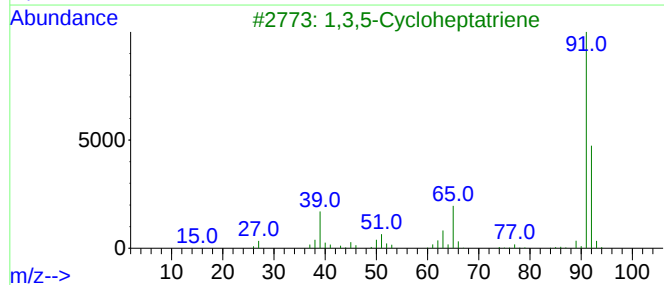
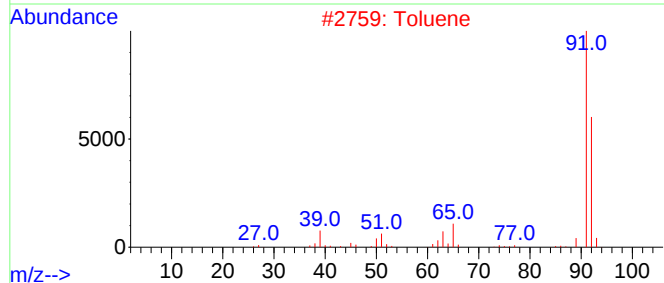
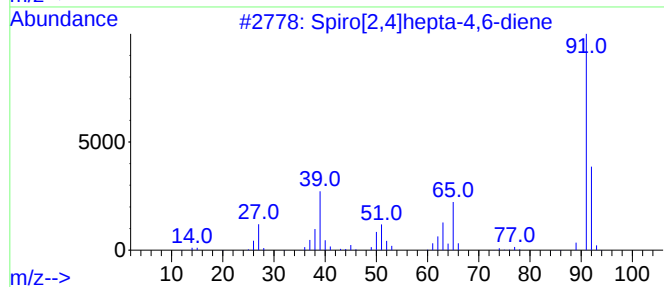
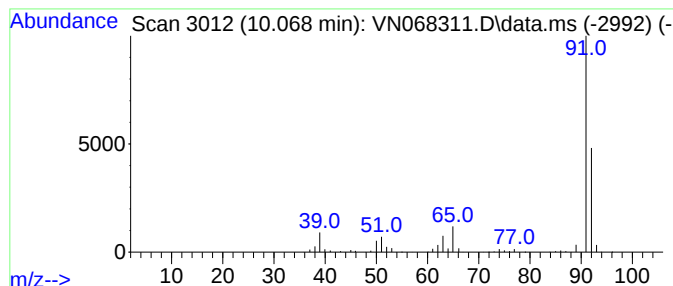
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 1 Spiro[2,4]hepta-4,6-diene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.068	57.77 ug/l	2553460	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	91
2			Toluene	92	C7H8	000108-88-3	91
3			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	91
4			2,5-Norbornadiene	92	C7H8	000121-46-0	80
5			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	80



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Instrument :
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ClientSampleId :
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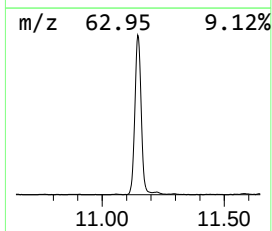
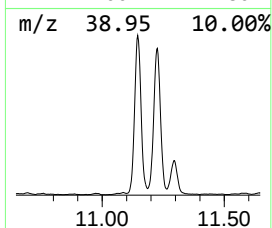
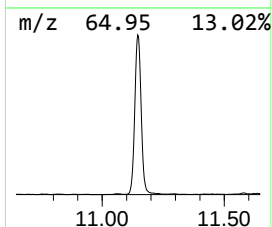
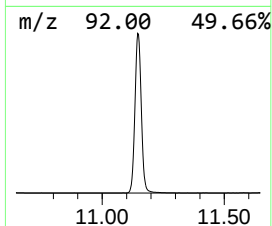
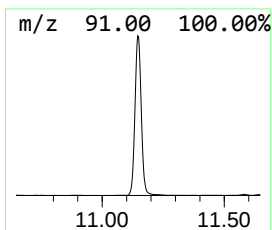
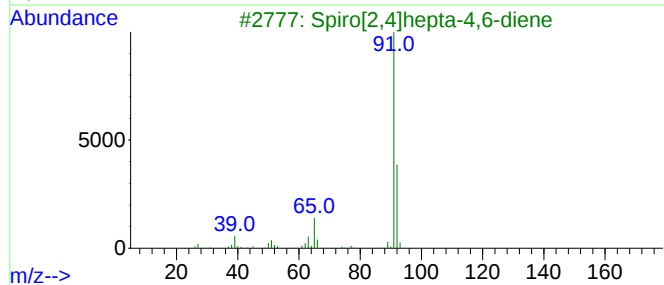
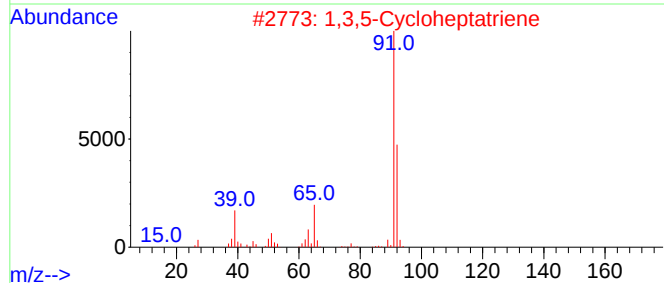
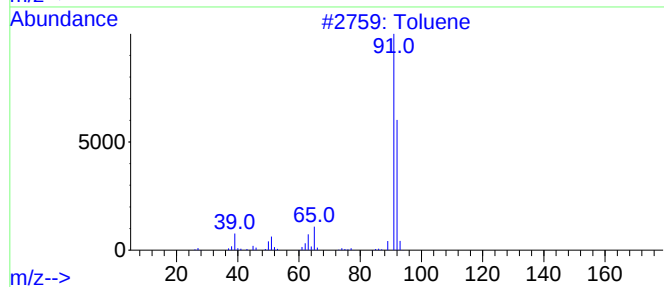
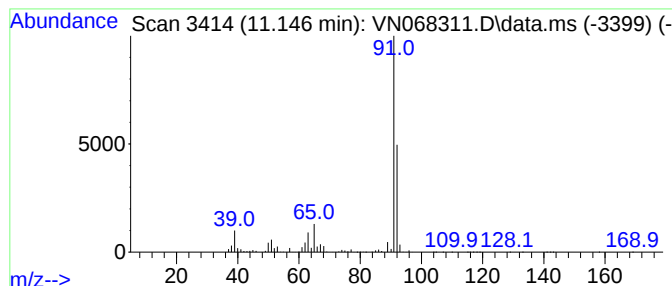
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
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Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.146	77.35 ug/l	4876500	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	90
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	74
4			2,5-Norbornadiene	92	C7H8	000121-46-0	72
5			Molybdenum, di-.mu.-chlorobis[(1... 532	C20H26Cl2Mo2	035625-66-2	72	



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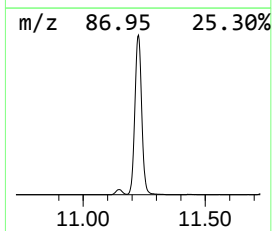
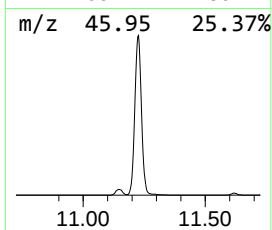
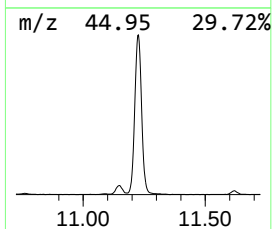
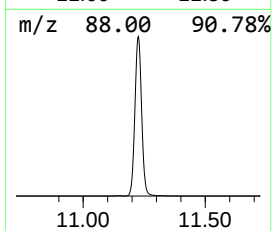
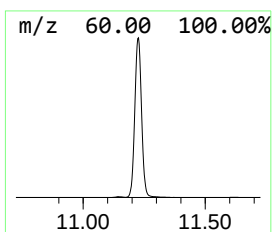
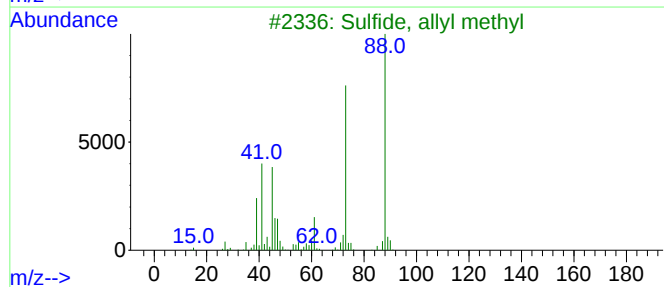
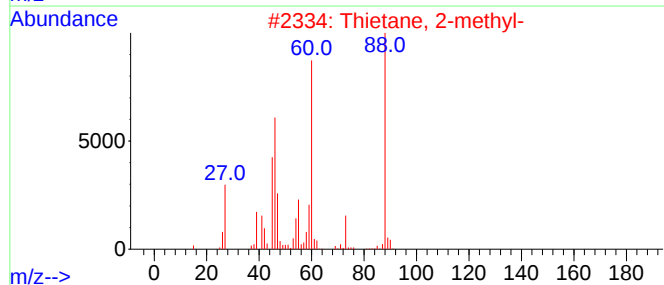
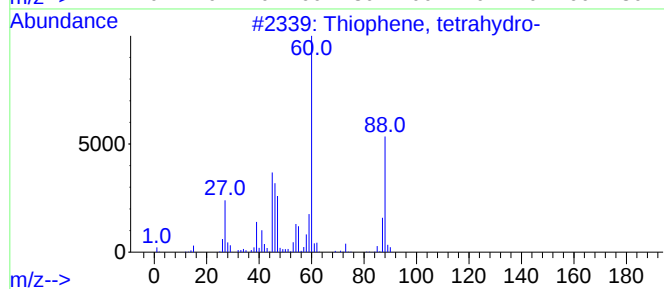
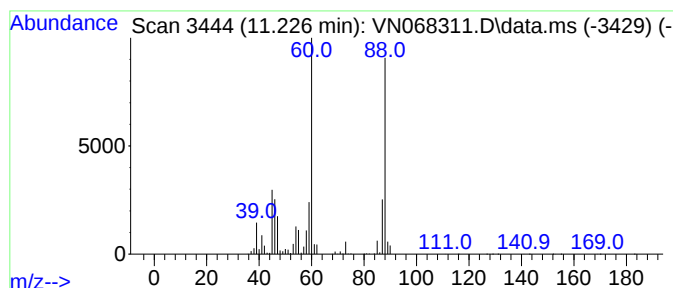
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.226	91.29 ug/l	5755360	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3			Sulfide, allyl methyl	88	C4H8S	010152-76-8	38
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25



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ALS Vial : 24 Sample Multiplier: 1

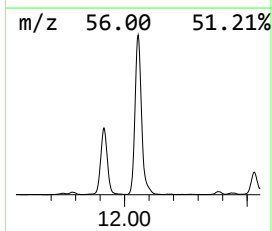
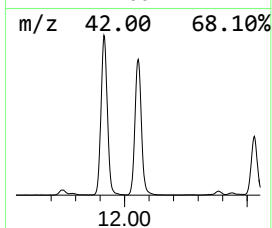
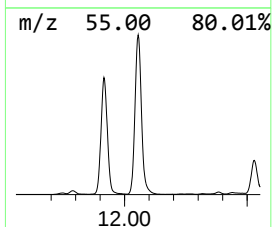
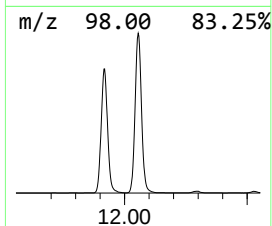
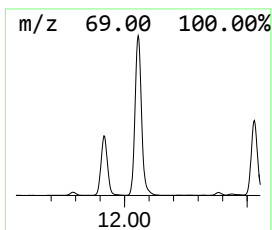
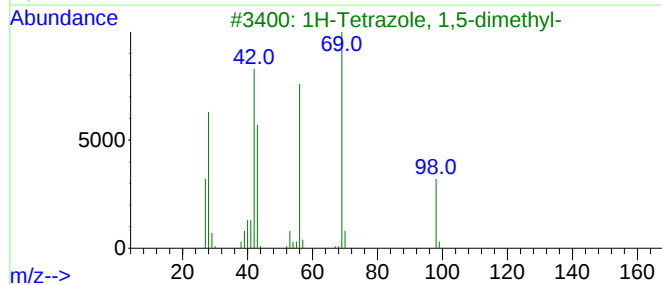
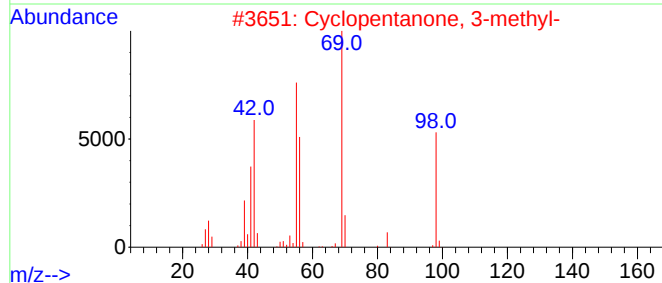
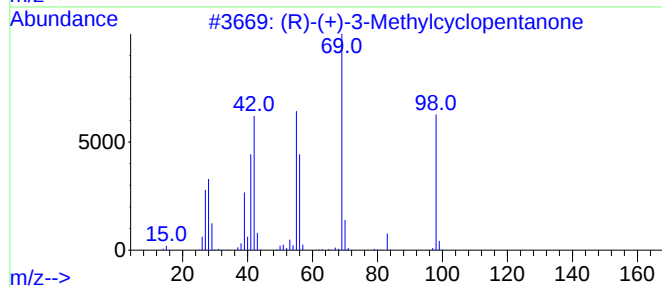
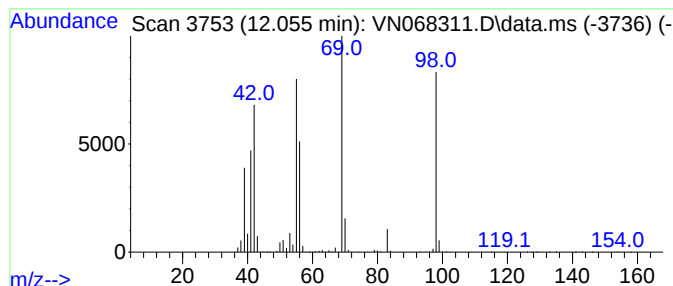
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Peak Number 4 (R)-(+)-3-Methylcyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.055	112.58 ug/l	7097710	Chlorobenzene-d5	11.746	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	94
2	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	91
3	1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	59
4	(Z)-4-Methyl-2-hexene	98	C7H14	003683-19-0	43
5	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	43



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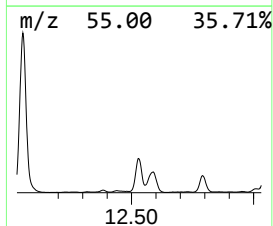
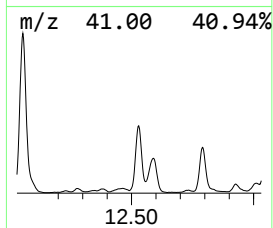
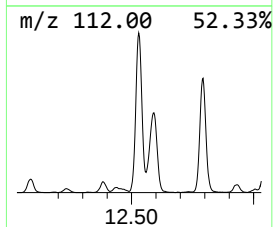
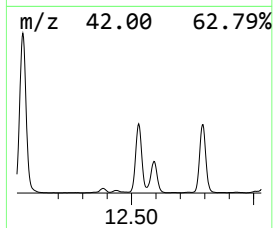
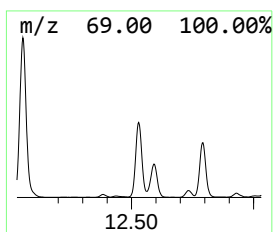
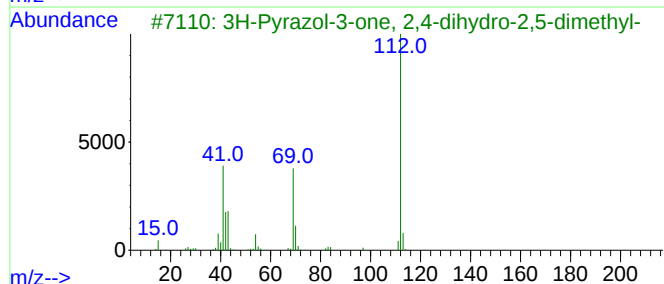
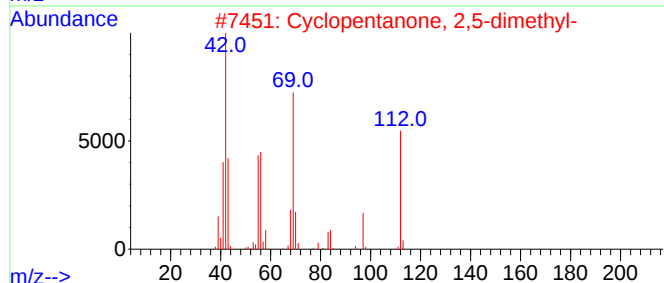
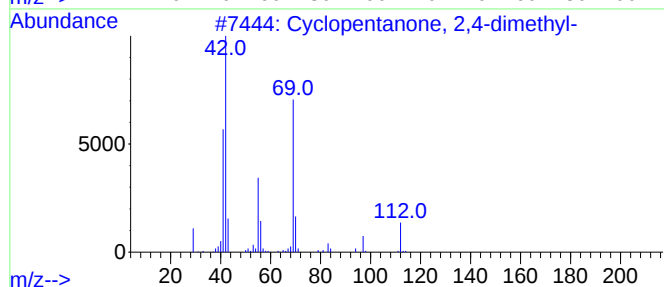
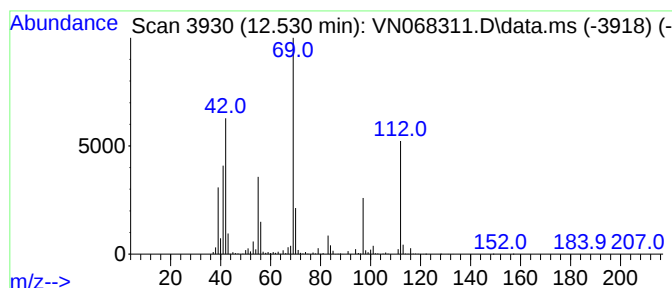
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentanone, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.530	39.83 ug/l	2511080	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 2,4-dimethyl-	112	C7H12O	001121-33-1	91
2			Cyclopentanone, 2,5-dimethyl-	112	C7H12O	004041-09-2	86
3			3H-Pyrazol-3-one, 2,4-dihydro-2,...	112	C5H8N2O	002749-59-9	59
4			Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	53
5			trans-3,4-Dimethylcyclopentanone	112	C7H12O	019550-73-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068311.D
Acq On : 25 Aug 2021 20:10
Operator : JC/MD
Sample : M3529-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31116

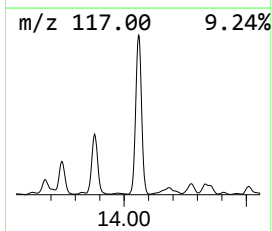
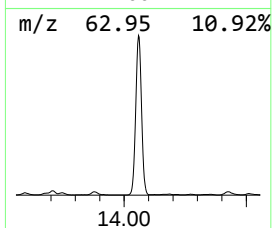
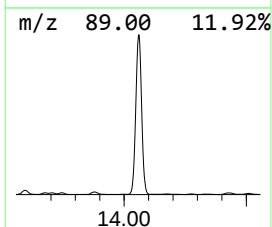
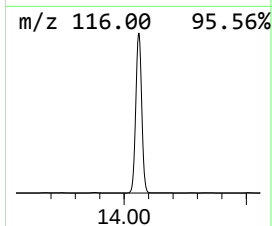
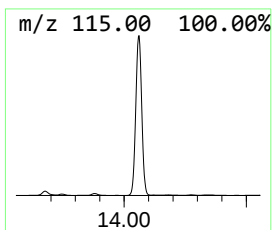
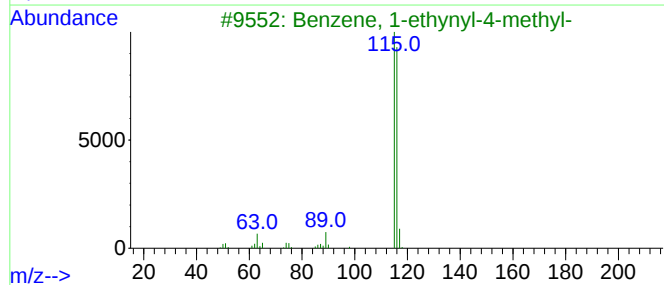
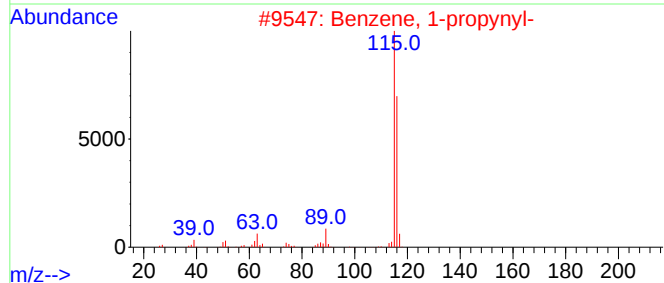
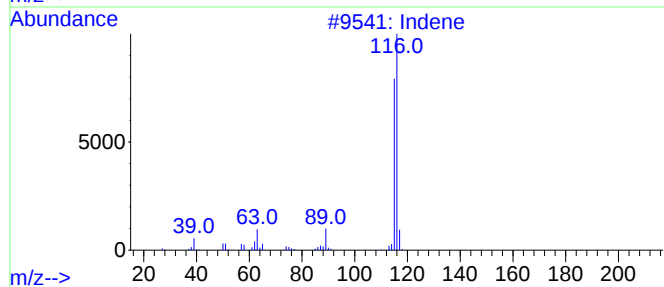
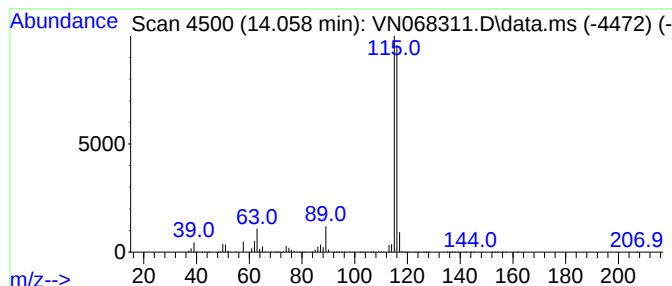
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Quant Title : SW846 8260

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

Peak Number 6 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.058	522.02 ug/l	35564800	1,4-Dichlorobenzene-d4	13.678

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			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068311.D
Acq On : 25 Aug 2021 20:10
Operator : JC/MD
Sample : M3529-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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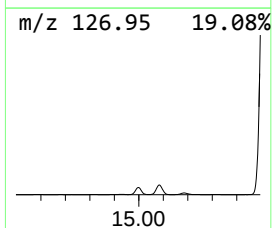
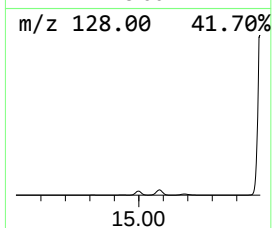
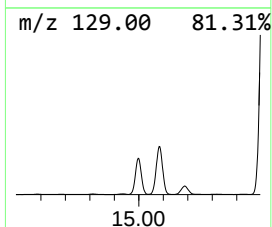
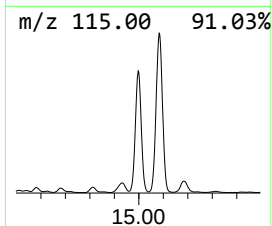
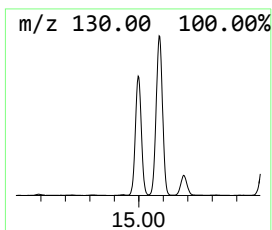
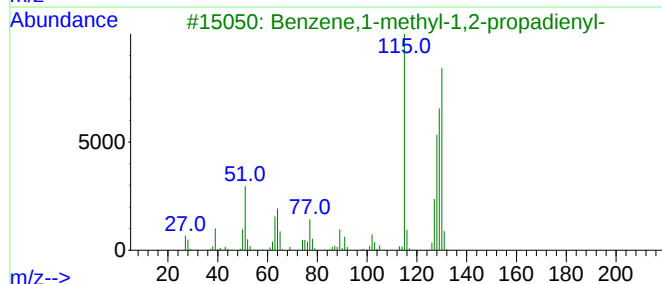
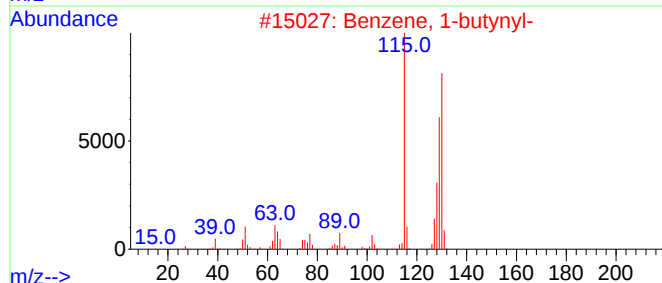
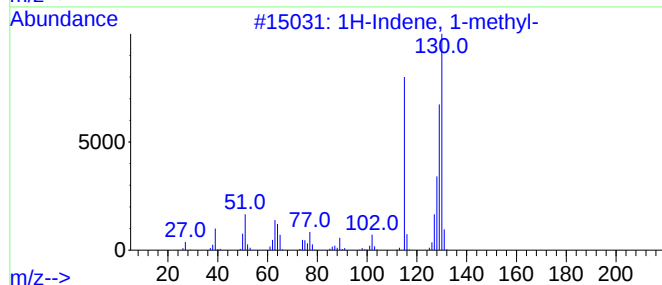
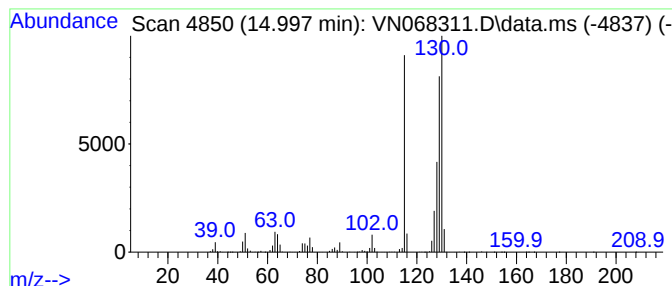
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	58.70 ug/l	3999360	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	91
2			Benzene, 1-butyryl-	130	C10H10	000622-76-4	91
3			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	90
4			2-Methylindene	130	C10H10	002177-47-1	90
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	89



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068311.D
Acq On : 25 Aug 2021 20:10
Operator : JC/MD
Sample : M3529-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleID :
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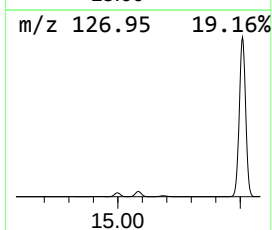
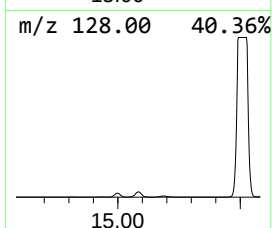
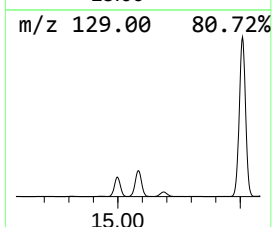
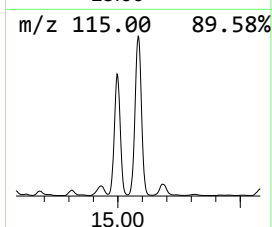
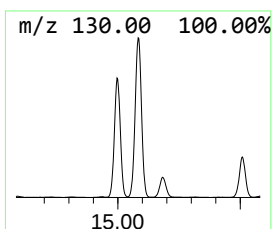
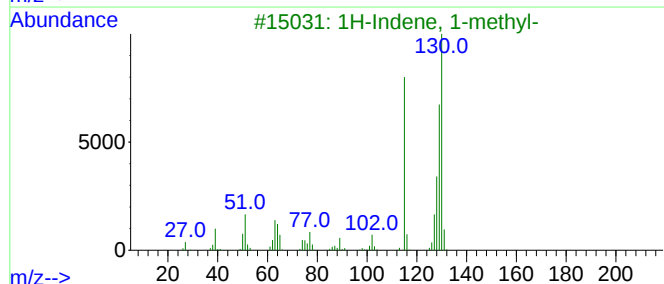
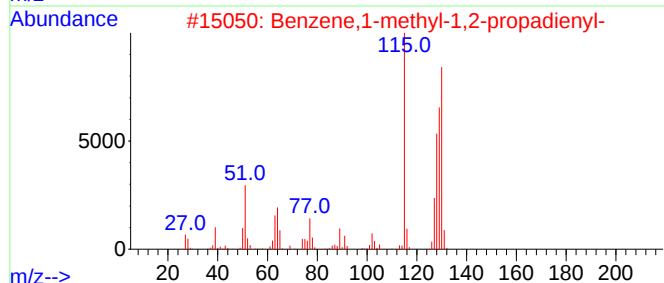
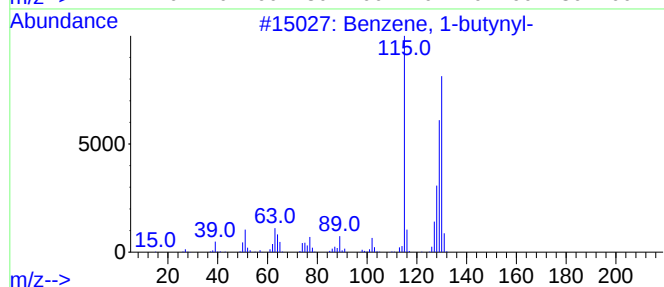
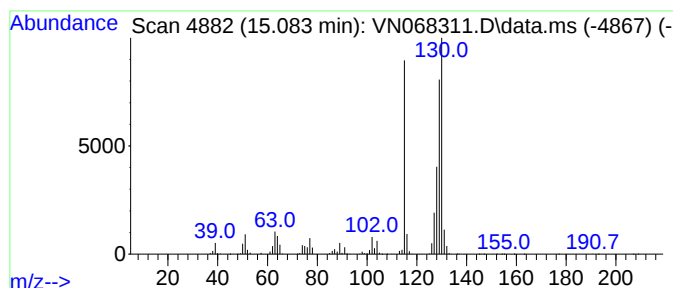
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-butynyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.083	86.12 ug/l	5867030	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-butynyl-	130	C10H10	000622-76-4	94
2			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
4			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93
5			2-Methylindene	130	C10H10	002177-47-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068311.D
Acq On : 25 Aug 2021 20:10
Operator : JC/MD
Sample : M3529-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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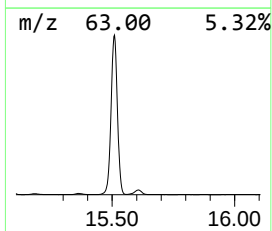
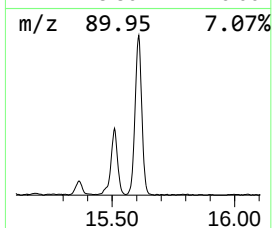
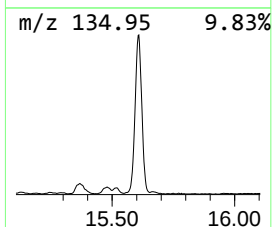
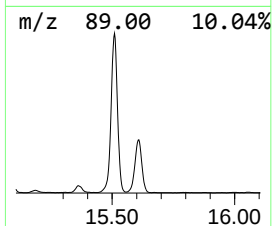
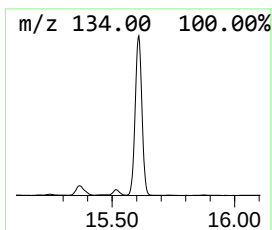
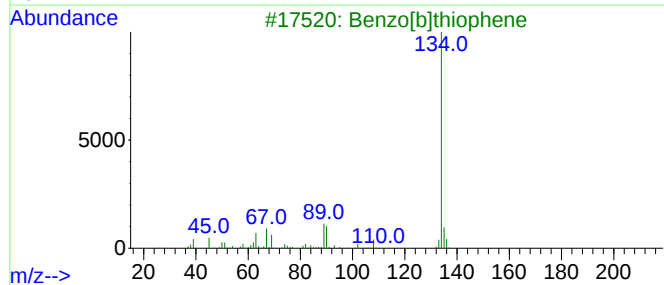
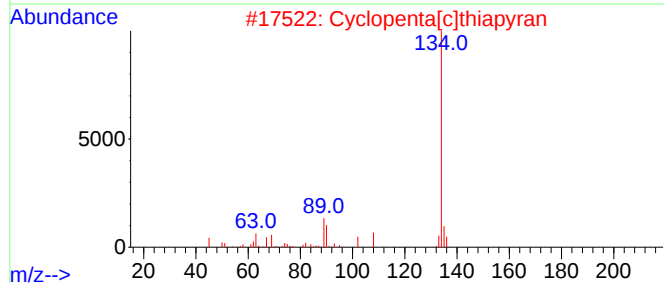
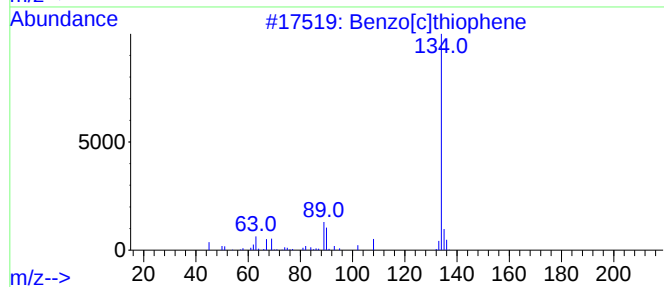
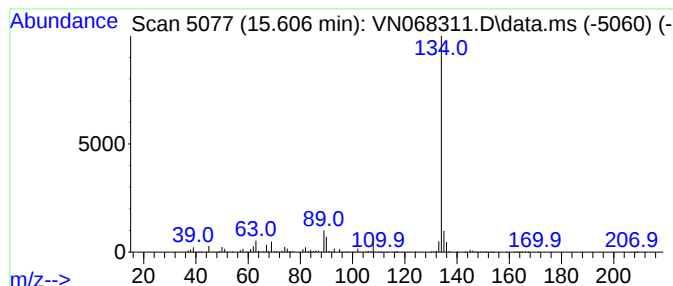
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[c]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.606	53.46 ug/l	3641970	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 : VN068311.D
Acq On : 25 Aug 2021 20:10
Operator : JC/MD
Sample : M3529-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31116

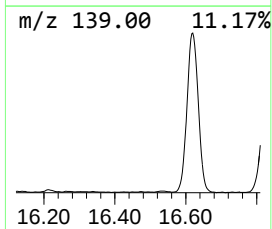
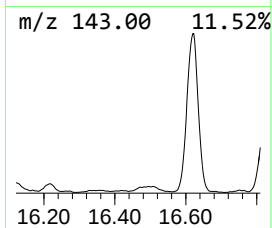
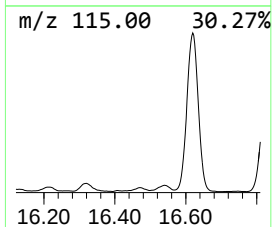
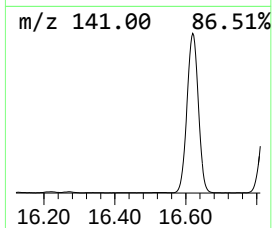
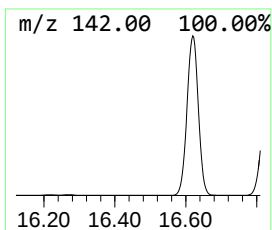
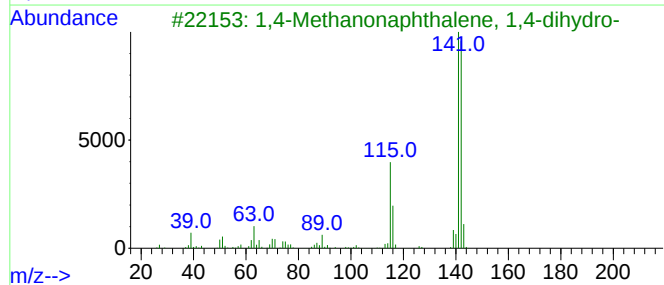
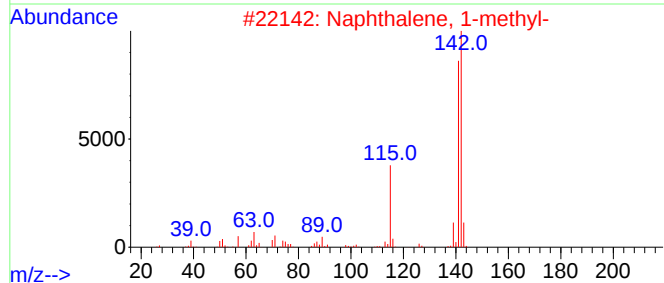
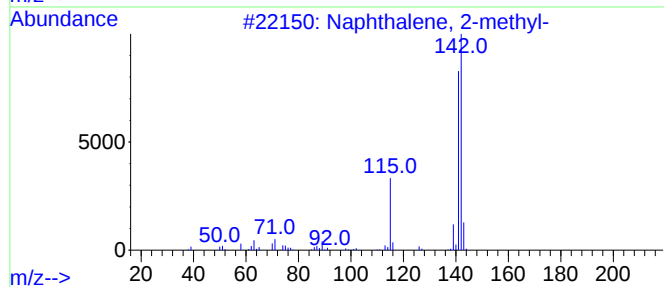
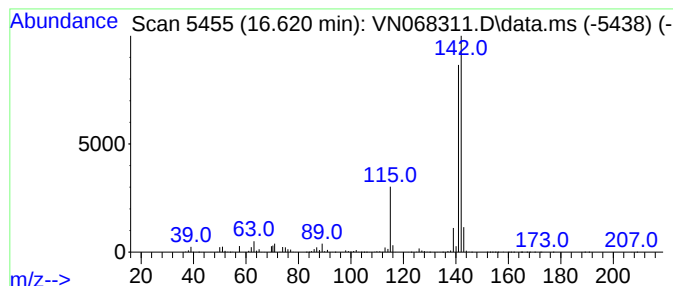
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Quant Title : SW846 8260

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	74.72 ug/l	5090360	1,4-Dichlorobenzene-d4	13.678

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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068311.D
Acq On : 25 Aug 2021 20:10
Operator : JC/MD
Sample : M3529-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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1,3,5-Cyclohept...	11.146	77.3	ug/l	4876500	3	11.746	3152240	50.0
Thiophene, tetr...	11.226	91.3	ug/l	5755360	3	11.746	3152240	50.0
(R)-(+)-3-Methy...	12.055	112.6	ug/l	7097710	3	11.746	3152240	50.0
Cyclopentanone,...	12.530	39.8	ug/l	2511080	3	11.746	3152240	50.0
Indene	14.058	522.0	ug/l	35564800	4	13.678	3406440	50.0
1H-Indene, 1-me...	14.997	58.7	ug/l	3999360	4	13.678	3406440	50.0
Benzene, 1-buty...	15.083	86.1	ug/l	5867030	4	13.678	3406440	50.0
Benzo[c]thiophene	15.606	53.5	ug/l	3641970	4	13.678	3406440	50.0
Naphthalene, 1-...	16.620	74.7	ug/l	5090360	4	13.678	3406440	50.0