

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073539.D
 Acq On : 20 Jul 2022 22:13
 Operator : JC\MD
 Sample : N3779-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-E

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	56	62	77	rBV	160752	704672	6.72%	1.658%
2	3.640	286	298	318	rBV	1994998	5129467	48.90%	12.072%
3	4.222	387	397	408	rBV	109215	324699	3.10%	0.764%
4	4.510	431	446	456	rBV3	33049	128049	1.22%	0.301%
5	7.951	1020	1031	1036	rBV	215463	516511	4.92%	1.216%
6	8.016	1036	1042	1052	rVB	396239	886355	8.45%	2.086%
7	8.381	1091	1104	1116	rBV2	410513	1174843	11.20%	2.765%
8	8.904	1184	1193	1206	rBV	557783	1162395	11.08%	2.736%
9	10.381	1433	1444	1450	rBV	763999	1429590	13.63%	3.365%
10	10.445	1450	1455	1468	rVB	443605	812265	7.74%	1.912%
11	10.698	1490	1498	1506	rBV	172093	313092	2.98%	0.737%
12	11.086	1557	1564	1570	rBV3	88997	193837	1.85%	0.456%
13	11.163	1570	1577	1591	rVB	758453	1444343	13.77%	3.399%
14	11.686	1655	1666	1670	rBV	827886	1523536	14.52%	3.586%
15	11.727	1670	1673	1679	rVV	292671	535032	5.10%	1.259%
16	11.780	1679	1682	1692	rVV	91079	197895	1.89%	0.466%
17	11.892	1693	1701	1711	rVB	396935	744635	7.10%	1.752%
18	12.027	1716	1724	1737	rBV2	155299	320255	3.05%	0.754%
19	12.222	1752	1757	1765	rVB2	362010	642141	6.12%	1.511%
20	12.463	1792	1798	1803	rVV2	109524	216080	2.06%	0.509%
21	12.674	1824	1834	1845	rBV	728144	1345471	12.83%	3.167%
22	12.951	1869	1881	1885	rBV2	168502	398209	3.80%	0.937%
23	12.998	1885	1889	1894	rVV	81755	142962	1.36%	0.336%
24	13.086	1894	1904	1914	rVV5	63413	330638	3.15%	0.778%
25	13.163	1914	1917	1926	rVB3	61762	122651	1.17%	0.289%
26	13.304	1934	1941	1948	rBV3	299464	613515	5.85%	1.444%
27	13.498	1956	1974	1986	rBV6	154150	727070	6.93%	1.711%
28	13.616	1987	1994	2005	rVV2	1008034	2111244	20.13%	4.969%
29	13.710	2005	2010	2017	rVB3	88343	153790	1.47%	0.362%
30	13.816	2022	2028	2032	rBV2	70223	125085	1.19%	0.294%
31	13.998	2053	2059	2066	rVV	343469	629551	6.00%	1.482%
32	14.098	2067	2076	2083	rVV5	46872	149980	1.43%	0.353%
33	14.363	2115	2121	2125	rBV3	63895	131908	1.26%	0.310%
34	14.857	2198	2205	2213	rBV2	72250	197449	1.88%	0.465%
35	15.016	2227	2232	2237	rBV2	59951	116961	1.12%	0.275%
36	15.433	2289	2303	2314	rBV	5473960	10489520	100.00%	24.687%

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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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Title : SW846 8260

37	15.533	2314	2320	2327	rVB	186648	370714	3.53%	0.872%
38	16.462	2471	2478	2482	rBV2	51558	115074	1.10%	0.271%
39	16.527	2482	2489	2503	rVV	1463779	3305362	31.51%	7.779%
40	16.739	2516	2525	2533	rBV	1100860	2513114	23.96%	5.915%

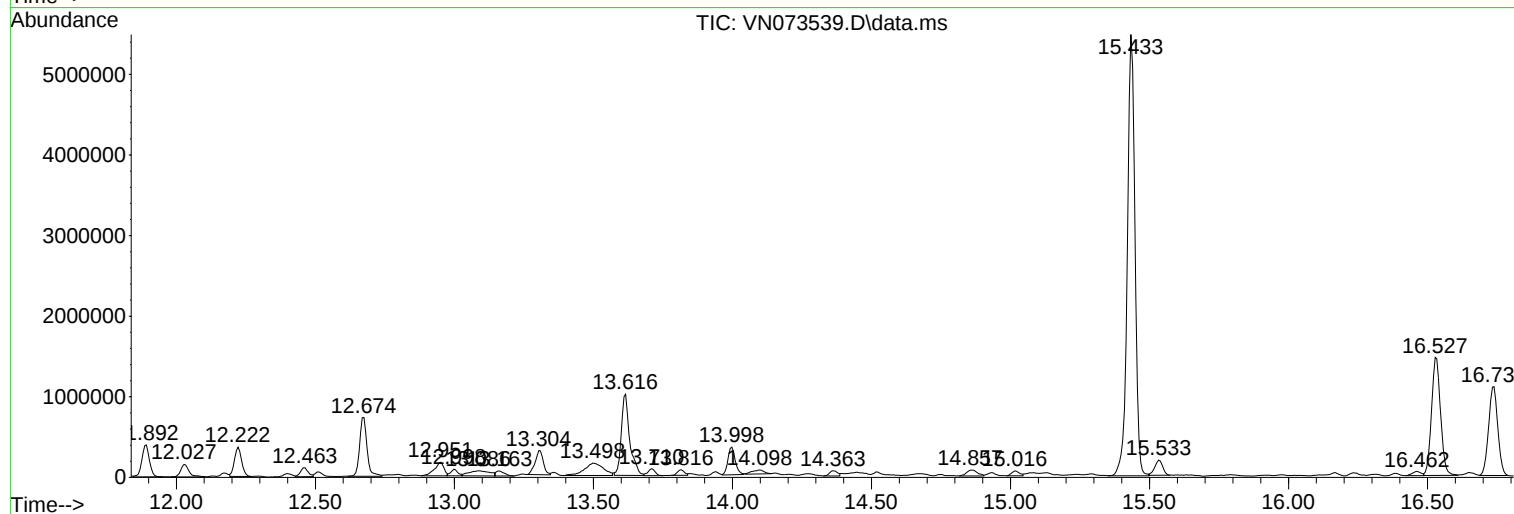
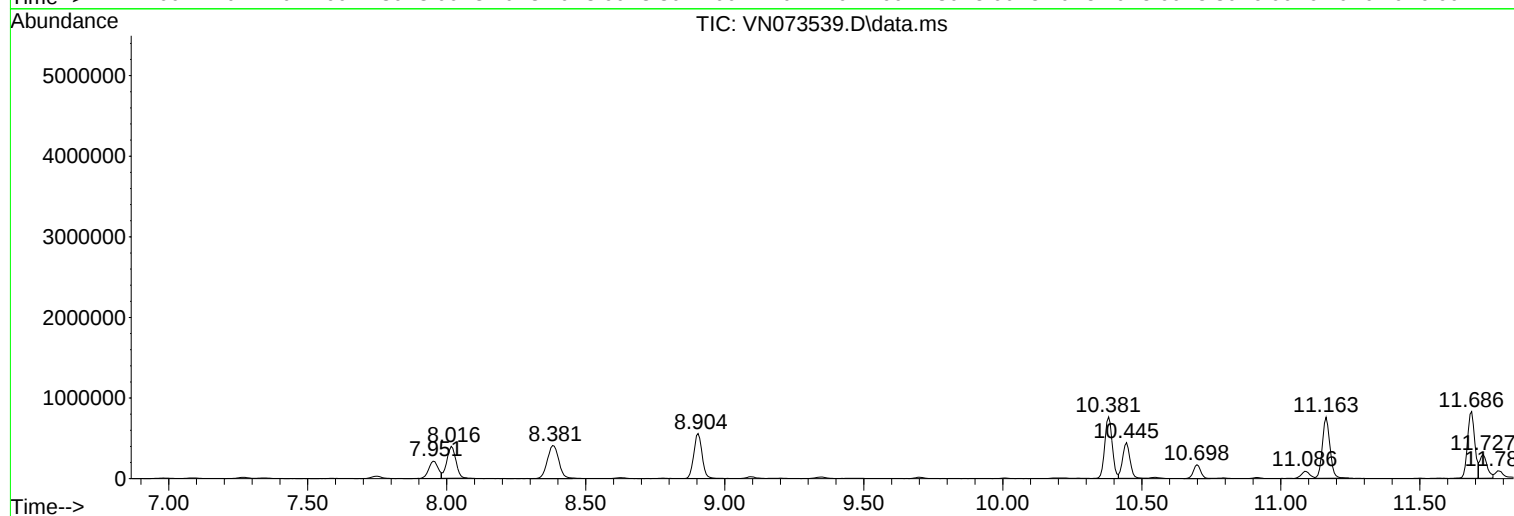
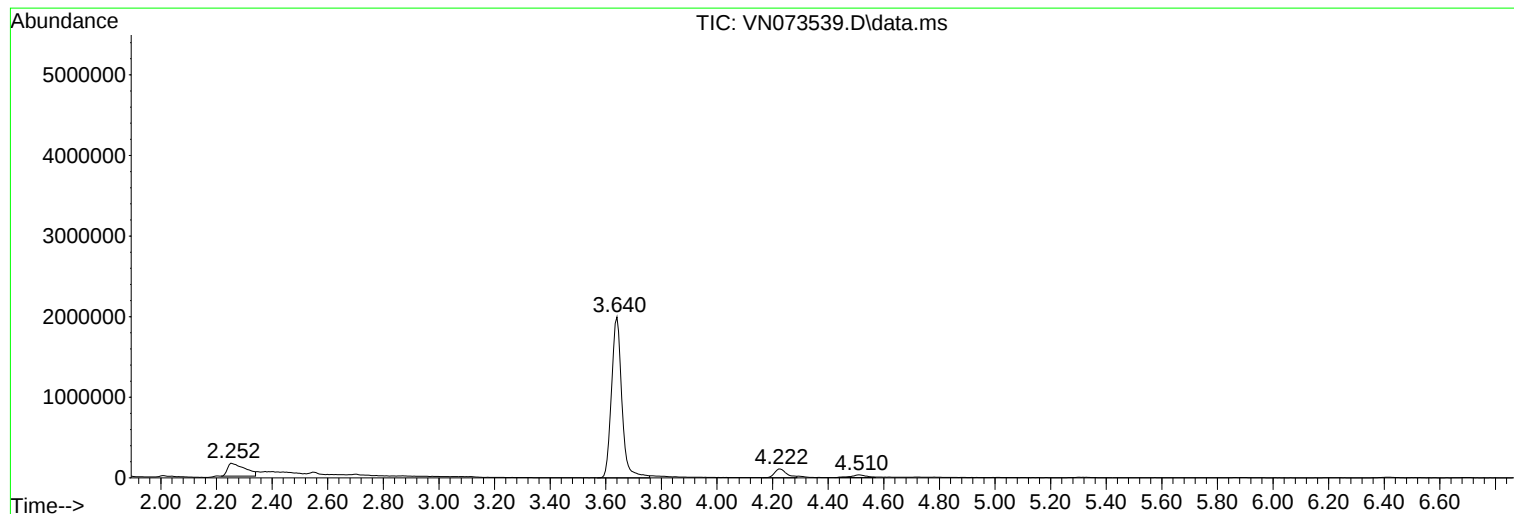
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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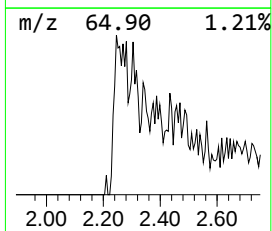
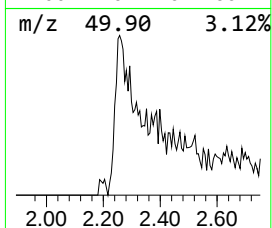
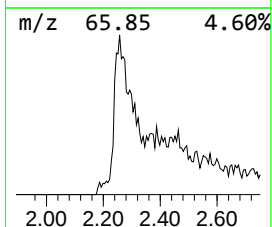
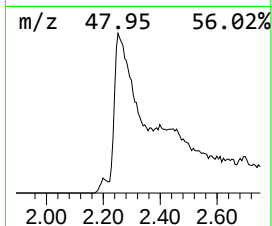
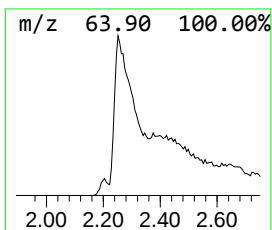
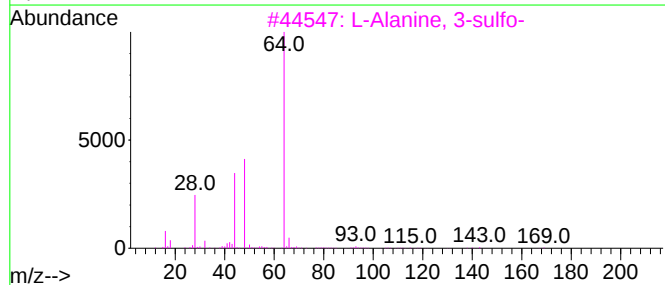
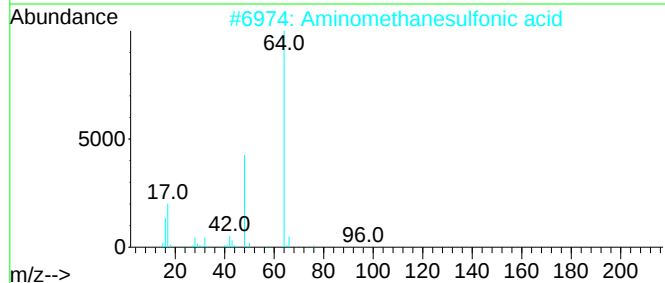
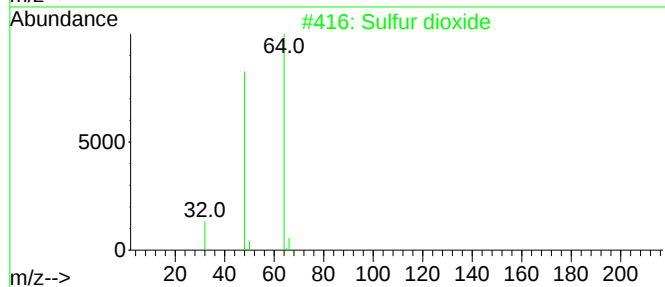
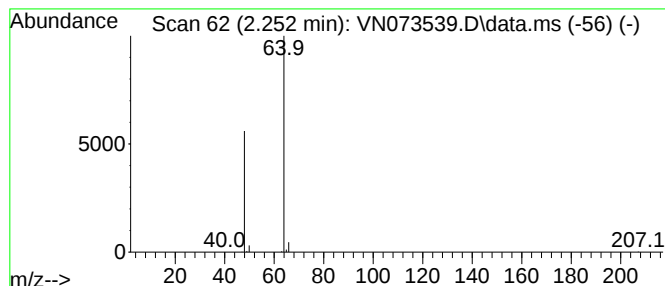
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	39.75 ug/l	704672	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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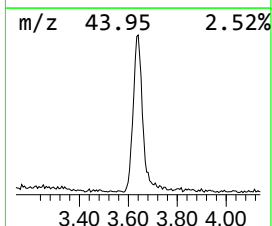
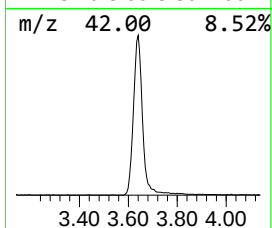
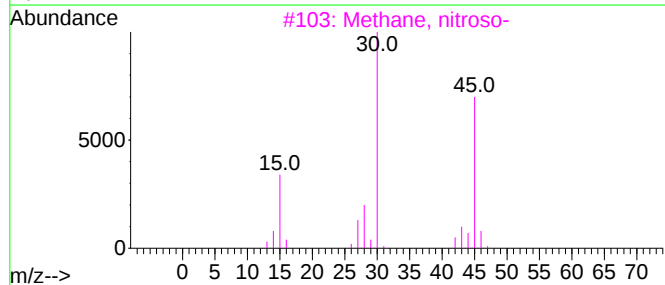
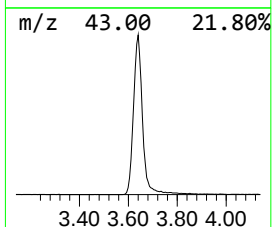
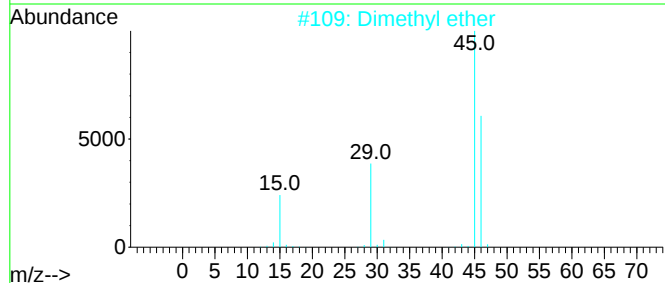
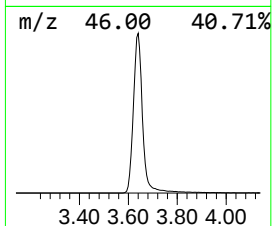
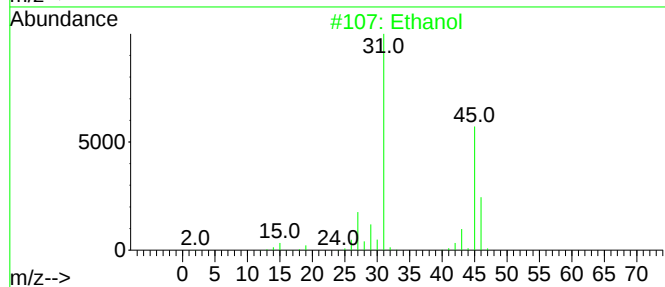
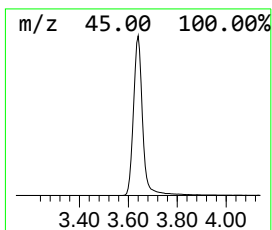
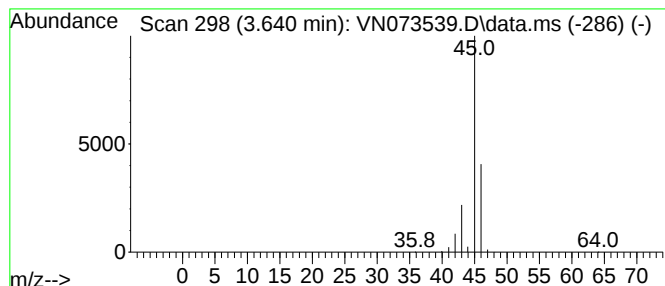
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.640	289.36 ug/l	5129470	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	74
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	Oxalic acid		90	C2H2O4	000144-62-7	4



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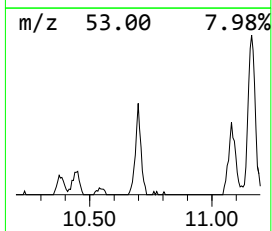
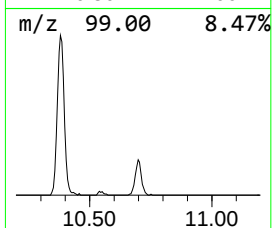
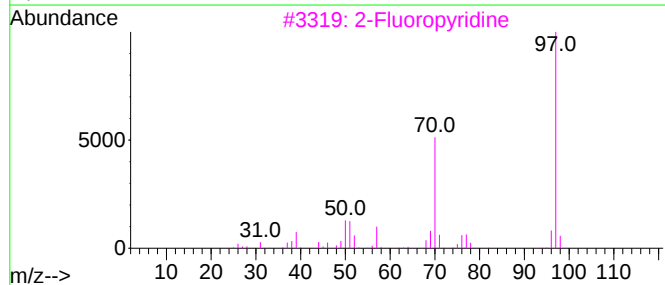
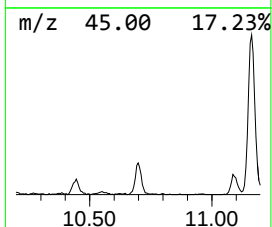
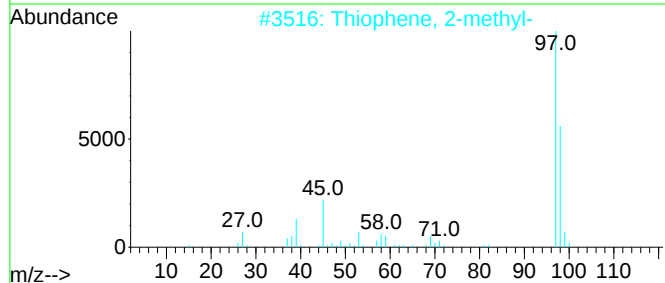
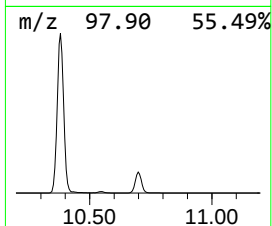
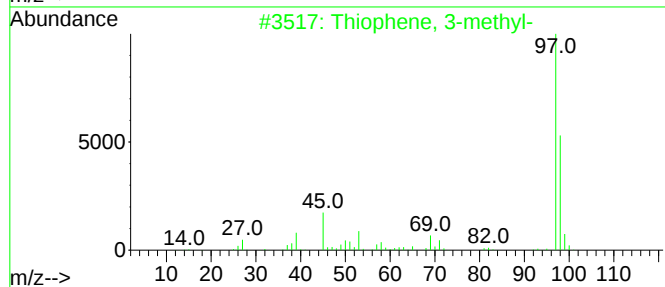
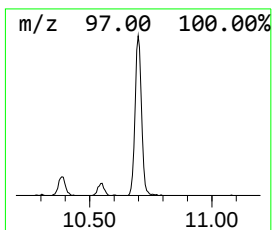
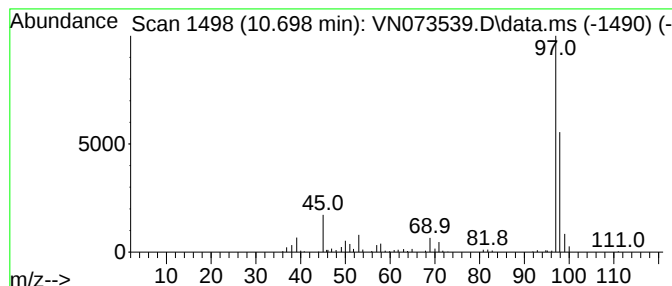
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Thiophene, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.698	10.28 ug/l	313092	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	94
2			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
3			2-Fluoropyridine	97	C5H4FN	000372-48-5	47
4			Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11N03S2	1000267-97-5	42
5			1,2-Ethanediol, 1,2-di-2-furanyl-	194	C10H10O4	004464-77-1	39



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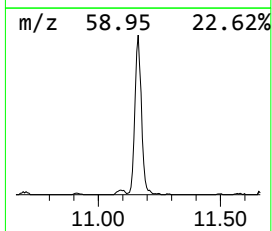
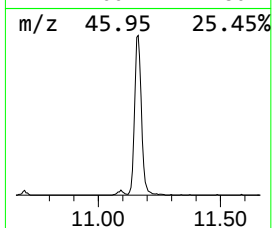
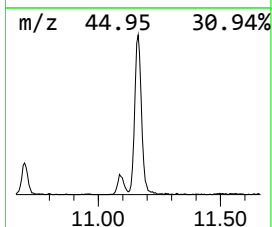
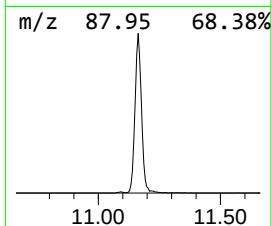
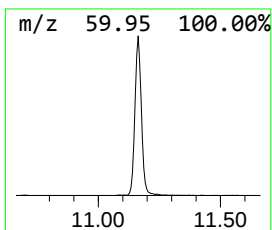
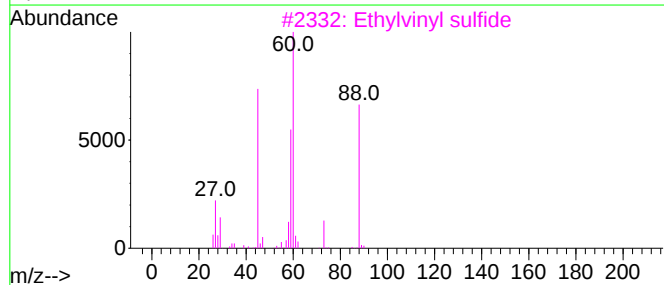
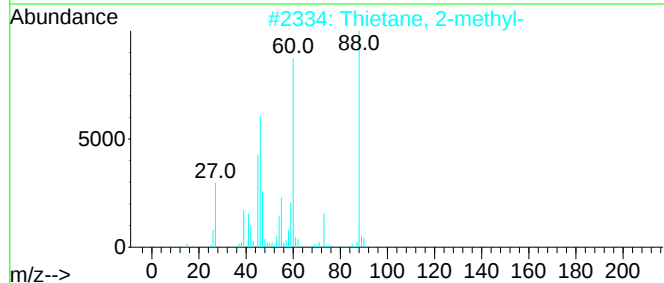
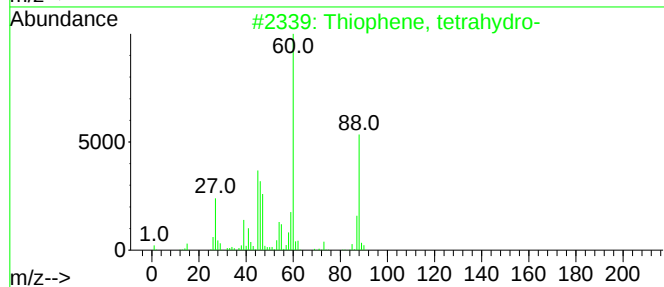
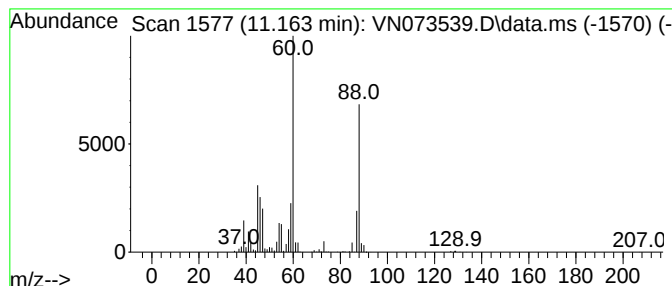
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophene, tetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	47.40 ug/l	1444340	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5			Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	25



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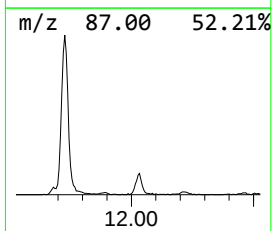
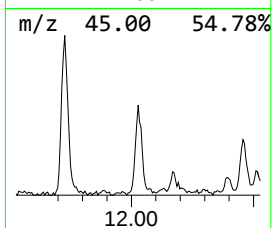
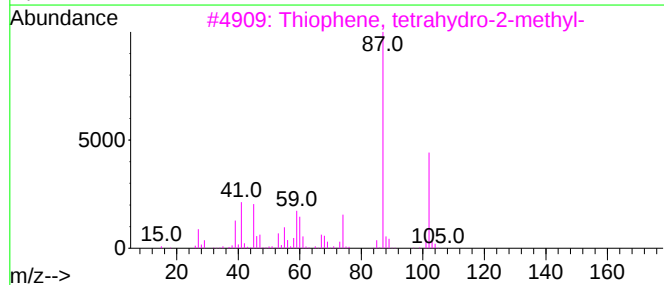
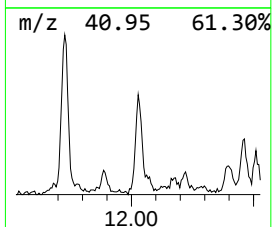
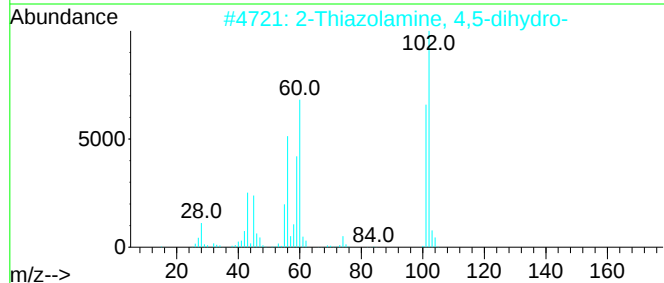
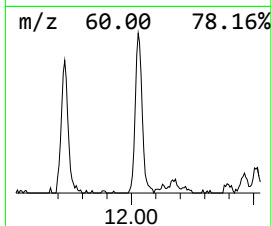
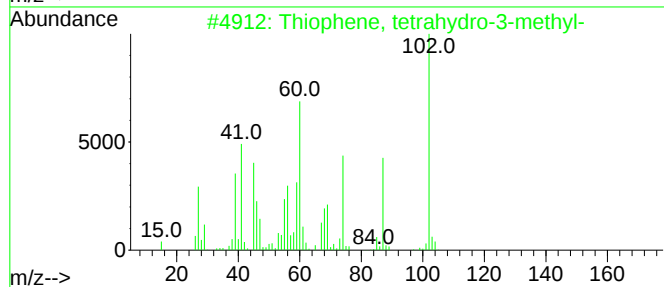
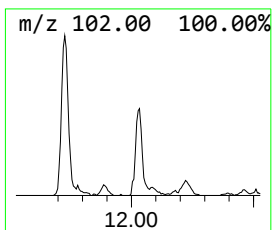
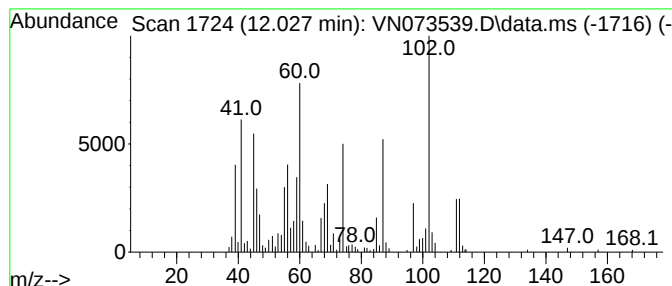
Instrument :
MSVOA_N
ClientSampleId :
070622-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 5 Thiophene, tetrahydro-3-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.028	10.51 ug/l	320255	Chlorobenzene-d5	11.686	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	97
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	49
3	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	30
4	2-Methyl-3-(methylthio)-1-propene	102	C5H10S	052326-10-0	30
5	2-Acetyl-2,3,5,6-tetrahydro-1,4-...	145	C6H11NOS	1000281-47-3	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073539.D
Acq On : 20 Jul 2022 22:13
Operator : JC\MD
Sample : N3779-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-E

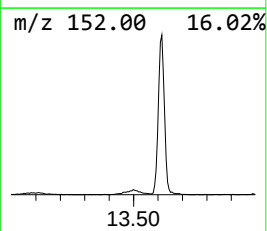
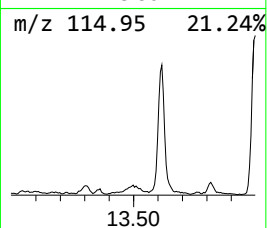
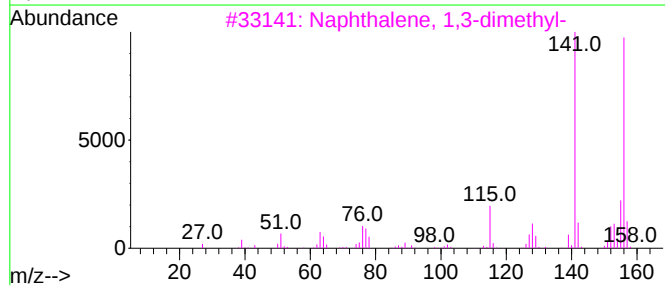
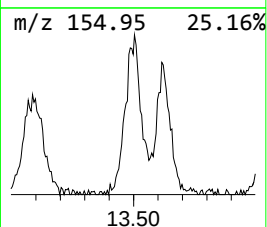
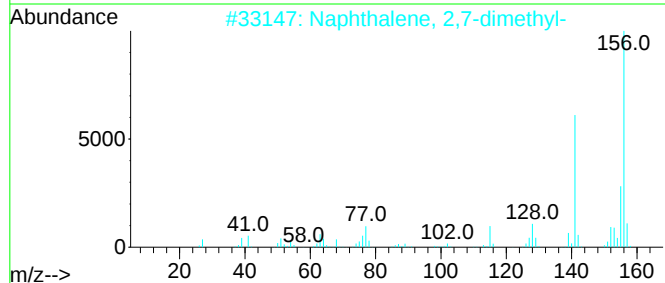
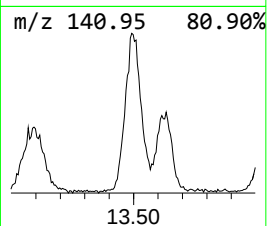
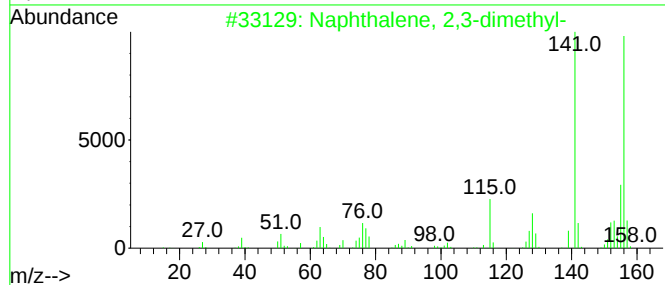
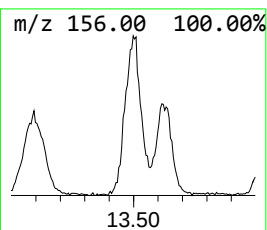
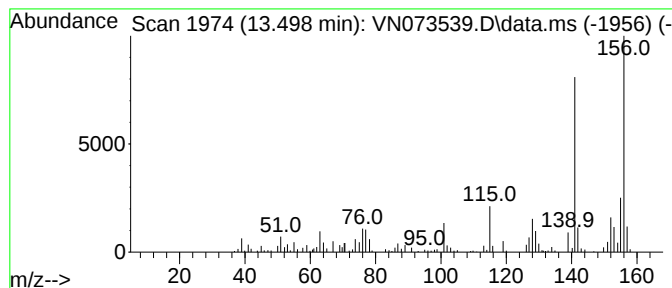
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	17.22 ug/l	727070	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073539.D
Acq On : 20 Jul 2022 22:13
Operator : JC\MD
Sample : N3779-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

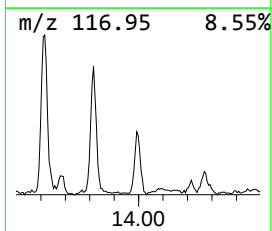
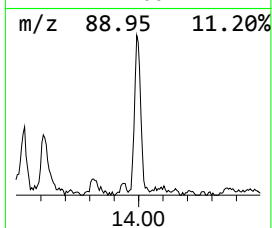
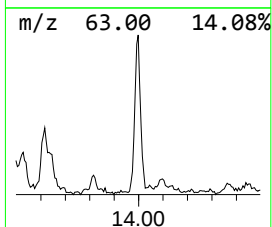
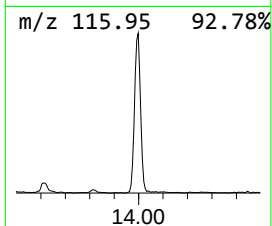
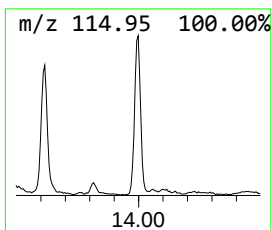
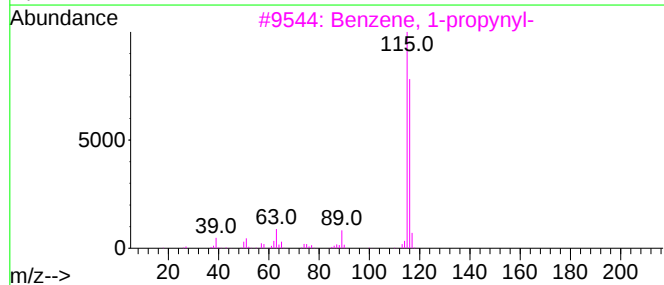
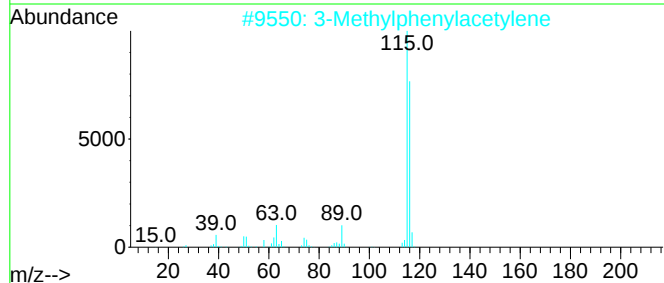
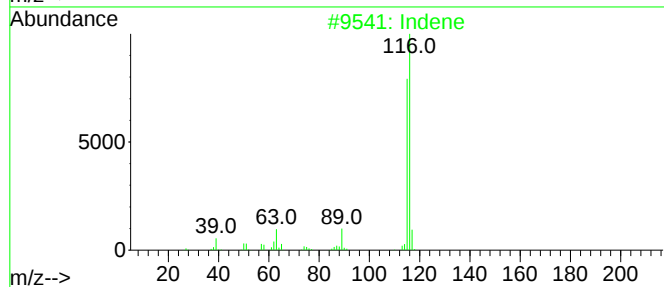
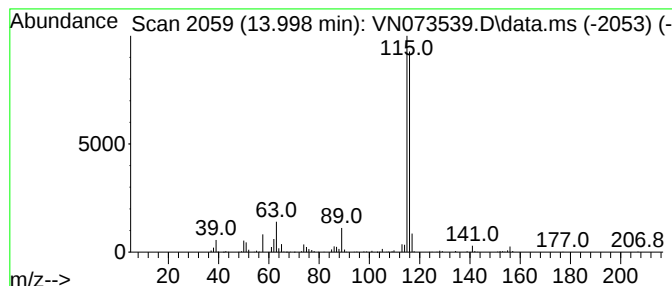
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.998	14.91 ug/l	629551	1,4-Dichlorobenzene-d4			13.616
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	Benzene, 1,2-propadienyl-		116	C9H8	002327-99-3	91
5	2-Methylphenylacetylene		116	C9H8	000766-47-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073539.D
Acq On : 20 Jul 2022 22:13
Operator : JC\MD
Sample : N3779-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-E

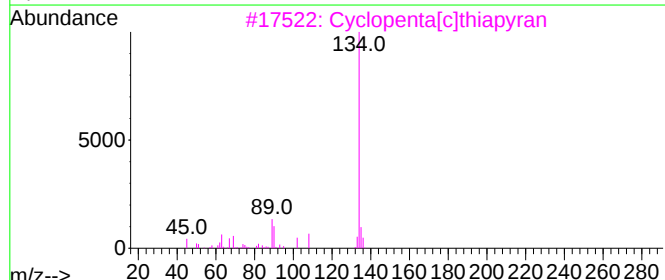
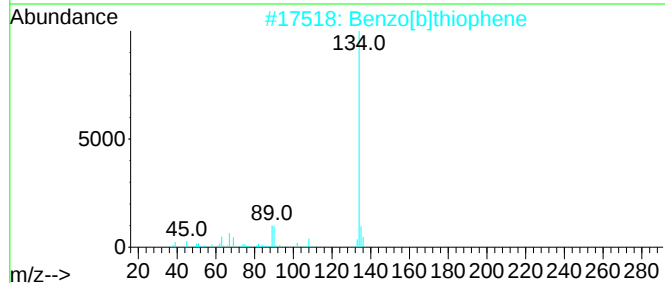
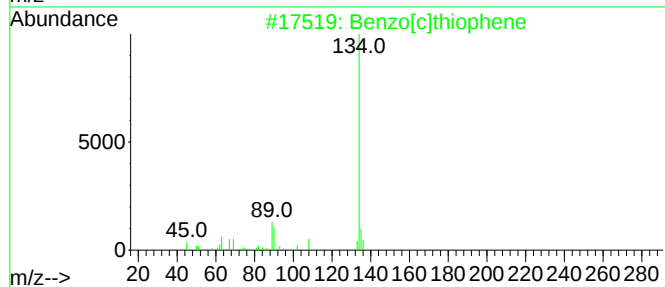
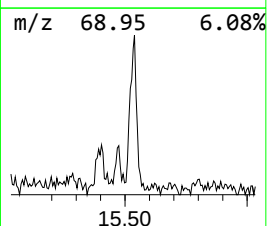
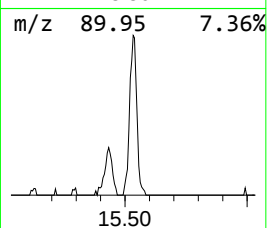
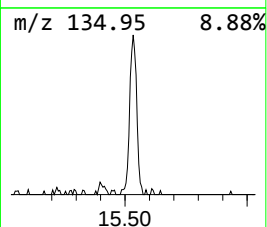
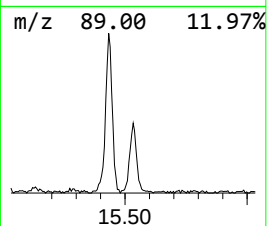
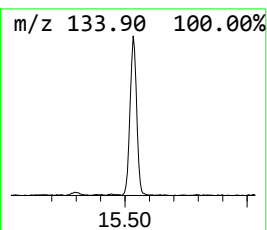
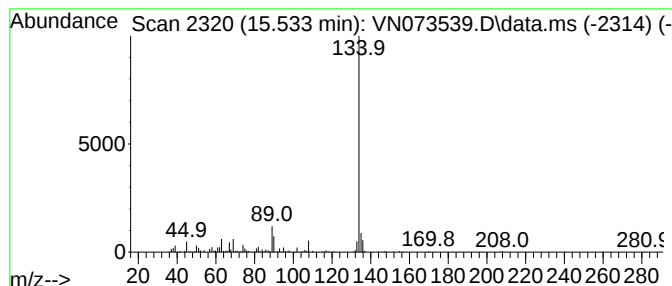
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[c]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	8.78 ug/l	370714	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	93
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	93
4			6-Phenyl-[1,3]thiazine-2,4-dione	205	C10H7N02S	1000300-90-1	64
5			3-Deazaadenine	134	C6H6N4	006811-77-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073539.D
Acq On : 20 Jul 2022 22:13
Operator : JC\MD
Sample : N3779-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-E

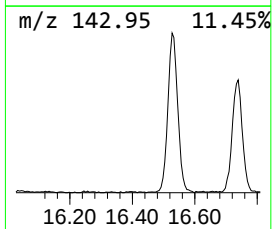
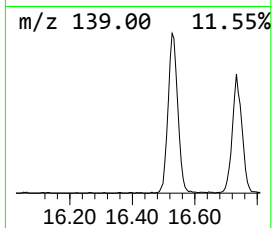
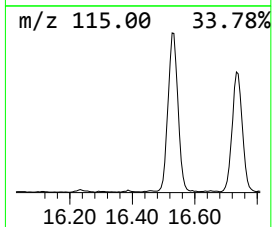
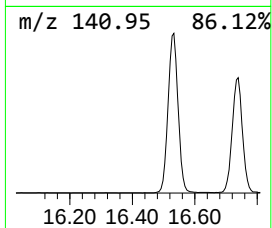
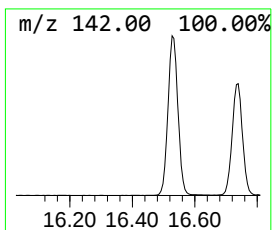
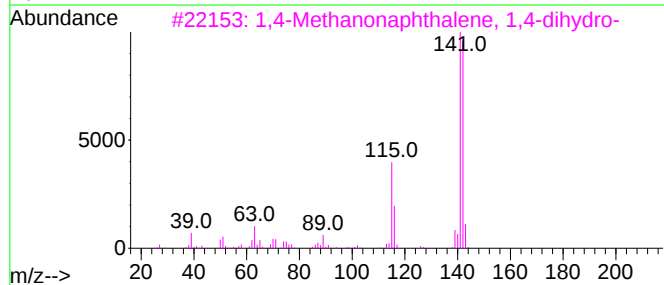
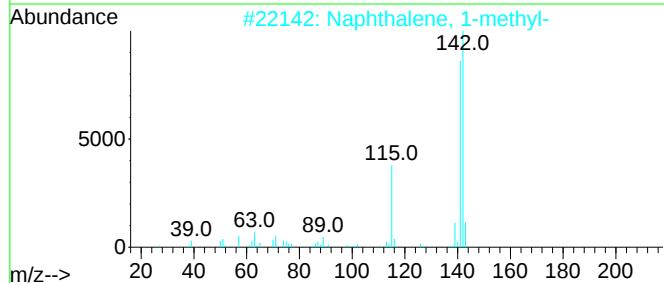
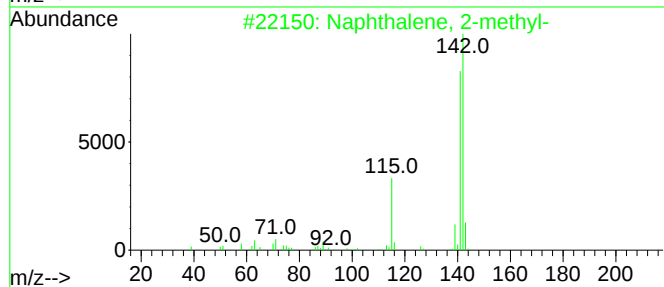
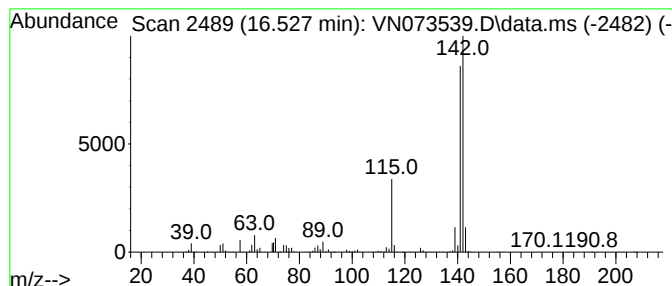
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	78.28 ug/l	3305360	1,4-Dichlorobenzene-d4	13.616

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	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073539.D
Acq On : 20 Jul 2022 22:13
Operator : JC\MD
Sample : N3779-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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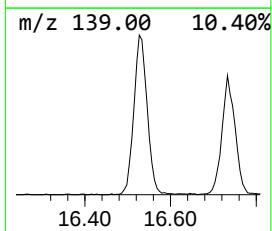
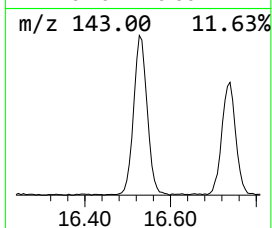
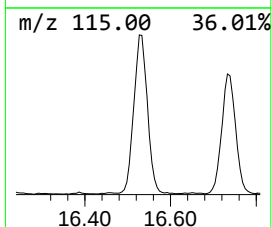
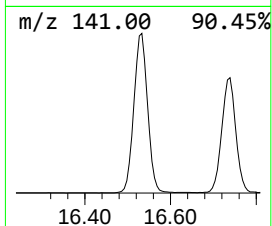
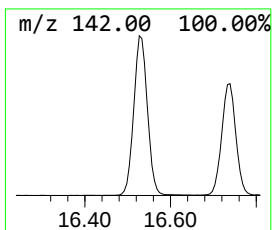
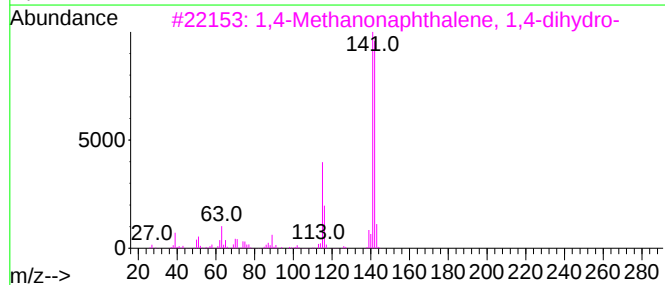
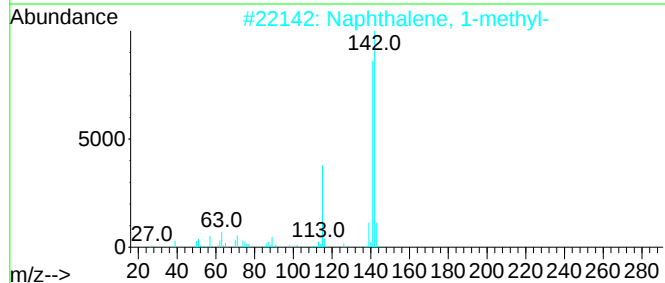
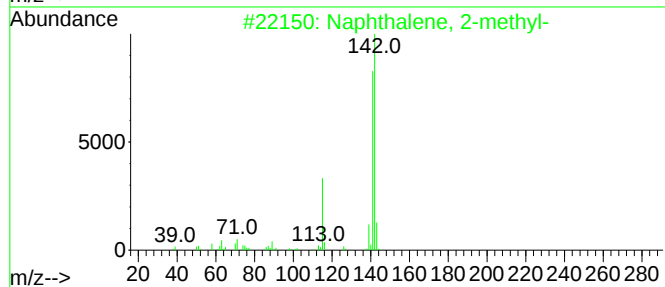
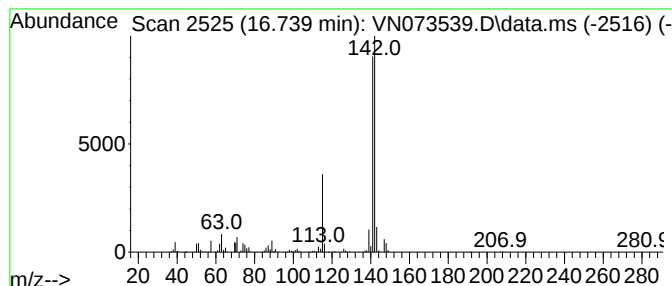
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	59.52 ug/l	2513110	1,4-Dichlorobenzene-d4	13.616

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	93
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90
5		Benzocycloheptatriene	142	C11H10	000264-09-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073539.D
Acq On : 20 Jul 2022 22:13
Operator : JC\MD
Sample : N3779-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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
Sulfur dioxide	2.252	39.8	ug/l	704672	1	8.016	886355	50.0
Ethanol	3.640	289.4	ug/l	5129470	1	8.016	886355	50.0
Thiophene, 3-me...	10.698	10.3	ug/l	313092	3	11.686	1523540	50.0
Thiophene, tetr...	11.163	47.4	ug/l	1444340	3	11.686	1523540	50.0
Thiophene, tetr...	12.028	10.5	ug/l	320255	3	11.686	1523540	50.0
Naphthalene, 2,...	13.498	17.2	ug/l	727070	4	13.616	2111240	50.0
Indene	13.998	14.9	ug/l	629551	4	13.616	2111240	50.0
Benzo[c]thiophene	15.533	8.8	ug/l	370714	4	13.616	2111240	50.0
Naphthalene, 2-...	16.527	78.3	ug/l	3305360	4	13.616	2111240	50.0
Naphthalene, 1-...	16.739	59.5	ug/l	2513110	4	13.616	2111240	50.0