

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
 Data File : VN068309.D
 Acq On : 25 Aug 2021 19:20
 Operator : JC/MD
 Sample : M3529-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31114

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: VN068309.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	832	858	916	rBV	559830	1692897	1.58%	0.624%
2	8.088	2261	2274	2307	rVB2	721928	1669450	1.56%	0.615%
3	8.458	2385	2412	2443	rBV3	980767	2703153	2.53%	0.996%
4	8.971	2583	2603	2648	rVB	970068	2022755	1.89%	0.745%
5	10.068	2989	3012	3037	rBV	1123588	2064453	1.93%	0.761%
6	10.288	3066	3094	3105	rBV2	555642	1300127	1.22%	0.479%
7	10.443	3136	3152	3164	rBV	1454453	2713170	2.54%	1.000%
8	10.507	3164	3176	3206	rVB	2928720	5438245	5.09%	2.003%
9	11.146	3399	3414	3428	rBV	2295714	4137551	3.87%	1.524%
10	11.224	3429	3443	3460	rVV	4846402	9110804	8.53%	3.356%
11	11.747	3623	3638	3647	rBV	1648166	2943143	2.76%	1.084%
12	11.787	3648	3653	3665	rVV	862208	1391861	1.30%	0.513%
13	11.848	3665	3676	3687	rVV	645926	1181182	1.11%	0.435%
14	11.916	3688	3701	3707	rVV2	3082611	5428818	5.08%	2.000%
15	11.950	3708	3714	3736	rVV	4065249	7263333	6.80%	2.676%
16	12.055	3737	3753	3783	rVB	3640294	7420375	6.95%	2.734%
17	12.288	3825	3840	3854	rBV5	3682653	7582115	7.10%	2.793%
18	12.530	3917	3930	3940	rBV	1503162	2645762	2.48%	0.975%
19	12.734	3992	4006	4017	rBV	1459863	2499302	2.34%	0.921%
20	12.790	4017	4027	4043	rVB	924144	1626413	1.52%	0.599%
21	12.924	4065	4077	4088	rBV	793142	1360441	1.27%	0.501%
22	13.055	4118	4126	4139	rVB2	1038966	1878216	1.76%	0.692%
23	13.230	4176	4191	4207	rBV4	689434	1492315	1.40%	0.550%
24	13.326	4209	4227	4231	rBV4	715662	1400672	1.31%	0.516%
25	13.369	4234	4243	4253	rVV	3057633	5382174	5.04%	1.983%
26	13.420	4254	4262	4273	rVV	1776697	2918427	2.73%	1.075%
27	13.678	4345	4358	4363	rBV	1877862	3112206	2.91%	1.147%
28	13.745	4379	4383	4405	rVB4	772365	1534538	1.44%	0.565%
29	13.879	4422	4433	4467	rVB3	907187	2343300	2.19%	0.863%
30	14.058	4485	4500	4518	rVB	25391519	42434246	39.73%	15.632%
31	14.423	4624	4636	4660	rBV4	960395	2022376	1.89%	0.745%
32	14.919	4808	4821	4836	rBV4	784715	1780264	1.67%	0.656%
33	14.997	4837	4850	4866	rVV	3179608	5396861	5.05%	1.988%
34	15.083	4868	4882	4902	rVB	4171151	7487503	7.01%	2.758%
35	15.188	4908	4921	4935	rBV3	537620	1138068	1.07%	0.419%
36	15.509	5014	5041	5060	rBV2	52072179	106819408	100.00%	39.351%

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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	15.609	5062	5078	5095	rVB	1806987	3858179	3.61%	1.421%
38	16.620	5438	5455	5488	rVB	2865291	6255602	5.86%	2.305%

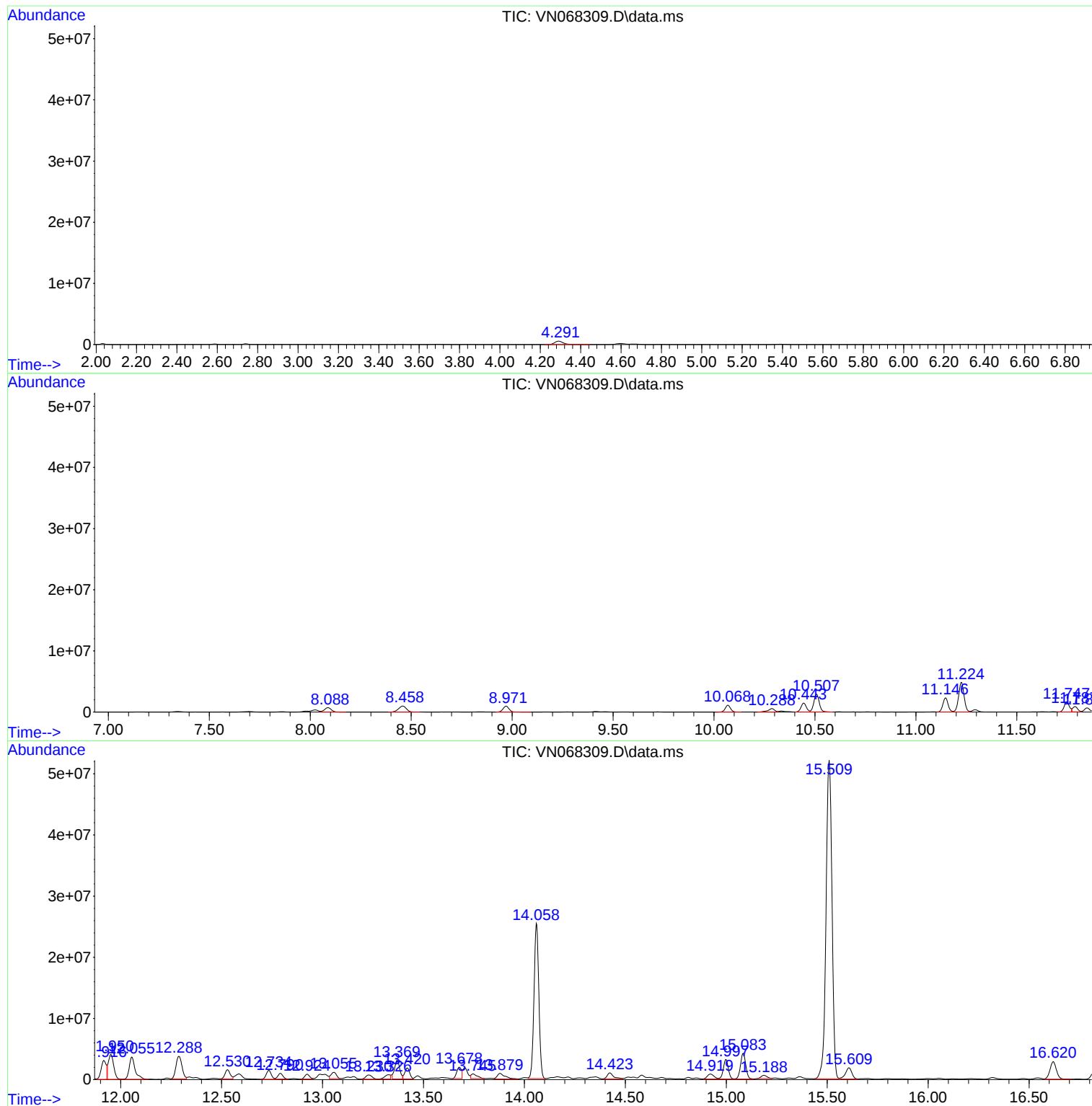
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Quant Title : SW846 8260

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



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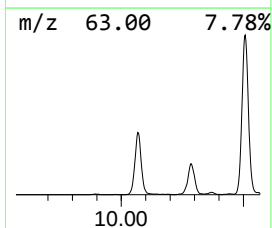
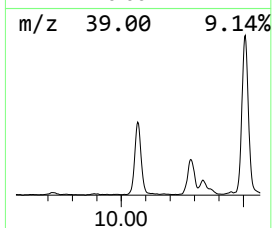
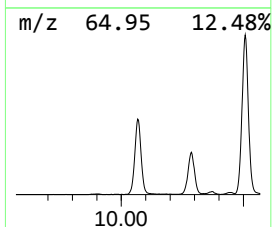
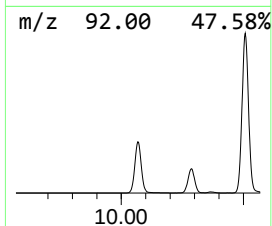
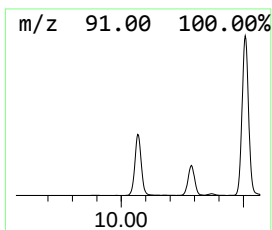
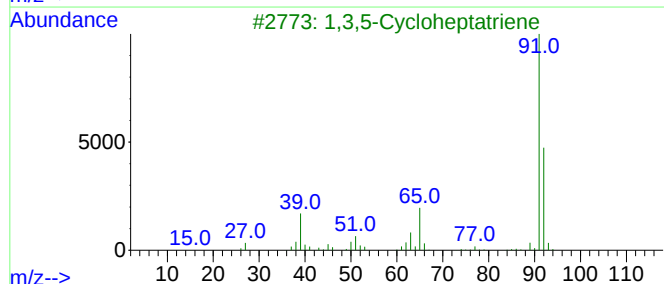
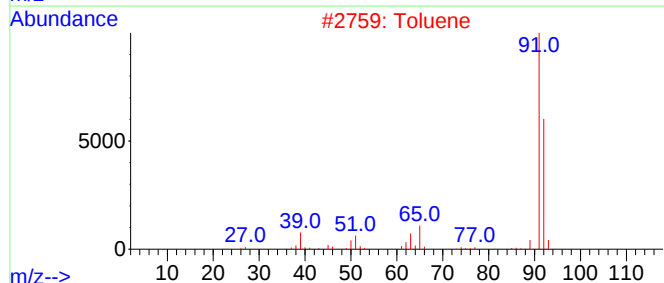
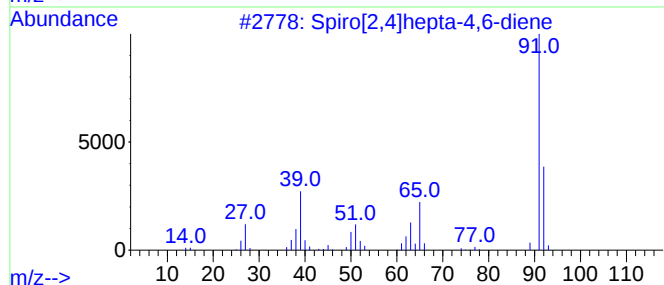
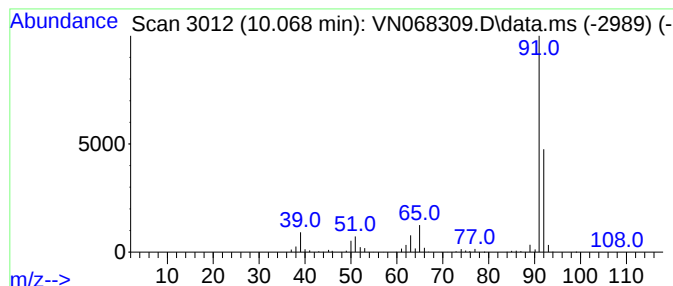
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 1 Spiro[2,4]hepta-4,6-diene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.068	51.03 ug/l	2064450	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	74



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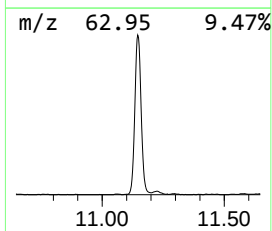
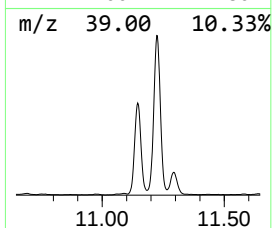
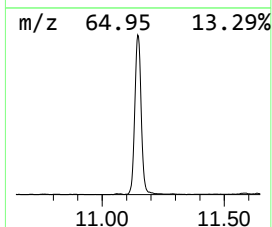
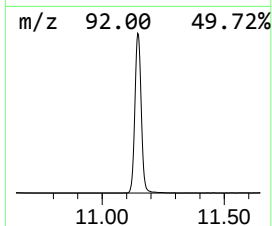
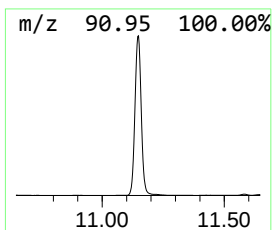
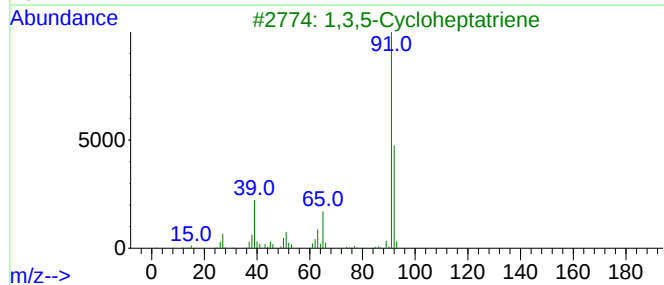
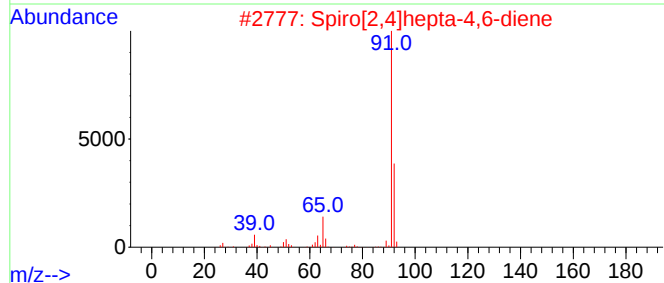
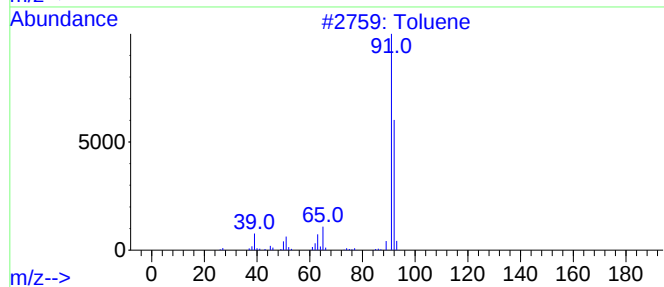
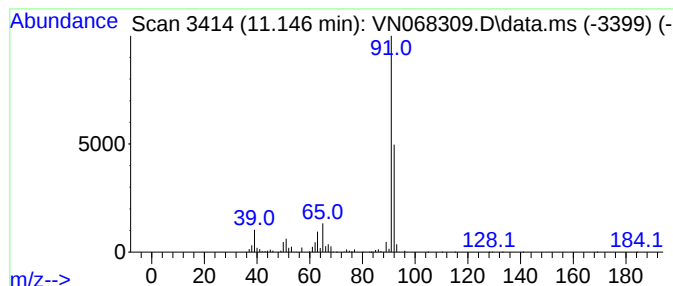
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.146	70.29 ug/l	4137550	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	90
2			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
3			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	83
4			2,5-Norbornadiene	92	C7H8	000121-46-0	72
5			1,6-Heptadien-3-yne	92	C7H8	005150-80-1	64



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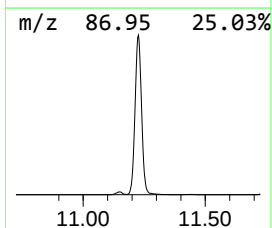
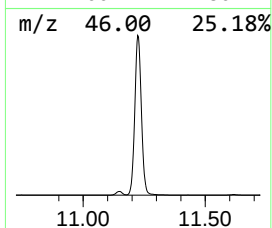
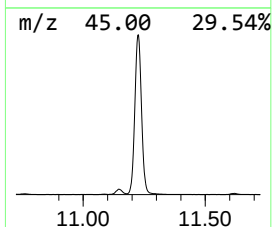
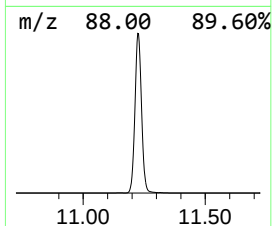
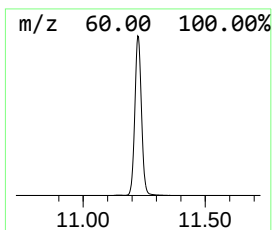
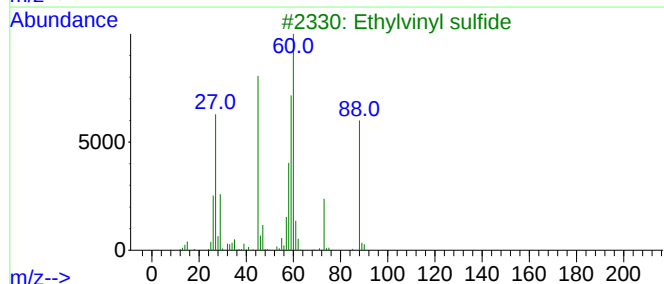
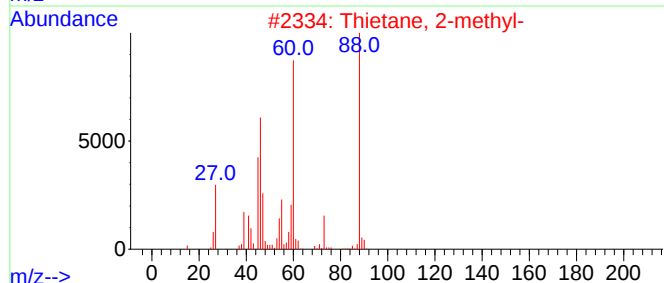
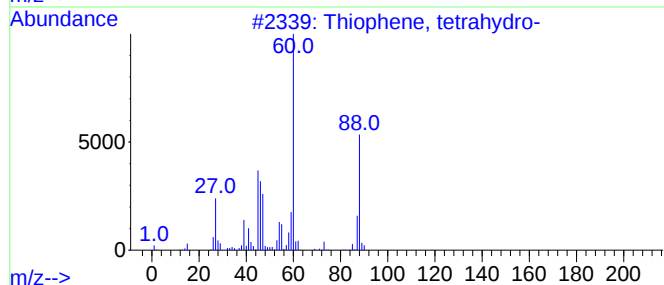
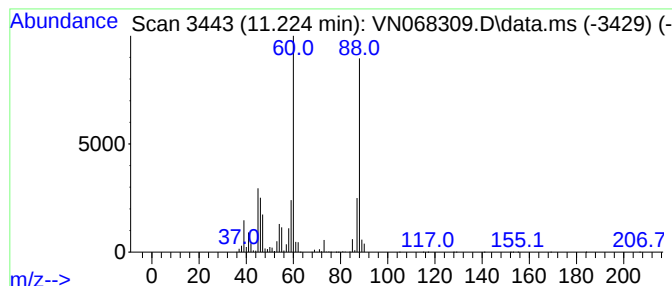
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.224	154.78 ug/l	9110800	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	74
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4			Sulfide, allyl methyl	88	C4H8S	010152-76-8	38
5			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36



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ALS Vial : 22 Sample Multiplier: 1

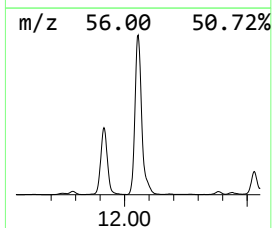
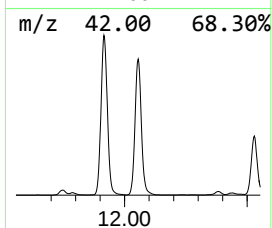
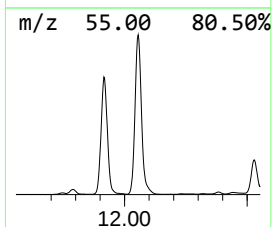
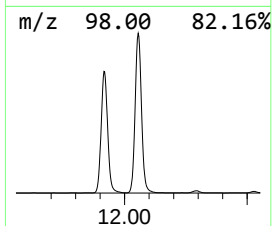
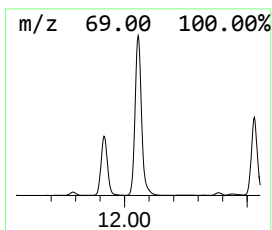
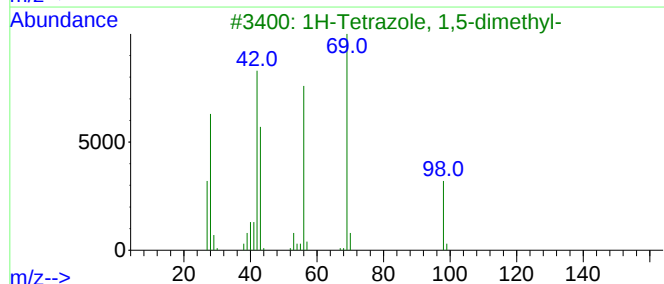
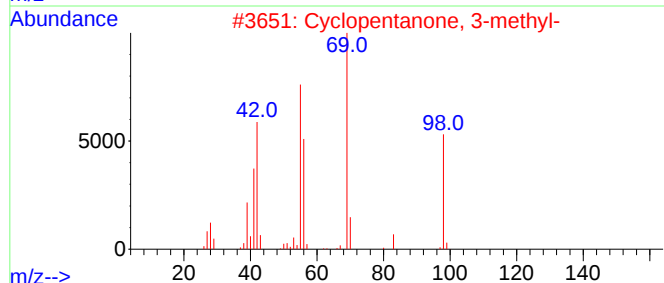
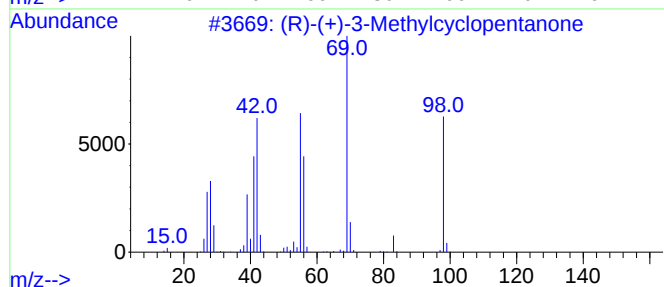
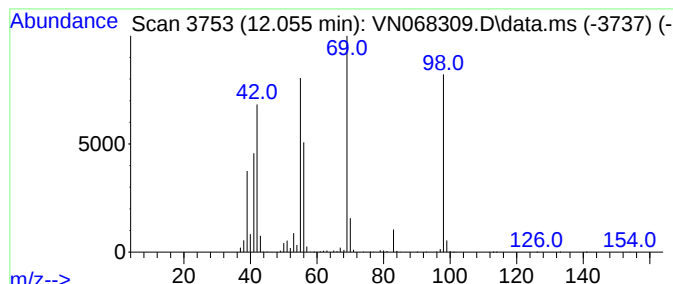
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Peak Number 4 (R)-(+)-3-Methylcyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.055	126.06 ug/l	7420380	Chlorobenzene-d5			11.746
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(R)-(+)-3-Methylcyclopentanone		98	C6H10O	006672-30-6	95
2	Cyclopentanone, 3-methyl-		98	C6H10O	001757-42-2	94
3	1H-Tetrazole, 1,5-dimethyl-		98	C3H6N4	005144-11-6	72
4	(Z)-4-Methyl-2-hexene		98	C7H14	003683-19-0	50
5	Cyclopentanone, 2-methyl-		98	C6H10O	001120-72-5	49



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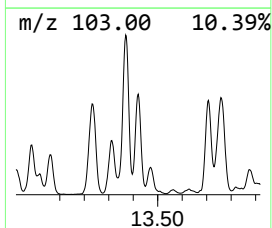
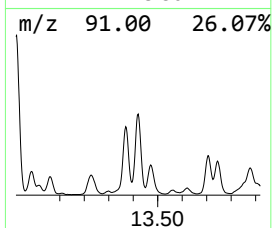
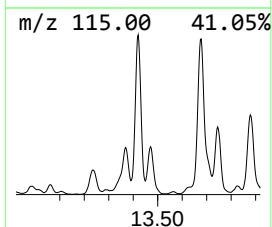
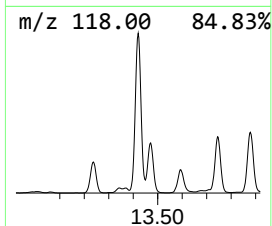
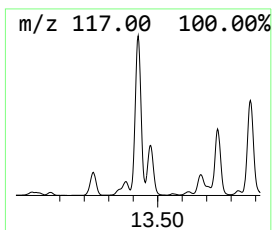
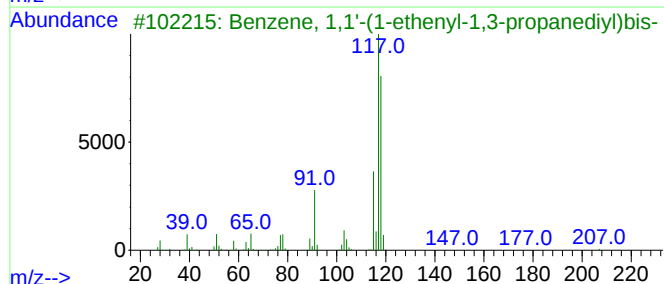
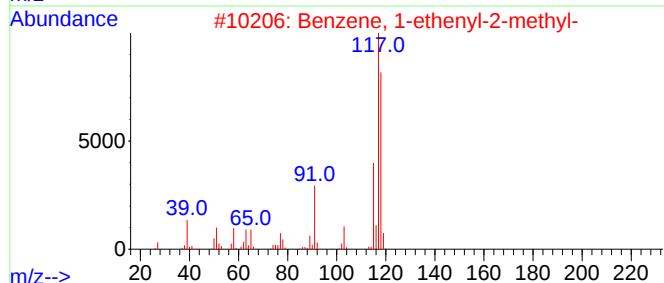
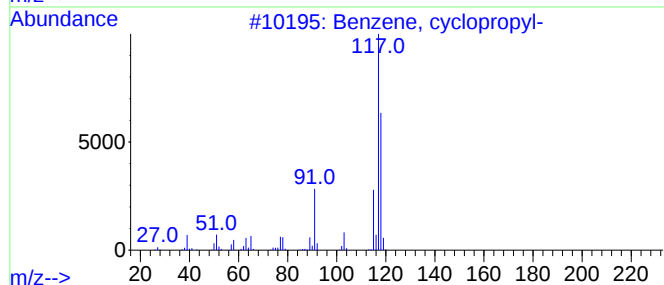
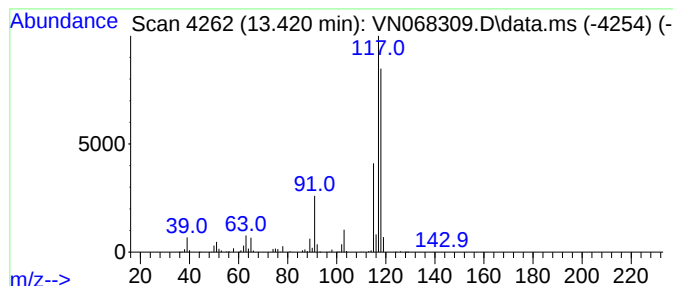
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	46.89 ug/l	2918430	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
3			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	90
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
5			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068309.D
Acq On : 25 Aug 2021 19:20
Operator : JC/MD
Sample : M3529-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31114

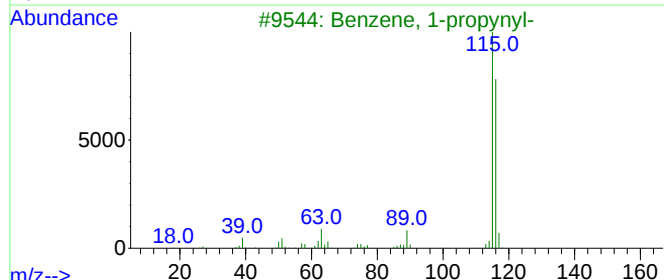
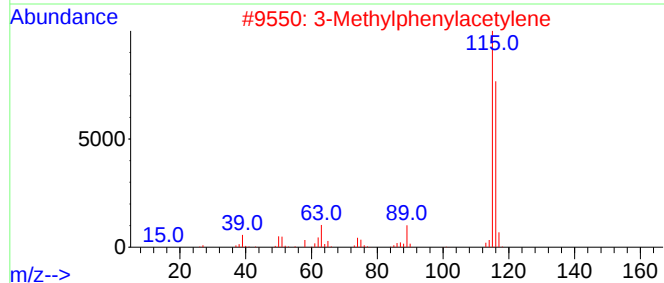
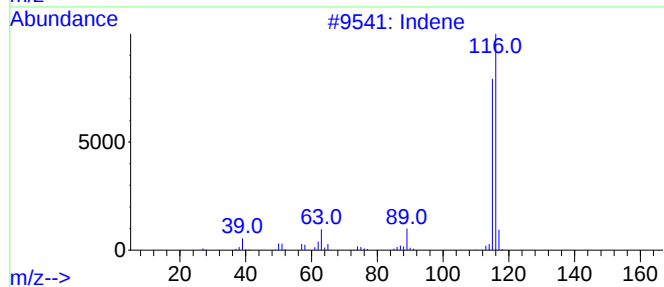
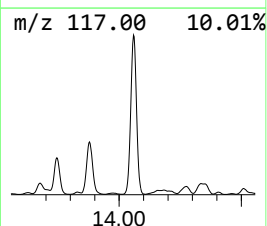
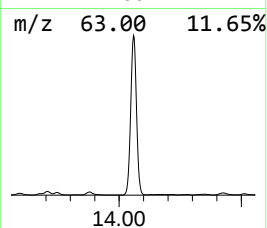
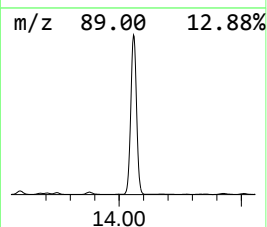
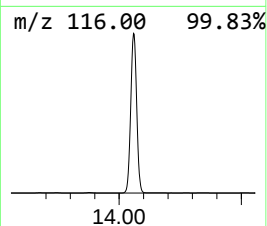
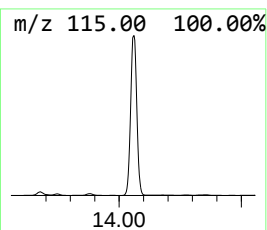
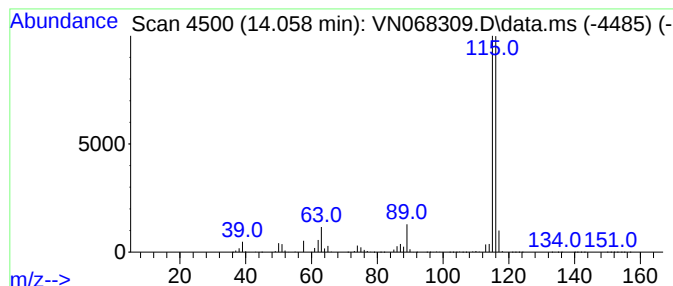
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Quant Title : SW846 8260

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	681.74 ug/l	42434200	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			2-Methylphenylacetylene	116	C9H8	000766-47-2	91
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068309.D
Acq On : 25 Aug 2021 19:20
Operator : JC/MD
Sample : M3529-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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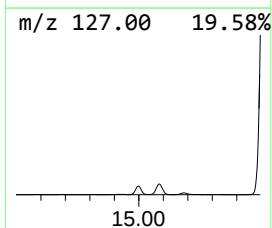
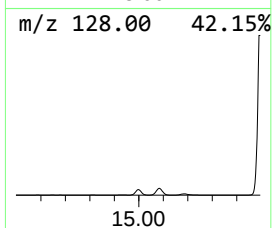
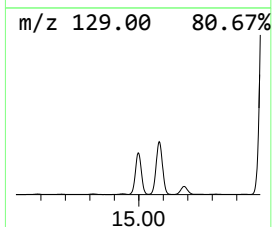
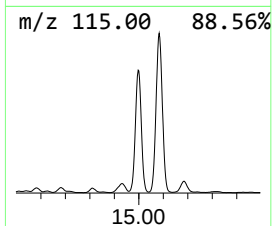
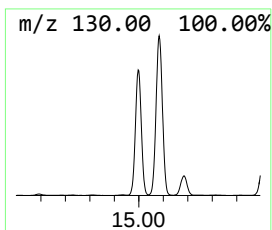
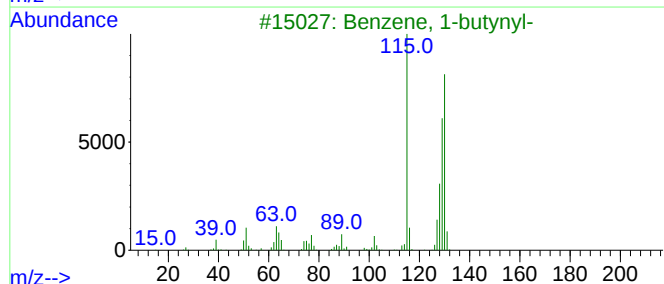
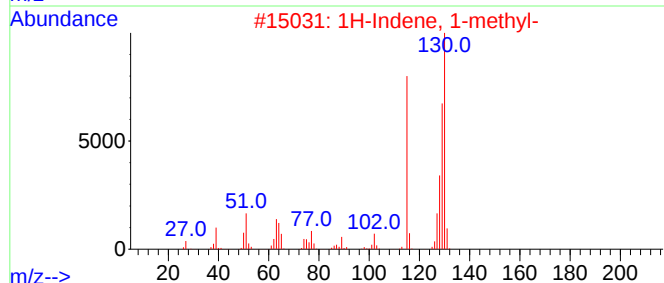
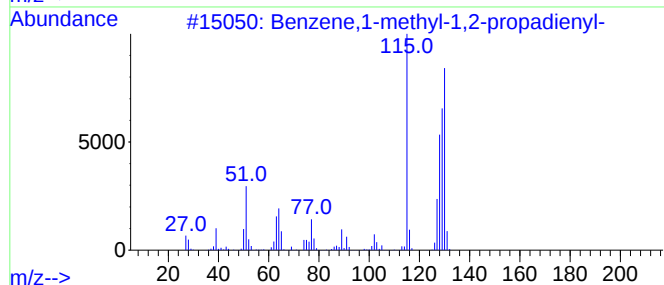
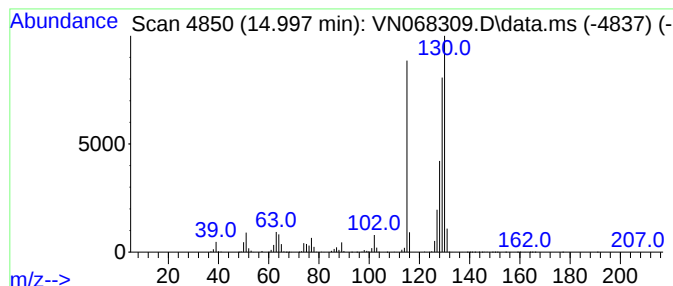
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Quant Title : SW846 8260

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

Peak Number 7 Benzene,1-methyl-1,2-propad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	86.70 ug/l	5396860	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
3			Benzene, 1-butyryl-	130	C10H10	000622-76-4	91
4			2-Methylindene	130	C10H10	002177-47-1	91
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068309.D
Acq On : 25 Aug 2021 19:20
Operator : JC/MD
Sample : M3529-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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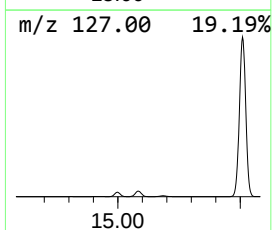
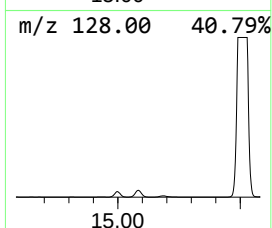
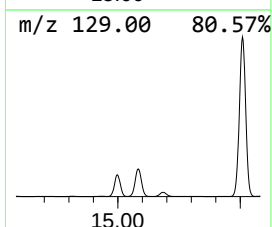
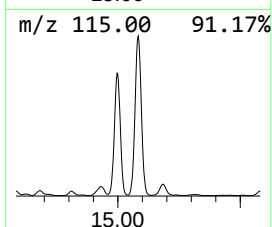
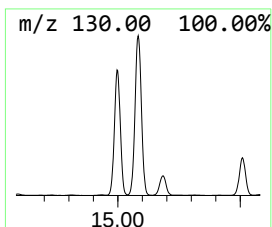
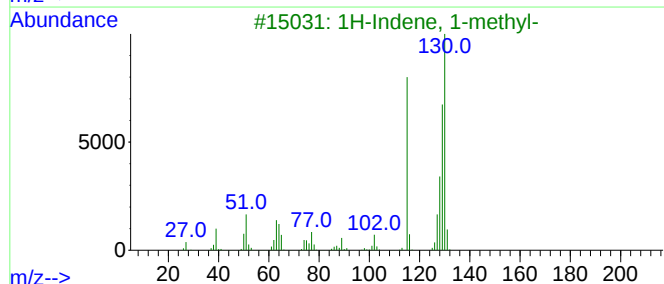
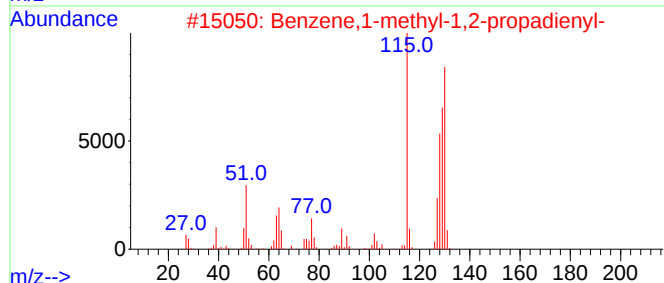
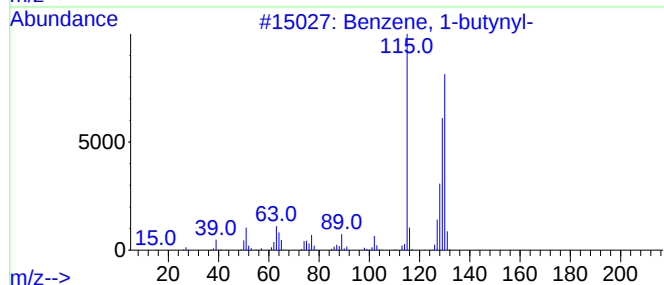
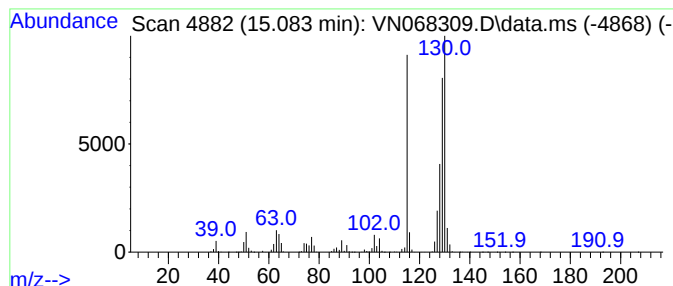
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Quant Title : SW846 8260

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	120.29 ug/l	7487500	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
2			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
4			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068309.D
Acq On : 25 Aug 2021 19:20
Operator : JC/MD
Sample : M3529-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31114

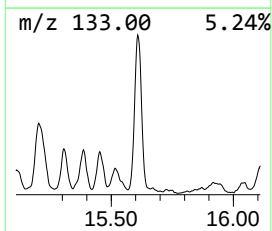
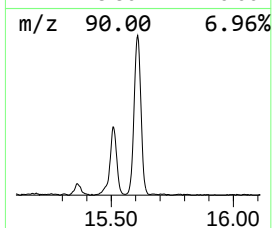
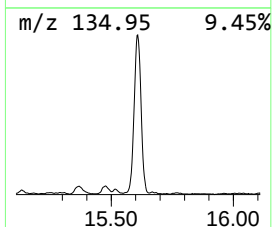
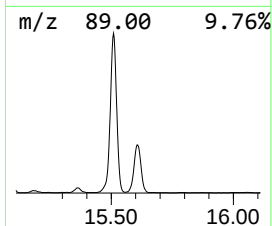
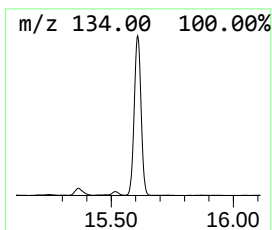
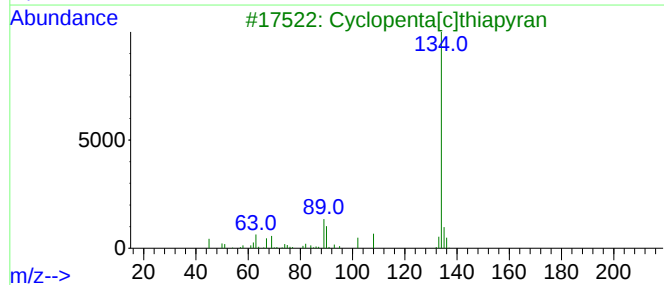
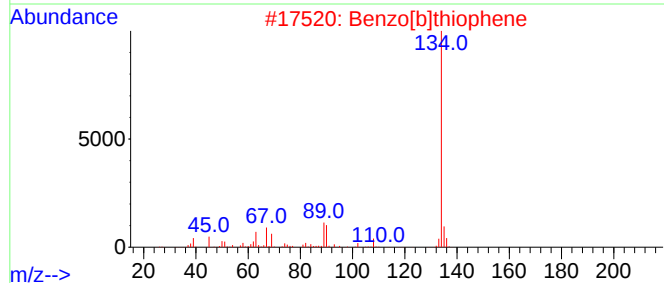
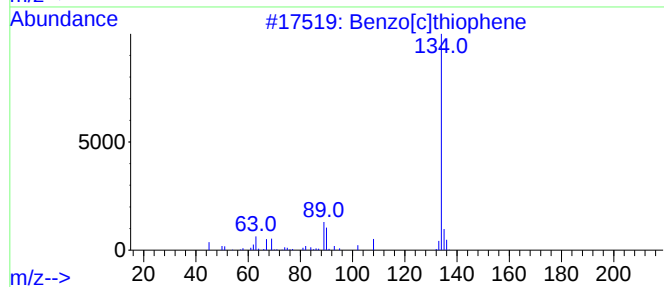
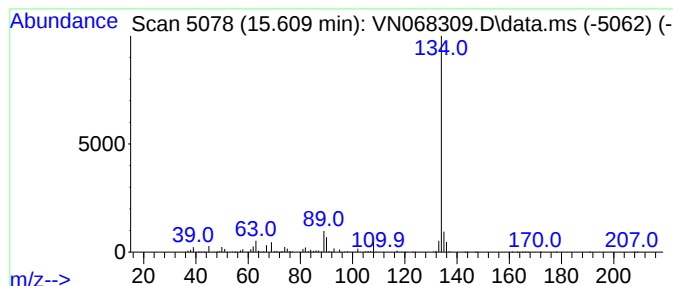
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[c]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	61.98 ug/l	3858180	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	91
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	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 : VN068309.D
Acq On : 25 Aug 2021 19:20
Operator : JC/MD
Sample : M3529-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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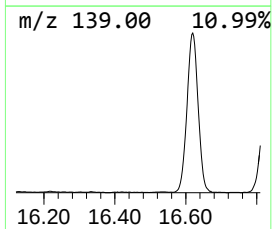
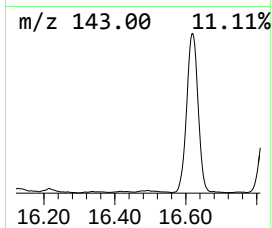
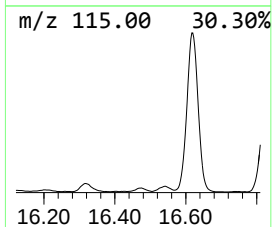
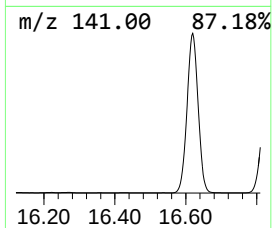
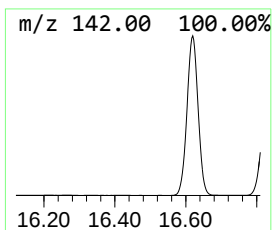
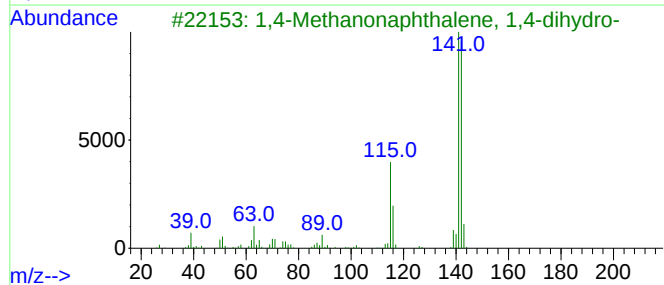
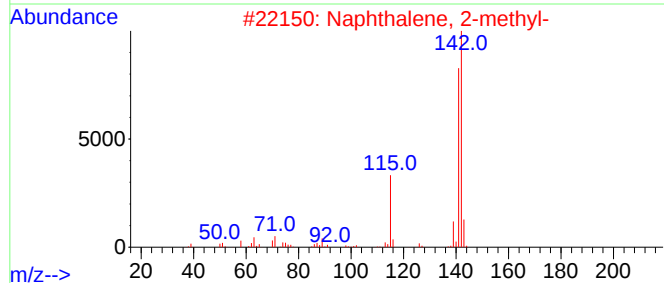
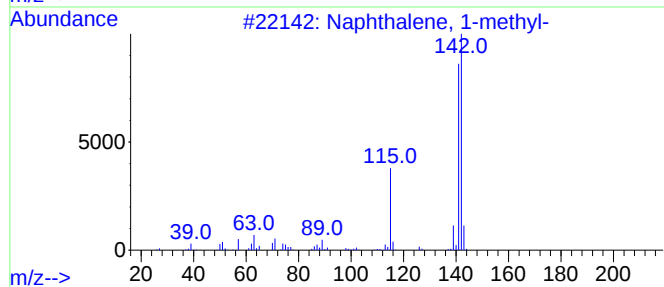
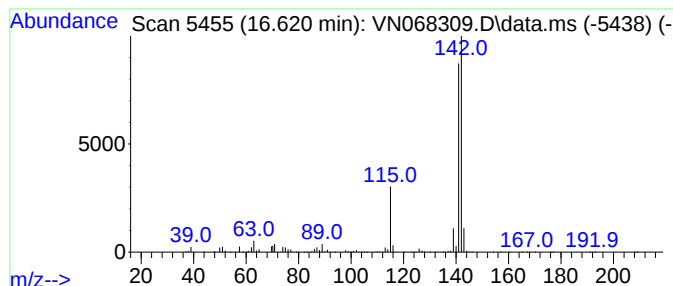
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.620	100.50 ug/l	6255600	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			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 : VN068309.D
Acq On : 25 Aug 2021 19:20
Operator : JC/MD
Sample : M3529-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31114

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...	11.146	70.3	ug/l	4137550	3	11.746	2943140	50.0
Thiophene, tetr...	11.224	154.8	ug/l	9110800	3	11.746	2943140	50.0
(R)-(+)-3-Methy...	12.055	126.1	ug/l	7420380	3	11.746	2943140	50.0
Benzene, cyclop...	13.420	46.9	ug/l	2918430	4	13.678	3112210	50.0
Indene	14.058	681.7	ug/l	42434200	4	13.678	3112210	50.0
Benzene,1-methy...	14.997	86.7	ug/l	5396860	4	13.678	3112210	50.0
Benzene, 1-buty...	15.083	120.3	ug/l	7487500	4	13.678	3112210	50.0
Benzo[c]thiophene	15.609	62.0	ug/l	3858180	4	13.678	3112210	50.0
Naphthalene, 1-...	16.620	100.5	ug/l	6255600	4	13.678	3112210	50.0