

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
 Data File : VN068310.D
 Acq On : 25 Aug 2021 19:45
 Operator : JC/MD
 Sample : M3529-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31115

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: VN068310.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	830	858	899	rBV2	491258	1490277	1.66%	0.639%
2	8.088	2261	2274	2302	rVB2	818335	1852454	2.06%	0.794%
3	8.458	2384	2412	2436	rBV3	991504	2749067	3.05%	1.179%
4	8.971	2584	2603	2624	rBV	1055776	2182963	2.43%	0.936%
5	10.068	2993	3012	3036	rBV	1238266	2276482	2.53%	0.976%
6	10.287	3066	3094	3105	rBV2	601417	1595618	1.77%	0.684%
7	10.443	3136	3152	3164	rBV	1575891	2918236	3.24%	1.251%
8	10.507	3164	3176	3206	rVB	2484931	4675808	5.20%	2.005%
9	11.146	3399	3414	3429	rBV	2353065	4249147	4.72%	1.822%
10	11.223	3429	3443	3459	rVV	2839203	5414467	6.02%	2.321%
11	11.746	3623	3638	3648	rBV	1684423	3076102	3.42%	1.319%
12	11.915	3688	3701	3707	rVV2	2915630	5051799	5.61%	2.166%
13	11.950	3709	3714	3734	rVB	3367110	5690924	6.32%	2.440%
14	12.055	3737	3753	3782	rBV	3546683	6883305	7.65%	2.951%
15	12.288	3825	3840	3854	rBV4	2970088	6100205	6.78%	2.615%
16	12.530	3917	3930	3941	rBV2	1400524	2575047	2.86%	1.104%
17	12.589	3943	3952	3990	rVB5	768933	1777485	1.97%	0.762%
18	12.733	3992	4006	4017	rBV	1491400	2563732	2.85%	1.099%
19	12.792	4017	4028	4044	rVB	887001	1553928	1.73%	0.666%
20	12.924	4064	4077	4089	rBV	818904	1407968	1.56%	0.604%
21	13.055	4118	4126	4138	rVB4	874563	1535045	1.71%	0.658%
22	13.155	4142	4163	4176	rVB2	1042542	2241013	2.49%	0.961%
23	13.230	4177	4191	4208	rVB4	651652	1361910	1.51%	0.584%
24	13.323	4209	4226	4232	rBV3	707927	1483595	1.65%	0.636%
25	13.369	4234	4243	4253	rVV	2636857	4778172	5.31%	2.048%
26	13.417	4255	4261	4273	rVV	1351829	2199052	2.44%	0.943%
27	13.677	4345	4358	4364	rBV	2011168	3464064	3.85%	1.485%
28	13.879	4423	4433	4467	rVB2	805670	1984864	2.21%	0.851%
29	14.058	4471	4500	4517	rBV	20647636	34554439	38.39%	14.814%
30	14.423	4623	4636	4660	rBV4	1119967	2364593	2.63%	1.014%
31	14.581	4687	4695	4722	rVB4	460842	1096837	1.22%	0.470%
32	14.922	4808	4822	4836	rBV4	598115	1356699	1.51%	0.582%
33	14.997	4837	4850	4865	rVV	2281725	3865551	4.30%	1.657%
34	15.083	4868	4882	4901	rVB	3093970	5617929	6.24%	2.408%
35	15.187	4908	4921	4934	rBV3	450035	978472	1.09%	0.419%
36	15.509	5015	5041	5059	rBV2	44386581	89999989	100.00%	38.583%

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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	1580324	3532780	3.93%	1.515%
38	16.620	5439	5455	5478	rVB	2138133	4763104	5.29%	2.042%

Sum of corrected areas: 233263122

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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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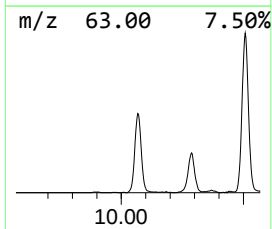
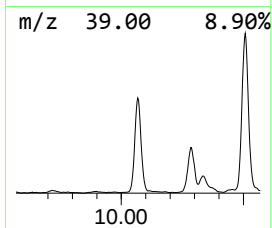
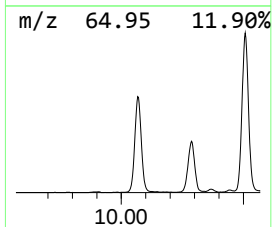
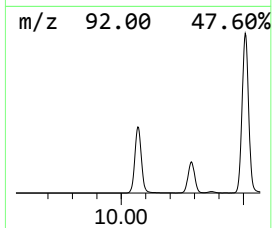
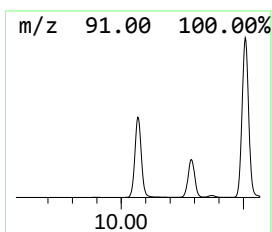
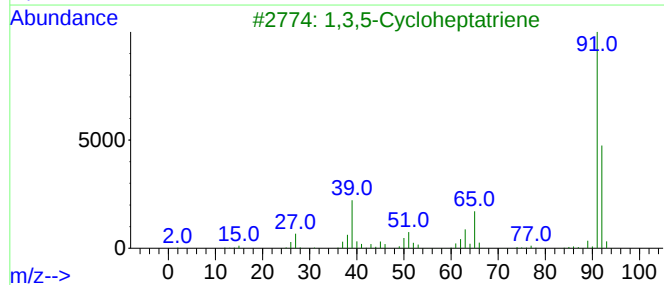
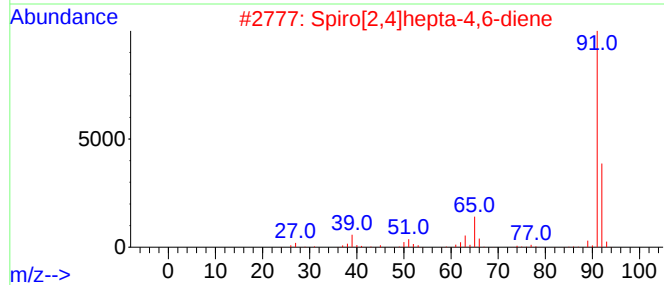
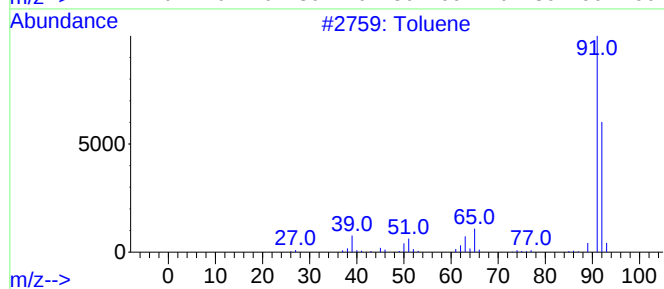
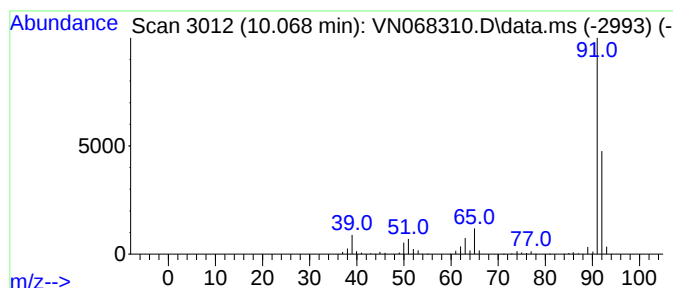
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.068	52.14 ug/l	2276480	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	91
2			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	91
3			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
4			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	80
5			Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	72



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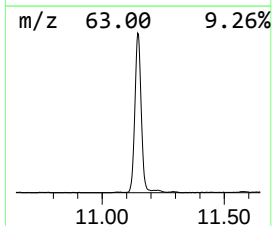
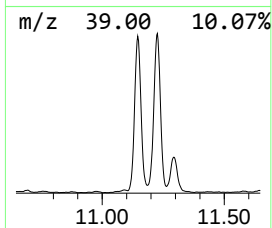
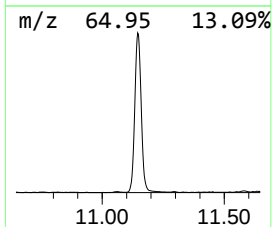
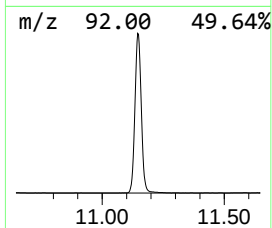
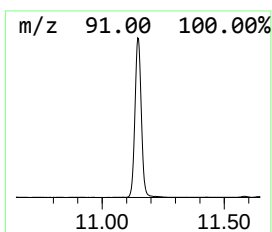
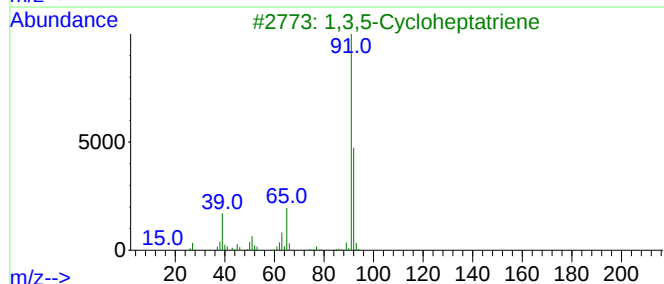
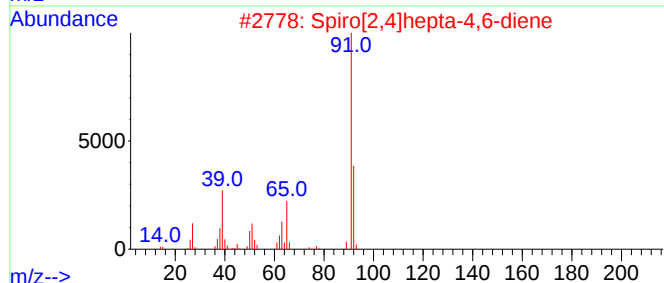
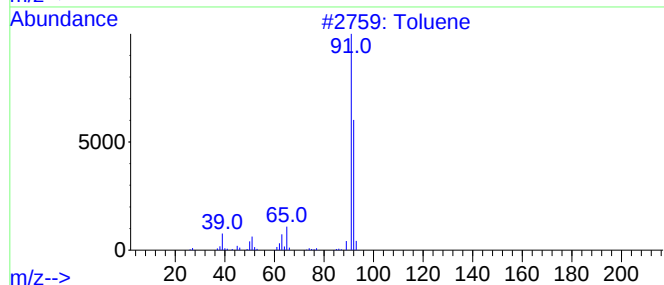
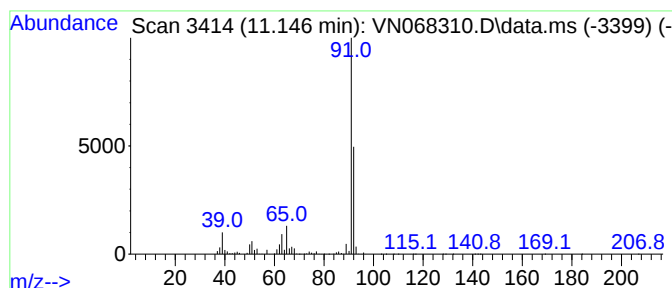
Instrument :
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ClientSampleId :
31115

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
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TIC Library : C:\Database\NIST20.L
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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	69.07 ug/l	4249150	Chlorobenzene-d5	11.746	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	94
2	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
3	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
4	2,5-Norbornadiene	92	C7H8	000121-46-0	80
5	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	72



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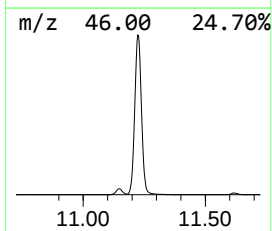
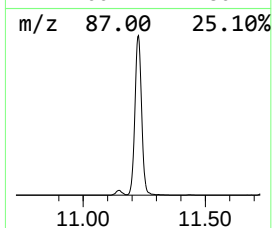
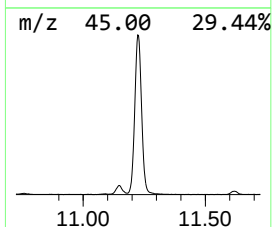
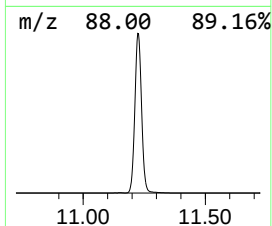
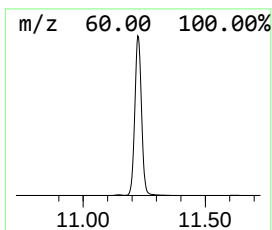
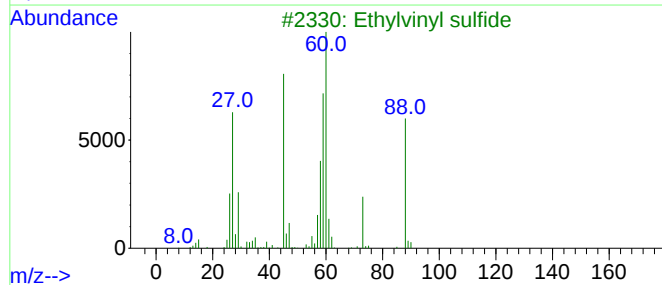
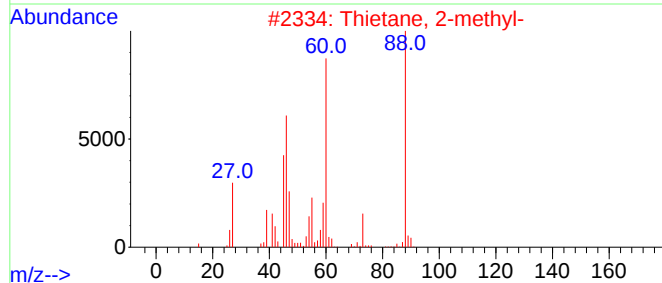
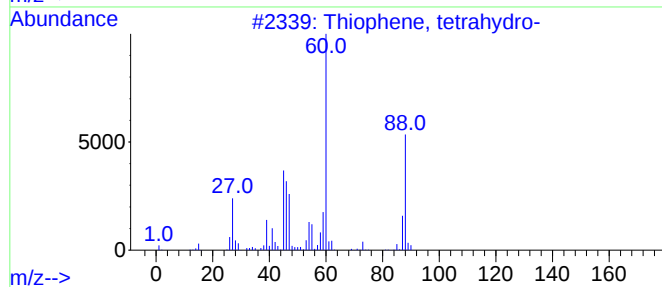
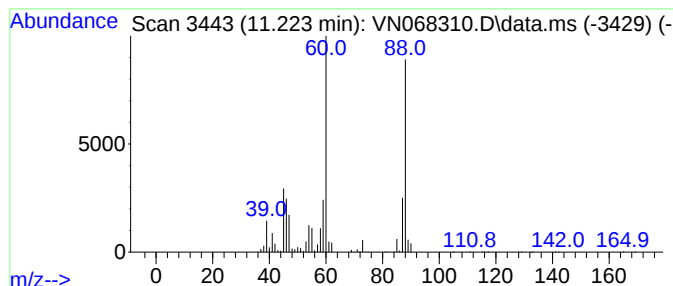
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.224	88.01 ug/l	5414470	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			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25



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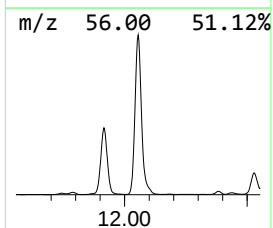
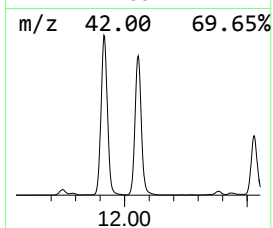
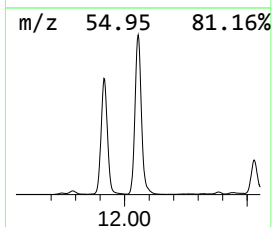
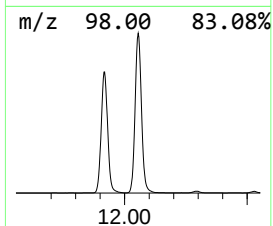
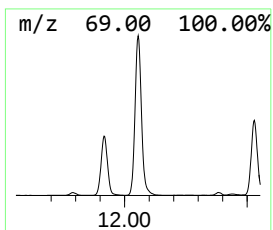
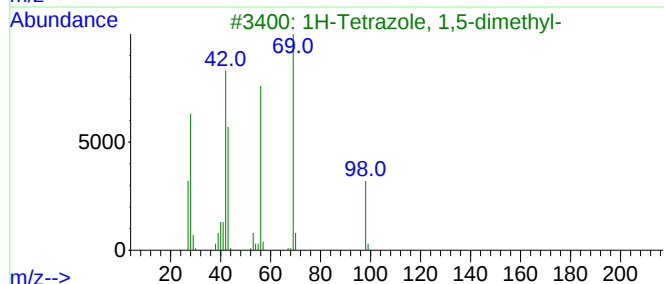
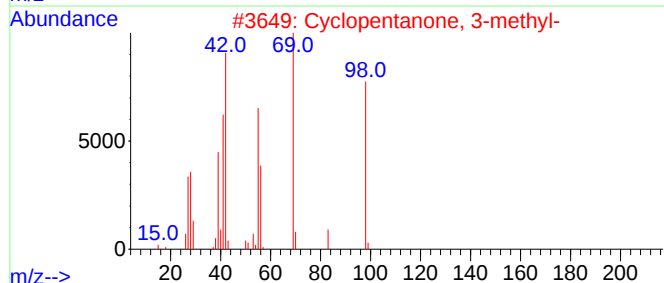
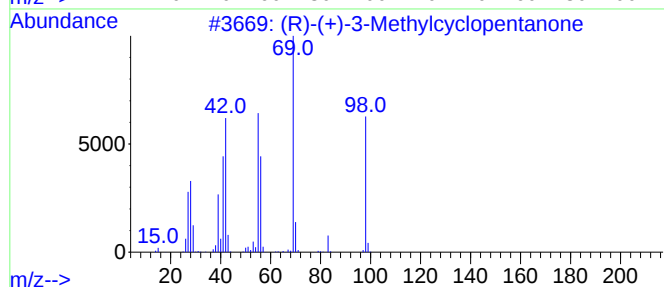
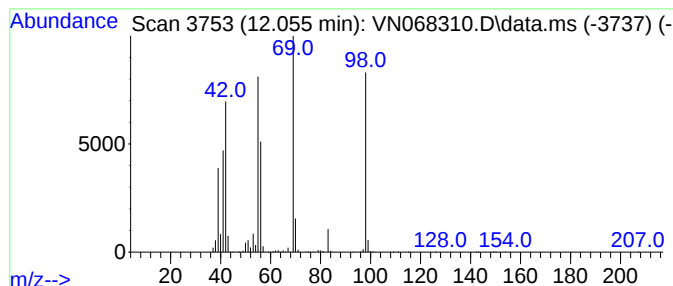
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 (R)-(+)-3-Methylcyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.055	111.88 ug/l	6883310	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	53
4	Cyclopentanone, 2-methyl-		98	C6H10O	001120-72-5	43
5	(Z)-4-Methyl-2-hexene		98	C7H14	003683-19-0	43



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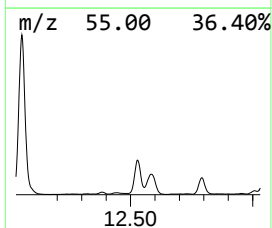
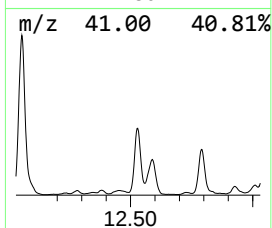
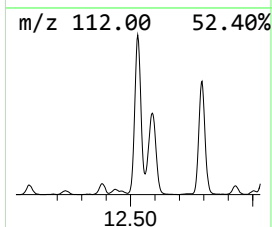
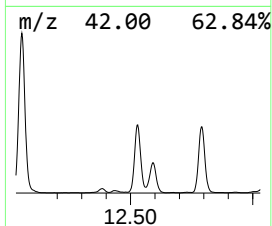
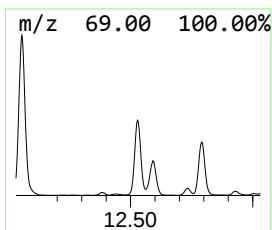
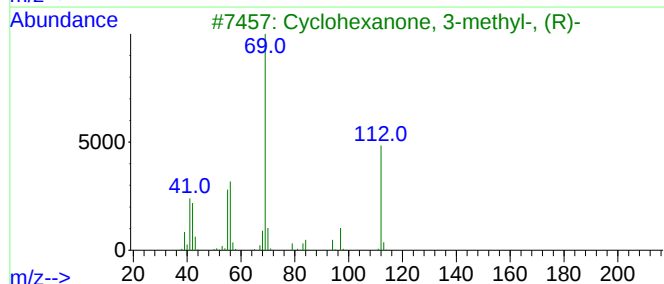
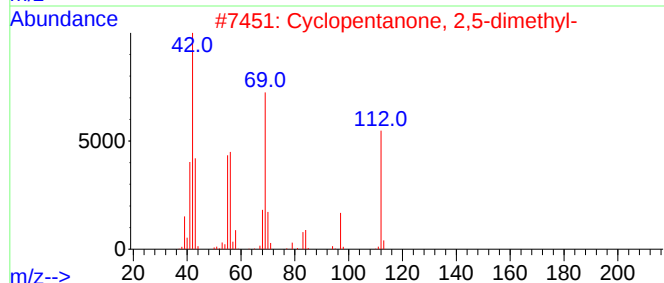
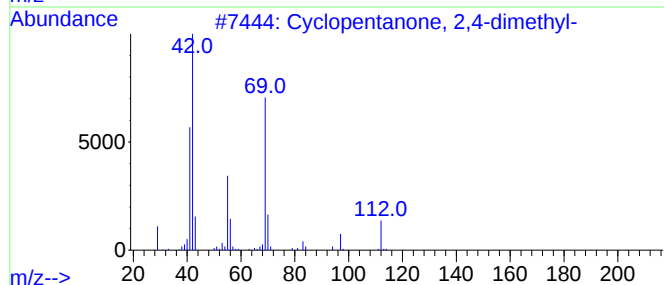
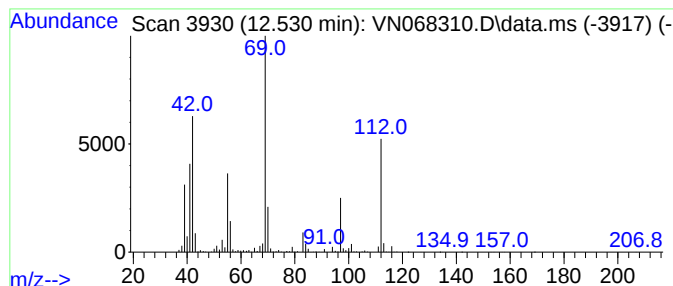
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.530	41.86 ug/l	2575050	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			Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	53
4			trans-3,4-Dimethylcyclopentanone	112	C7H12O	019550-73-3	53
5			1,2,4-Cyclopentanetrione	112	C5H4O3	015849-14-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068310.D
Acq On : 25 Aug 2021 19:45
Operator : JC/MD
Sample : M3529-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31115

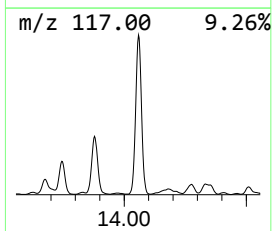
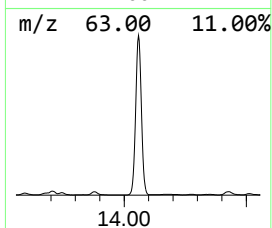
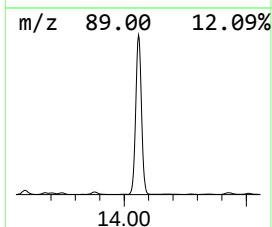
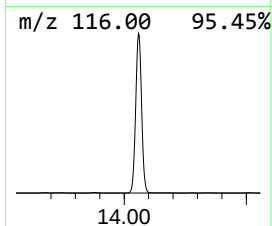
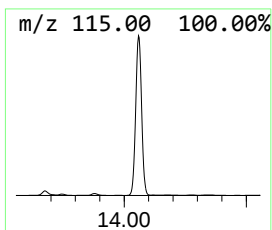
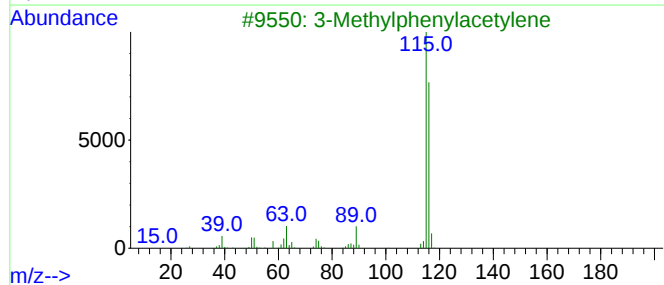
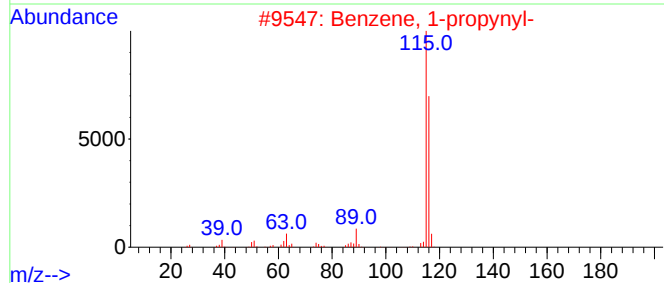
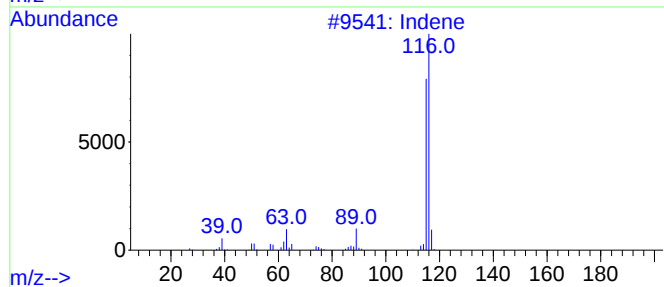
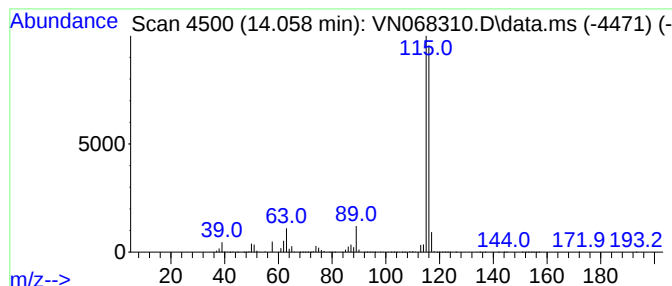
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Quant Title : SW846 8260

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	498.76 ug/l	34554400	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			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 : VN068310.D
Acq On : 25 Aug 2021 19:45
Operator : JC/MD
Sample : M3529-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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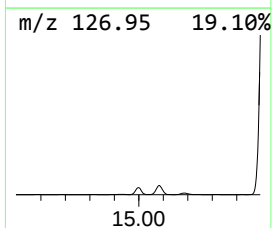
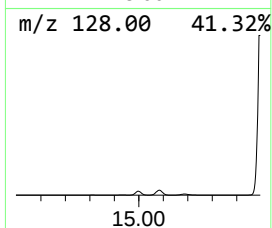
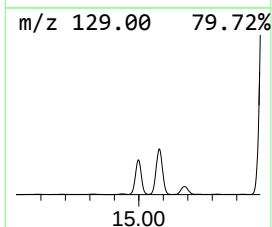
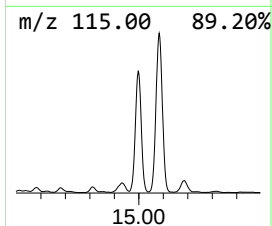
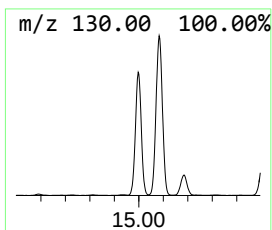
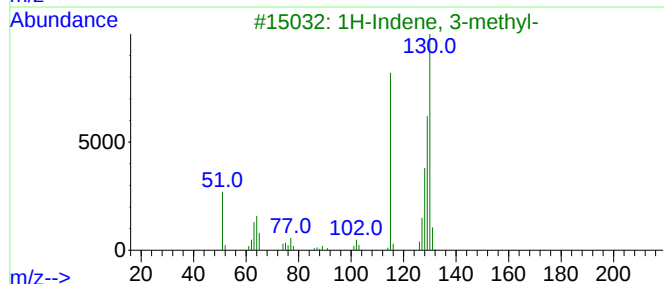
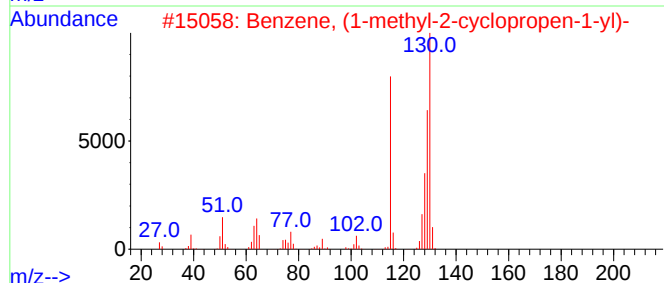
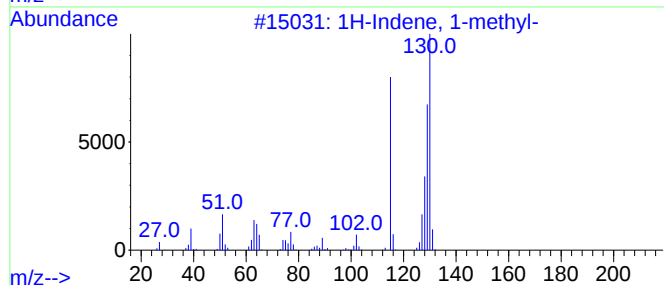
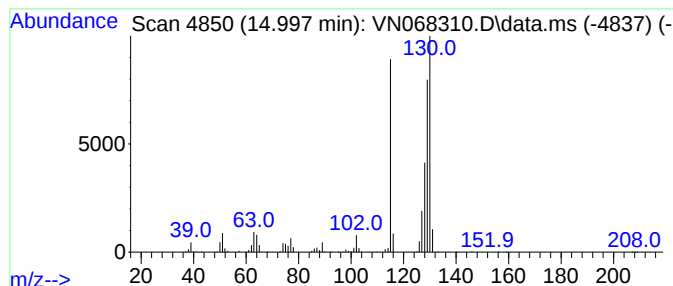
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Quant Title : SW846 8260

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	55.80 ug/l	3865550	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	93
2			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	91
3			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	91
4			2-Methylindene	130	C10H10	002177-47-1	91
5			Benzene, 1-butynyl-	130	C10H10	000622-76-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068310.D
Acq On : 25 Aug 2021 19:45
Operator : JC/MD
Sample : M3529-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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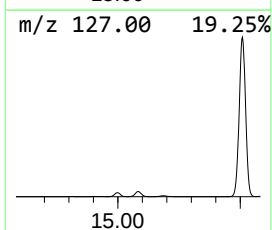
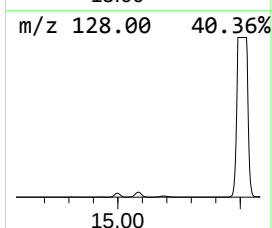
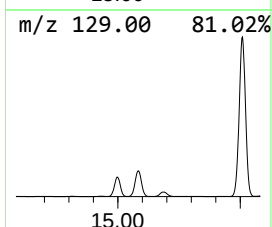
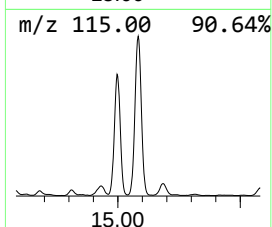
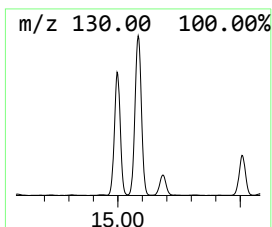
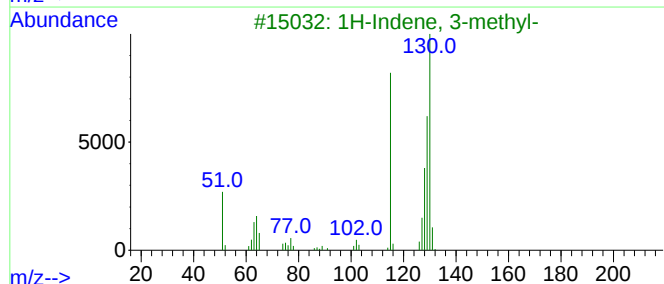
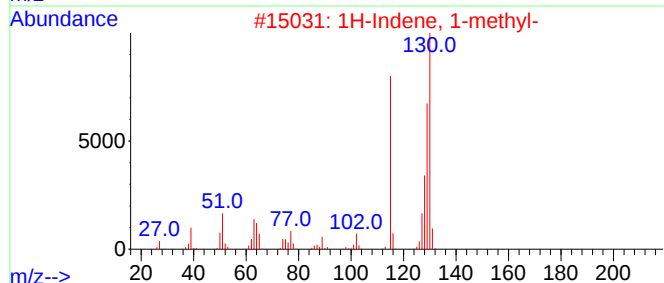
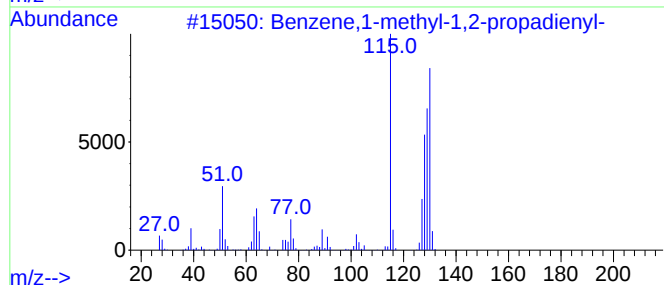
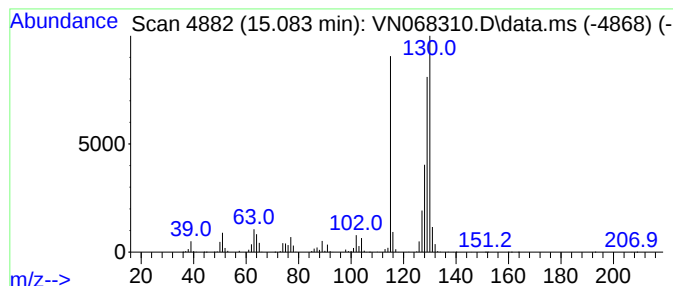
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Quant Title : SW846 8260

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

Peak Number 8 Benzene,1-methyl-1,2-propad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.083	81.09 ug/l	5617930	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		1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93
4		Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	91
5		2-Methylindene	130	C10H10	002177-47-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068310.D
Acq On : 25 Aug 2021 19:45
Operator : JC/MD
Sample : M3529-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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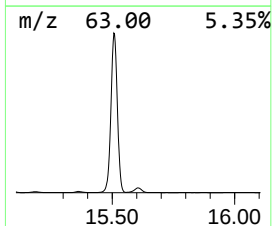
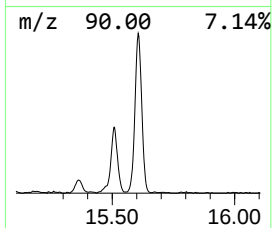
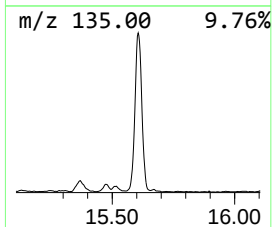
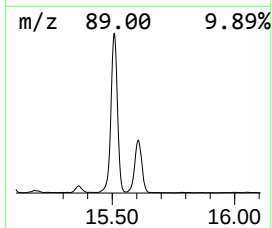
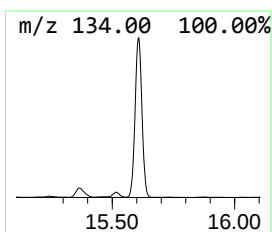
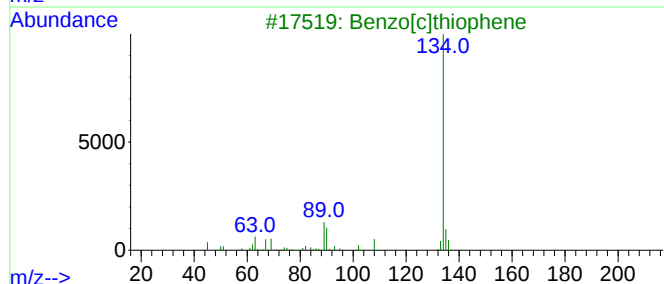
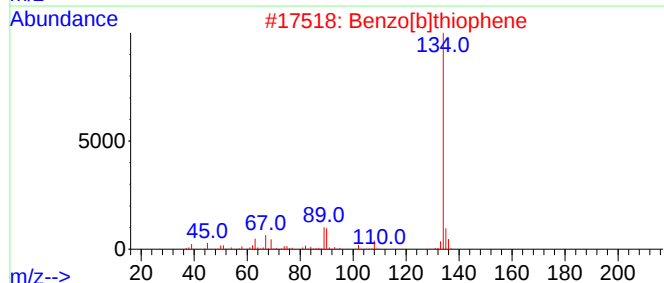
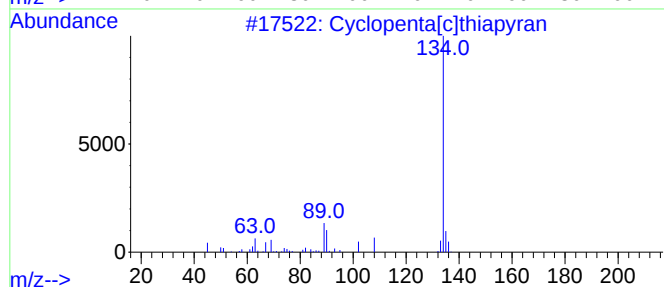
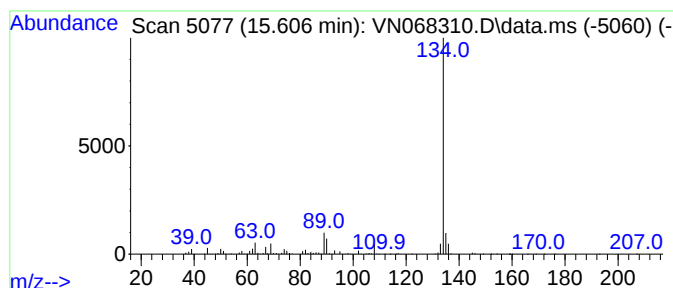
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopenta[c]thiapyran Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.606	50.99 ug/l	3532780	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	91
3			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
4			[1]Benzothieno[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 : VN068310.D
Acq On : 25 Aug 2021 19:45
Operator : JC/MD
Sample : M3529-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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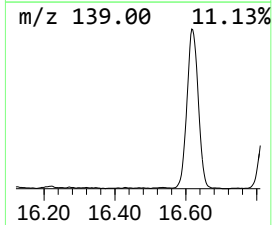
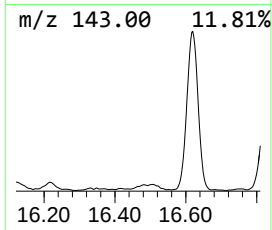
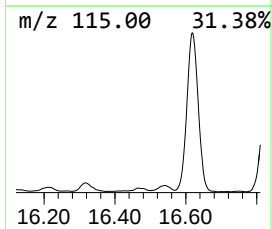
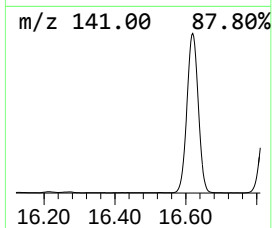
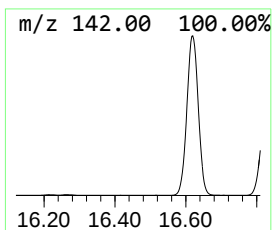
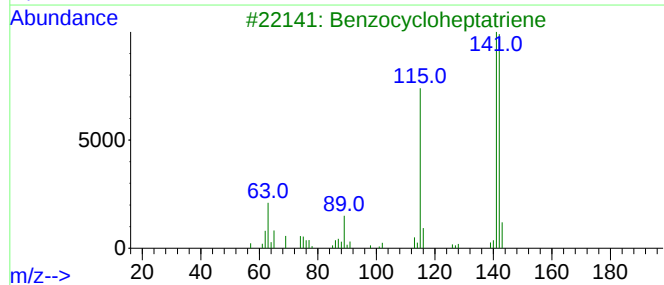
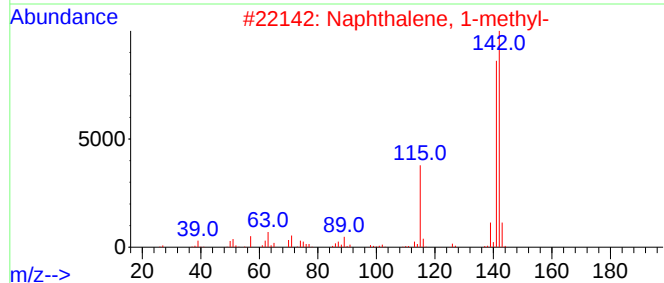
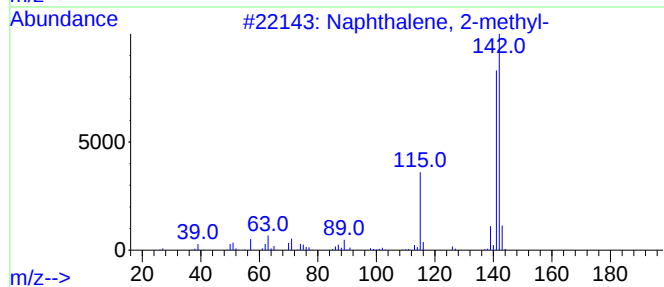
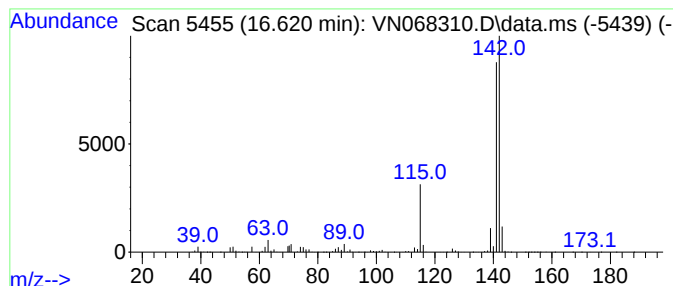
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.620	68.75 ug/l	4763100	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082521\
Data File : VN068310.D
Acq On : 25 Aug 2021 19:45
Operator : JC/MD
Sample : M3529-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31115

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
Spiro[2,4]hepta...	10.068	52.1	ug/l	2276480	2	8.971	2182960	50.0
1,3,5-Cyclohept...	11.146	69.1	ug/l	4249150	3	11.746	3076100	50.0
Thiophene, tetr...	11.224	88.0	ug/l	5414470	3	11.746	3076100	50.0
(R)-(+)-3-Methy...	12.055	111.9	ug/l	6883310	3	11.746	3076100	50.0
Cyclopentanone,...	12.530	41.9	ug/l	2575050	3	11.746	3076100	50.0
Indene	14.058	498.8	ug/l	34554400	4	13.678	3464060	50.0
1H-Indene, 1-me...	14.997	55.8	ug/l	3865550	4	13.678	3464060	50.0
Benzene,1-methy...	15.083	81.1	ug/l	5617930	4	13.678	3464060	50.0
Cyclopenta[c]th...	15.606	51.0	ug/l	3532780	4	13.678	3464060	50.0
Naphthalene, 1-...	16.620	68.8	ug/l	4763100	4	13.678	3464060	50.0