

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073543.D
 Acq On : 20 Jul 2022 23:51
 Operator : JC\MD
 Sample : N3779-11
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-I

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: VN073543.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.634	288	297	313	rBV2	77718	213483	2.80%	0.764%
2	4.228	389	398	407	rBV2	64895	192690	2.52%	0.690%
3	7.751	986	997	1007	rBV	51185	133996	1.76%	0.480%
4	7.951	1021	1031	1036	rBV	199008	471991	6.18%	1.690%
5	8.016	1036	1042	1060	rVB	365653	845733	11.08%	3.028%
6	8.381	1093	1104	1127	rBV3	403005	1158250	15.17%	4.147%
7	8.904	1184	1193	1203	rBV	522330	1072614	14.05%	3.840%
8	10.380	1435	1444	1450	rBV	736047	1330077	17.43%	4.762%
9	10.445	1450	1455	1466	rVB	626270	1128877	14.79%	4.041%
10	11.163	1569	1577	1587	rVV	465381	865301	11.34%	3.098%
11	11.686	1657	1666	1670	rBV	768352	1376267	18.03%	4.927%
12	11.727	1670	1673	1679	rVV	204796	371487	4.87%	1.330%
13	11.786	1679	1683	1690	rVV	74642	142851	1.87%	0.511%
14	11.892	1690	1701	1711	rVB	321095	654827	8.58%	2.344%
15	12.022	1713	1723	1737	rBV3	146218	349621	4.58%	1.252%
16	12.222	1751	1757	1765	rVB3	314572	580175	7.60%	2.077%
17	12.292	1765	1769	1775	rBV	62636	96021	1.26%	0.344%
18	12.463	1792	1798	1803	rVV2	86341	167351	2.19%	0.599%
19	12.510	1803	1806	1815	rVB3	50140	89189	1.17%	0.319%
20	12.674	1824	1834	1845	rBV	643056	1167123	15.29%	4.178%
21	12.951	1869	1881	1885	rBV3	126241	302690	3.97%	1.084%
22	12.998	1885	1889	1894	rVB	52828	85645	1.12%	0.307%
23	13.163	1913	1917	1925	rVB2	37138	80327	1.05%	0.288%
24	13.304	1933	1941	1946	rVV2	208871	479641	6.28%	1.717%
25	13.357	1946	1950	1954	rVB3	50031	78105	1.02%	0.280%
26	13.504	1966	1975	1977	rBV8	47759	121916	1.60%	0.436%
27	13.616	1987	1994	2006	rVV2	867706	1646402	21.57%	5.894%
28	13.710	2006	2010	2017	rVB3	54422	92327	1.21%	0.331%
29	13.816	2023	2028	2032	rBV2	49339	82274	1.08%	0.295%
30	13.998	2053	2059	2066	rVV	353505	630675	8.26%	2.258%
31	14.074	2066	2072	2082	rVB10	31303	121253	1.59%	0.434%
32	14.292	2104	2109	2115	rVB3	37729	77272	1.01%	0.277%
33	14.857	2199	2205	2213	rBV5	40049	99302	1.30%	0.356%
34	15.015	2227	2232	2238	rBV2	45297	96716	1.27%	0.346%
35	15.433	2291	2303	2313	rBV	3956566	7632990	100.00%	27.326%
36	15.533	2314	2320	2329	rVB	132209	257935	3.38%	0.923%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
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37	16.533	2482	2490	2504	rVB	917250	2025342	26.53%	7.251%
38	16.739	2516	2525	2533	rBV	701153	1613906	21.14%	5.778%

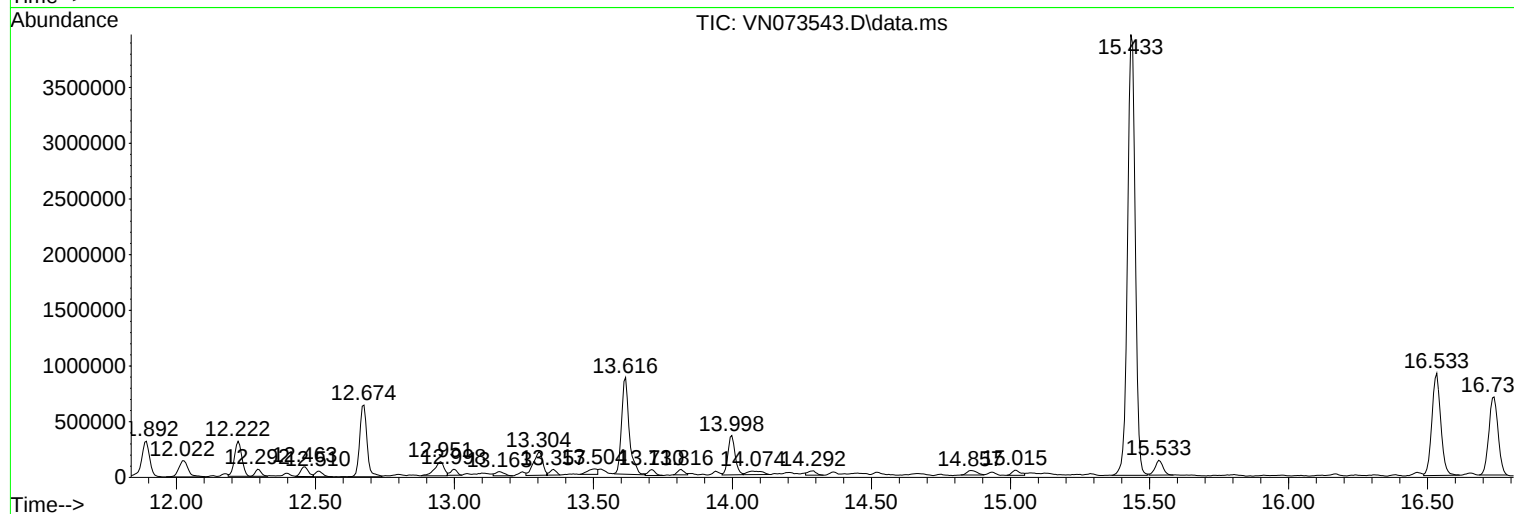
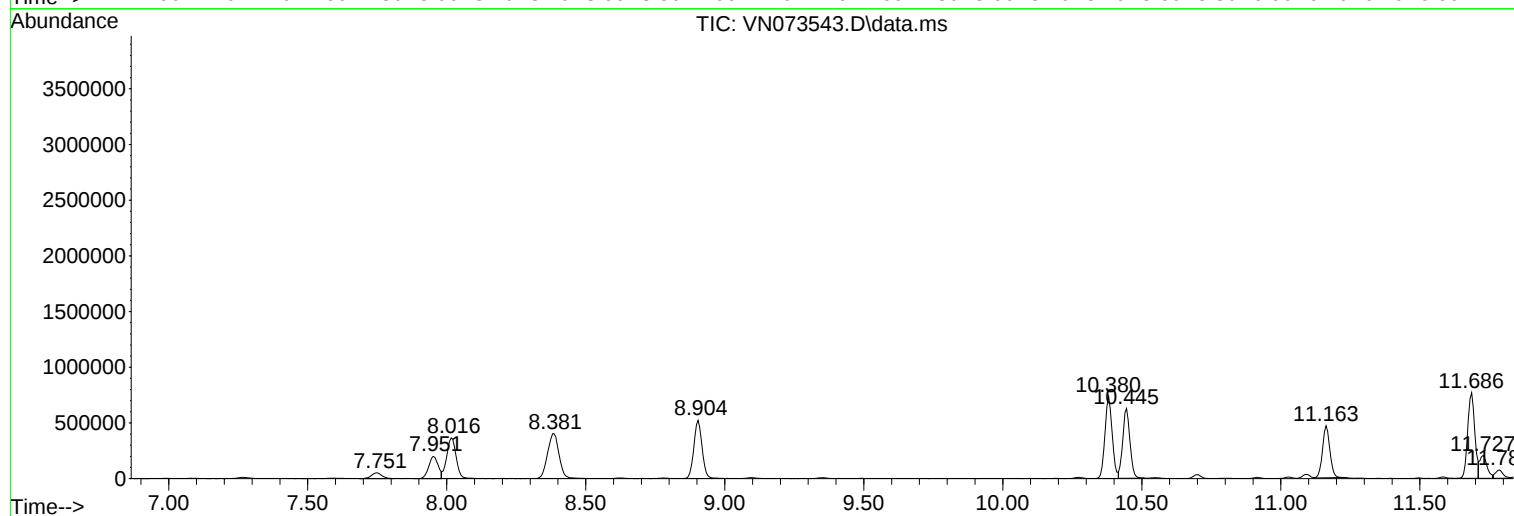
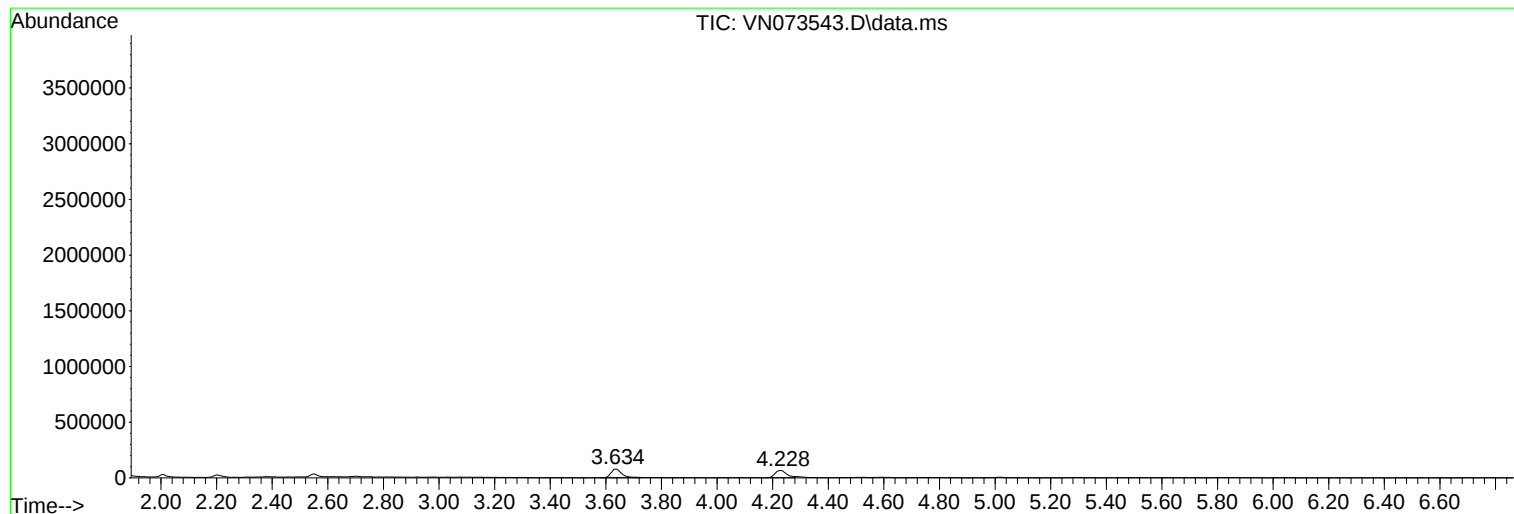
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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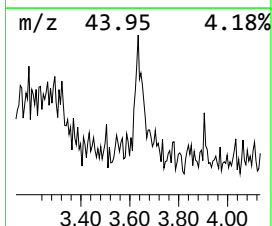
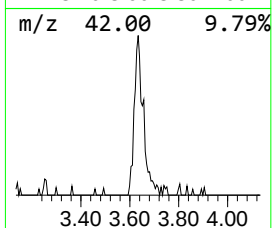
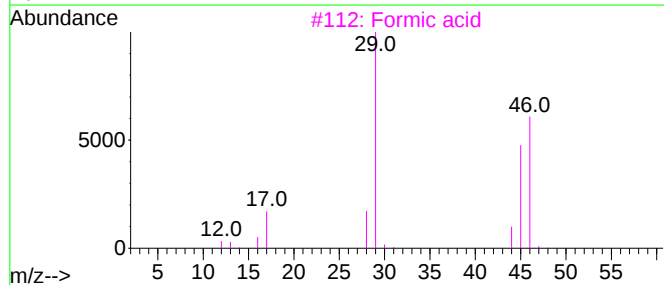
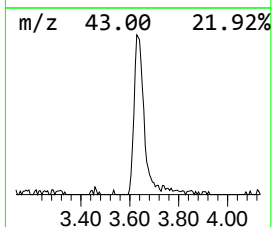
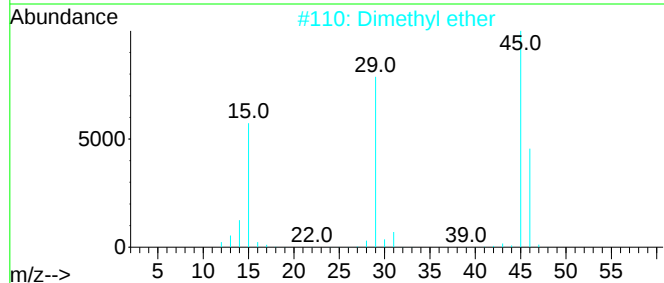
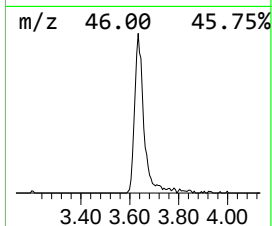
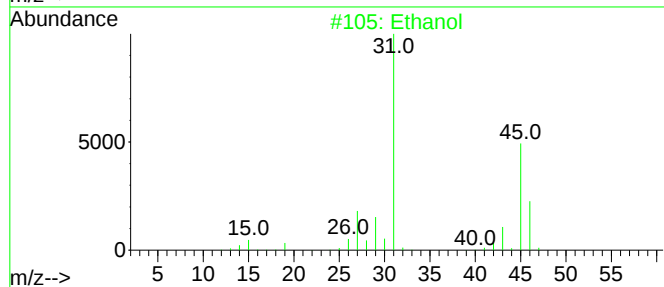
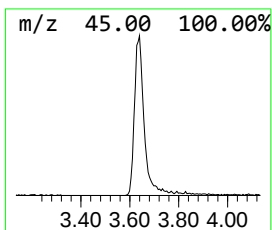
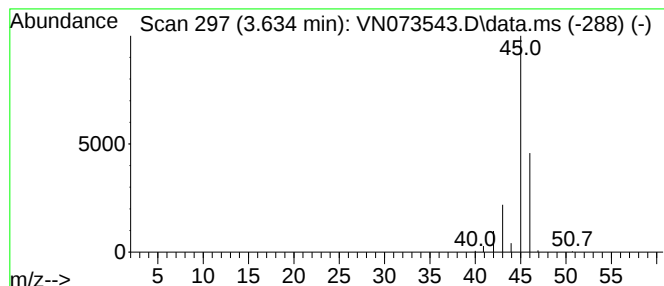
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	12.62 ug/l	213483	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Formic acid	46	CH2O2	000064-18-6	4
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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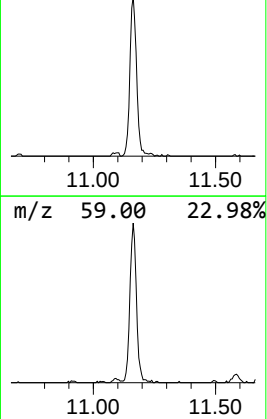
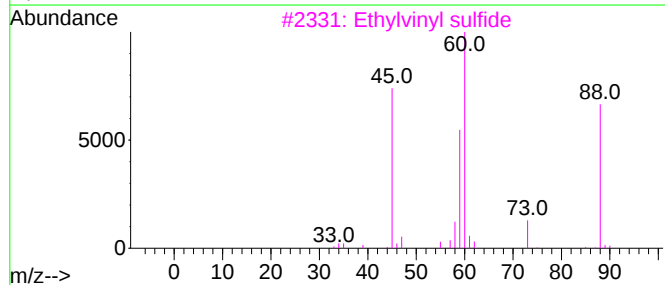
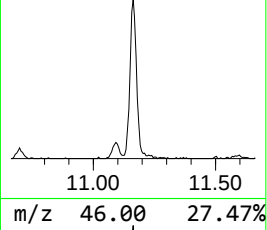
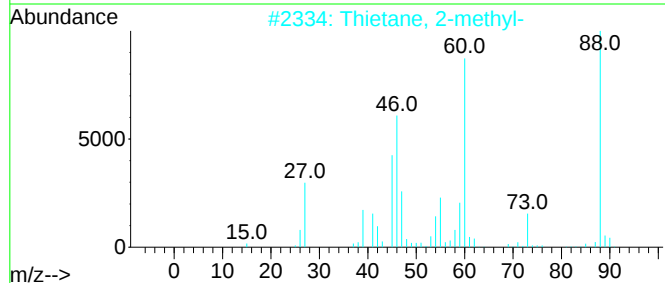
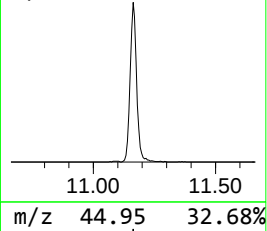
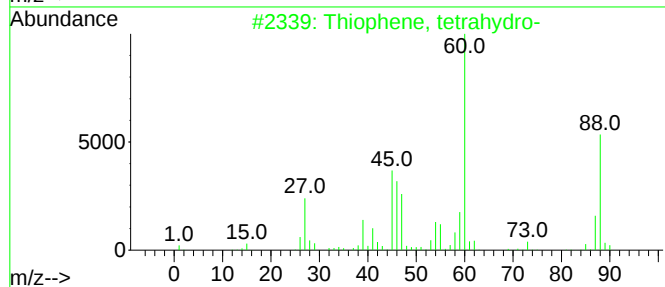
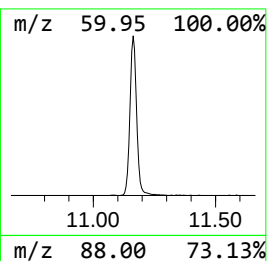
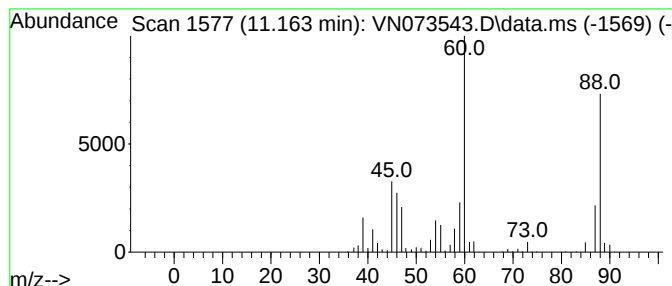
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	31.44 ug/l	865301	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	58
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	25



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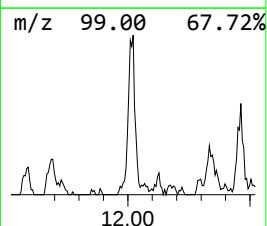
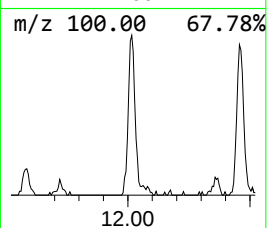
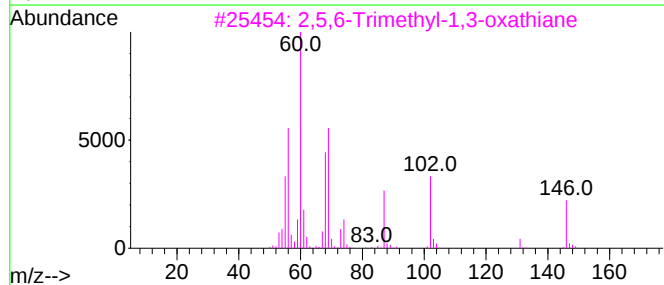
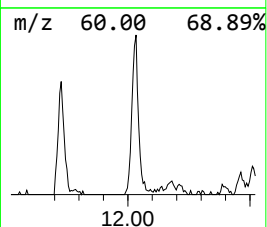
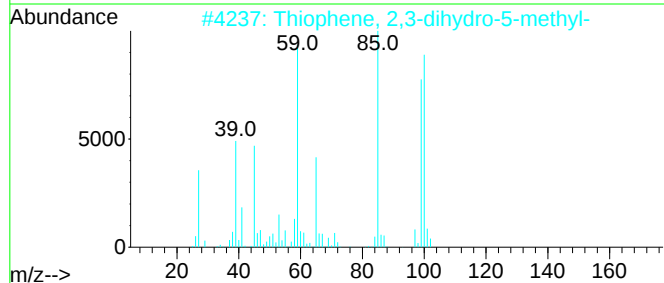
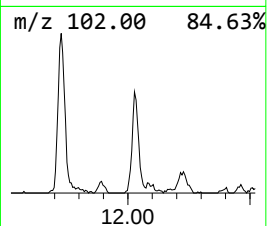
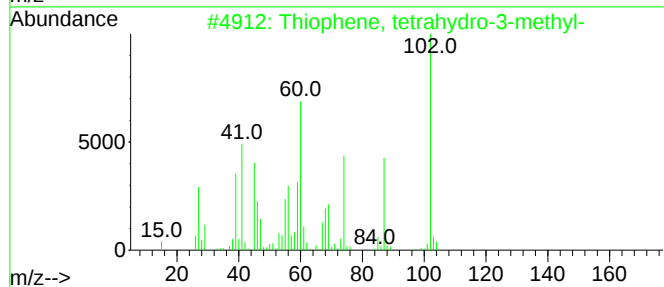
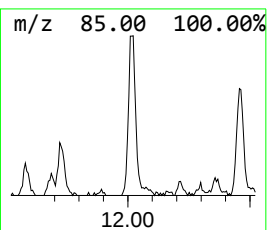
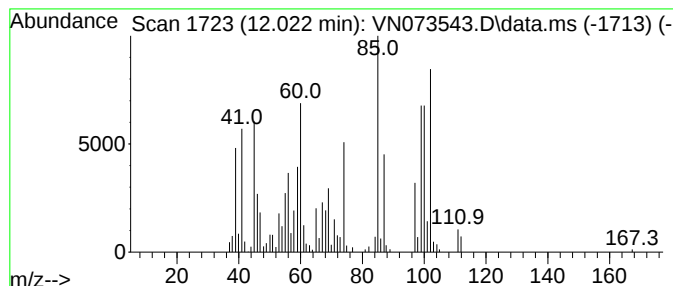
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Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	12.70 ug/l	349621	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	95
2			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	30
3			2,5,6-Trimethyl-1,3-oxathiane	146	C7H14OS	114376-06-6	27
4			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	22
5			Propionaldehyde, ethylhydrazone	100	C5H12N2	007422-92-6	14



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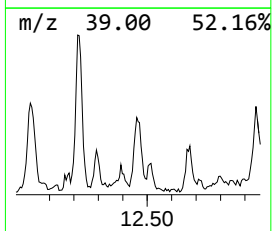
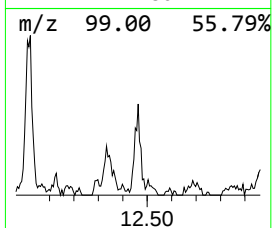
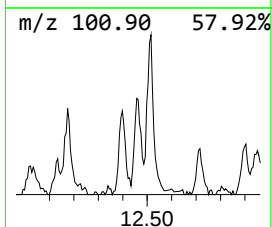
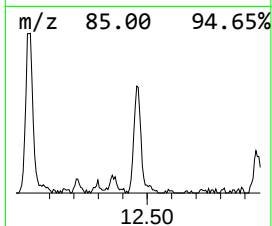
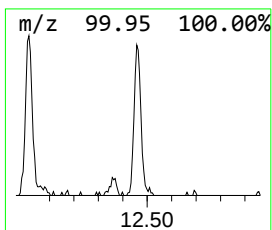
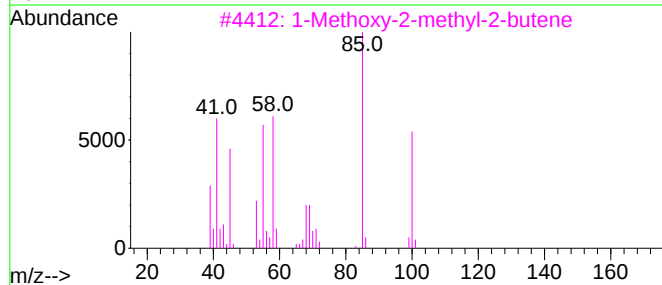
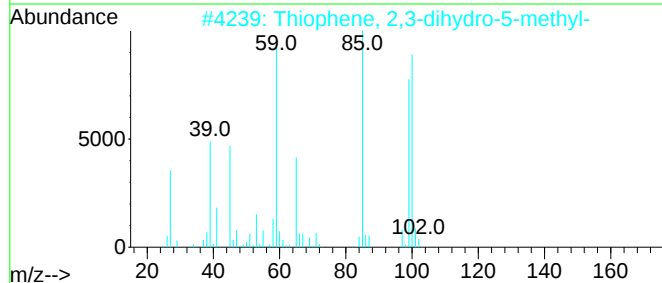
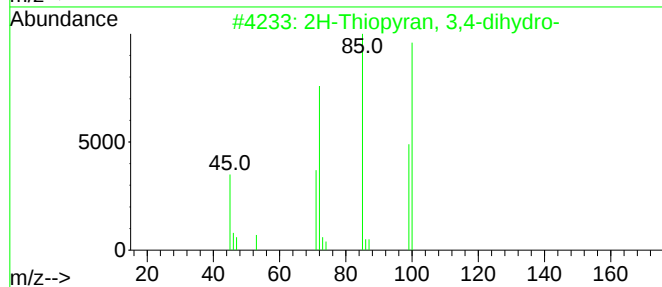
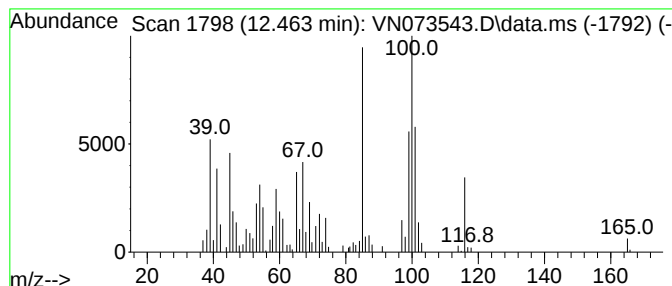
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2H-Thiopyran, 3,4-dihydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	6.08 ug/l	167351	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Thiopyran, 3,4-dihydro-	100	C5H8S	013042-80-3	50
2			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	49
3			1-Methoxy-2-methyl-2-butene	100	C6H12O	1000279-59-7	43
4			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	42
5			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	38



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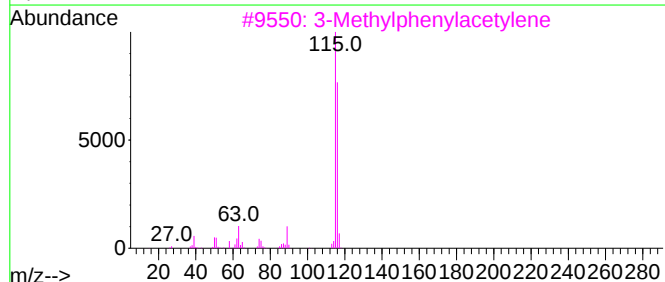
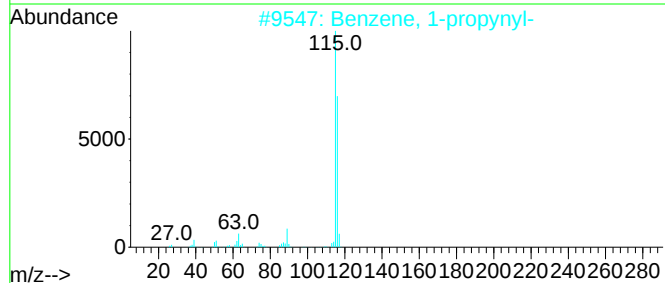
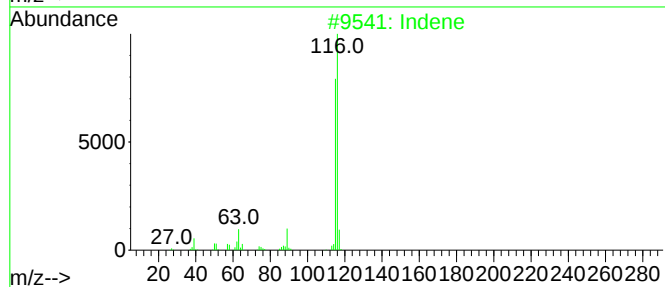
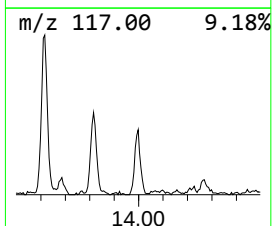
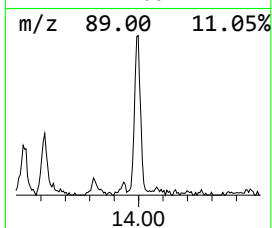
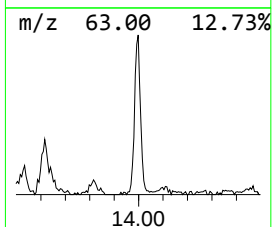
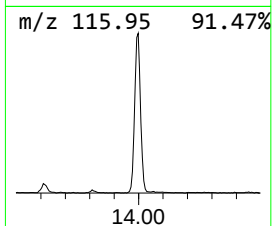
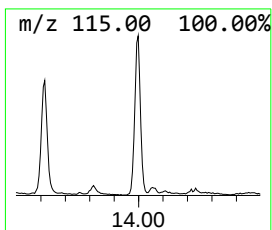
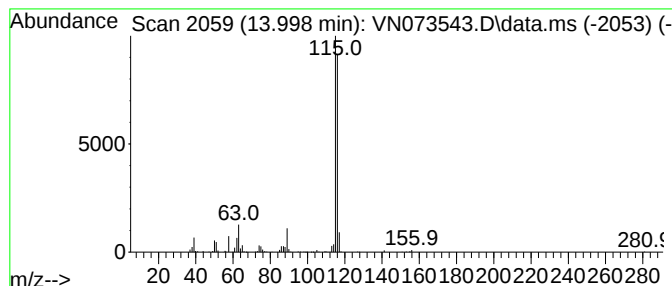
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 5 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	19.15 ug/l	630675	1,4-Dichlorobenzene-d4	13.610

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	94
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073543.D
Acq On : 20 Jul 2022 23:51
Operator : JC\MD
Sample : N3779-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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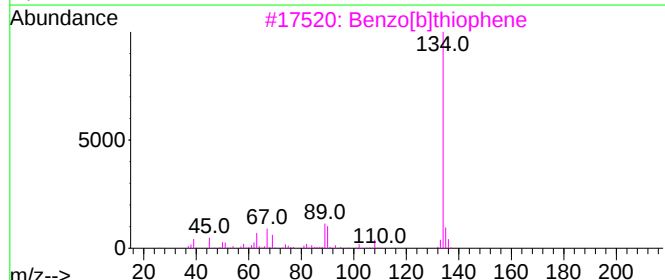
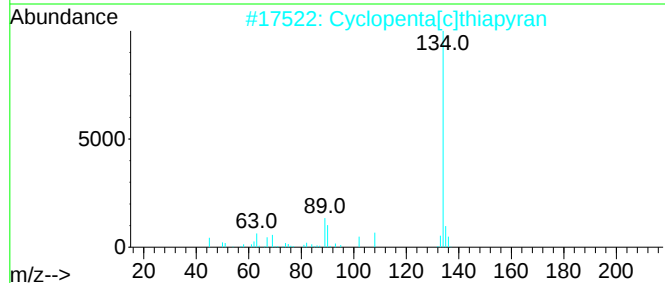
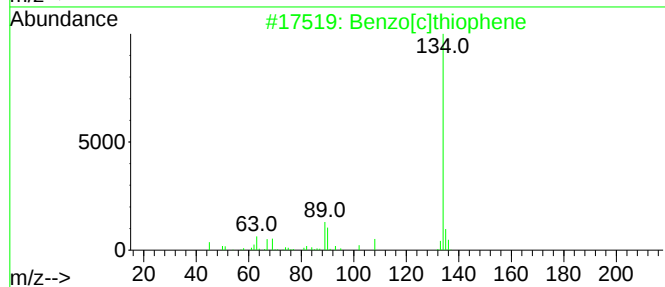
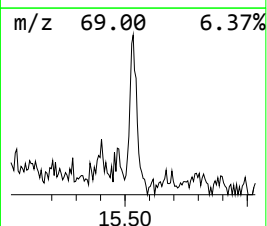
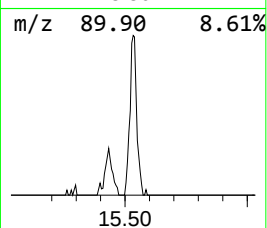
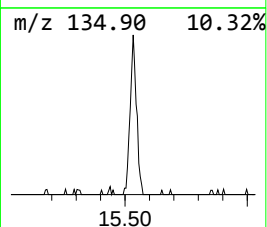
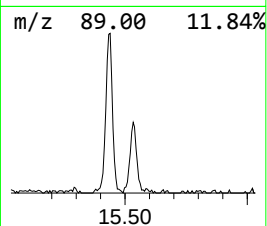
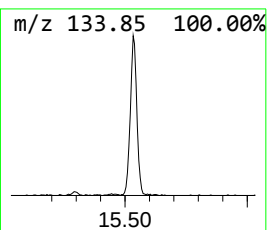
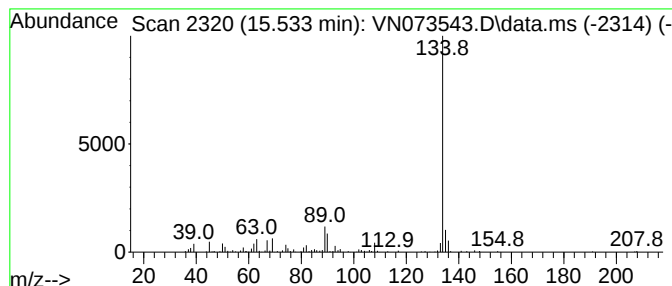
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Quant Title : SW846 8260

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

Peak Number 6 Benzo[c]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	7.83 ug/l	257935	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
2			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
3			Benzo[b]thiophene	134	C8H6S	000095-15-8	91
4			3-Deazaadenine	134	C6H6N4	006811-77-4	59
5			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073543.D
Acq On : 20 Jul 2022 23:51
Operator : JC\MD
Sample : N3779-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-I

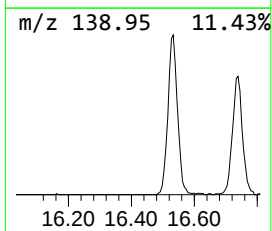
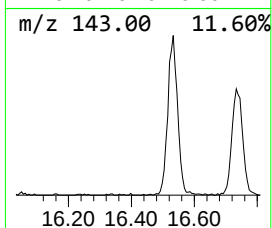
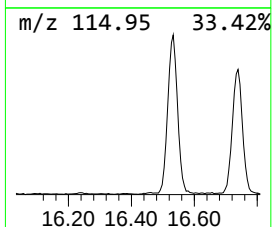
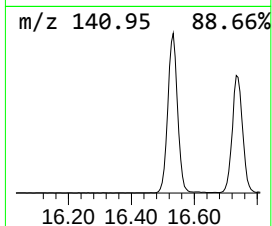
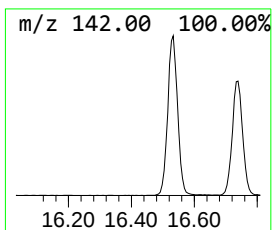
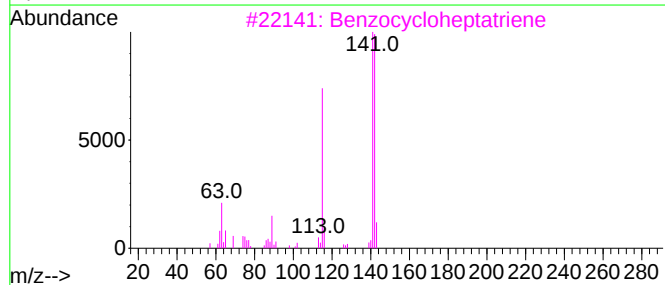
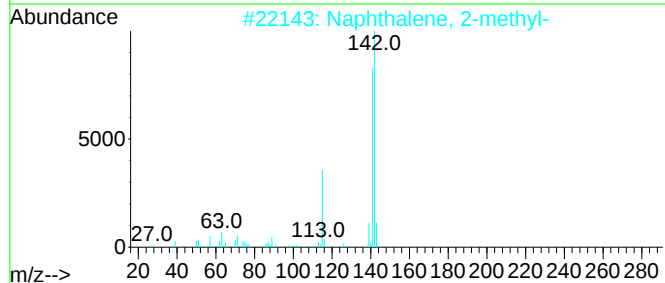
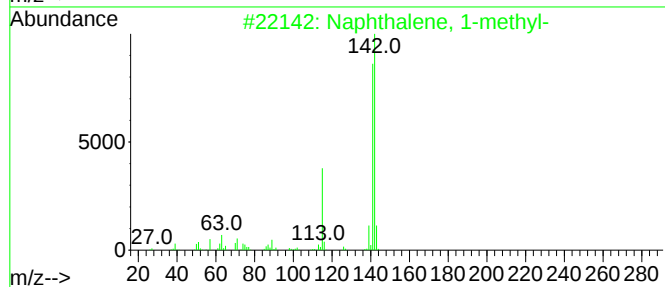
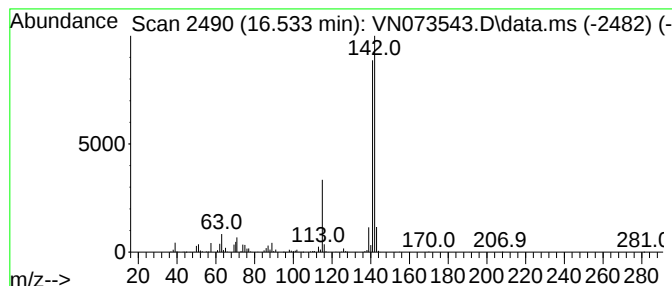
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.533	61.51 ug/l	2025340	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073543.D
Acq On : 20 Jul 2022 23:51
Operator : JC\MD
Sample : N3779-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-I

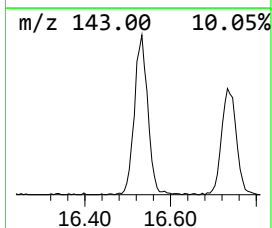
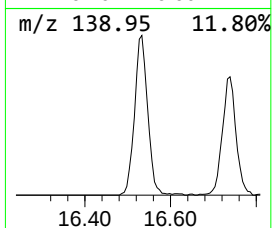
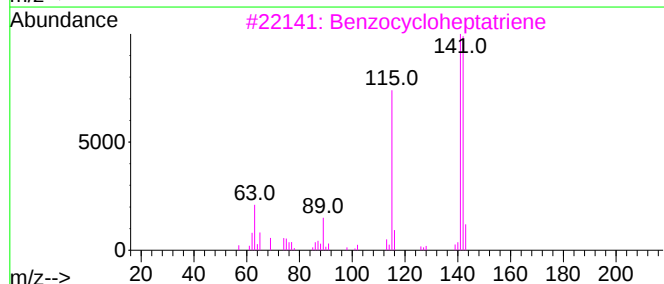
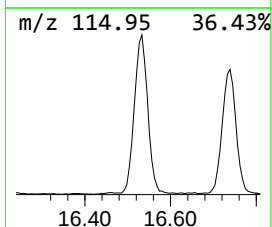
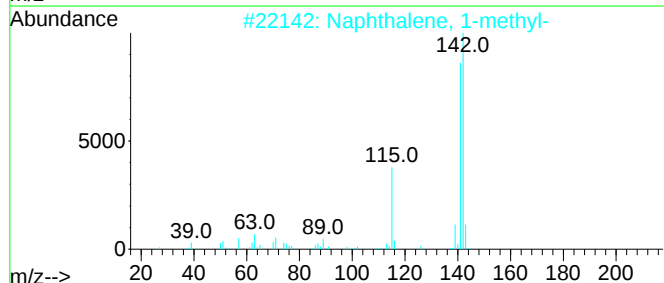
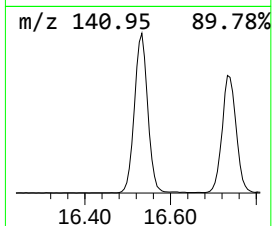
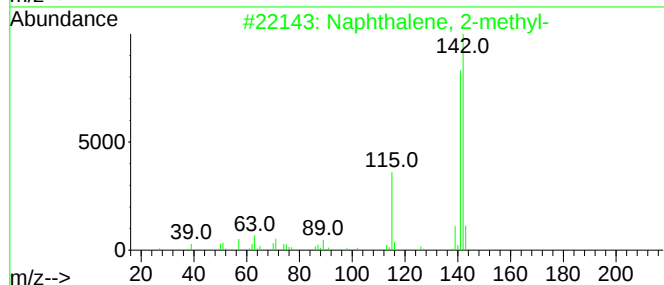
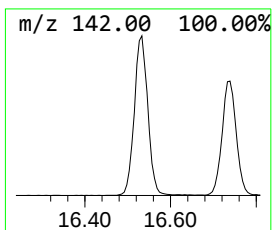
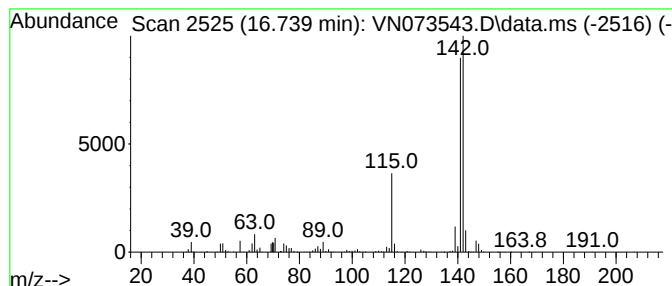
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	49.01 ug/l	1613910	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	93
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073543.D
Acq On : 20 Jul 2022 23:51
Operator : JC\MD
Sample : N3779-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-I

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
Ethanol	3.634	12.6	ug/l	213483	1	8.016	845733	50.0
Thiophene, tetr...	11.163	31.4	ug/l	865301	3	11.686	1376270	50.0
Thiophene, tetr...	12.022	12.7	ug/l	349621	3	11.686	1376270	50.0
2H-Thiopyran, 3...	12.463	6.1	ug/l	167351	3	11.686	1376270	50.0
Indene	13.998	19.1	ug/l	630675	4	13.610	1646400	50.0
Benzo[c]thiophene	15.533	7.8	ug/l	257935	4	13.610	1646400	50.0
Naphthalene, 1-...	16.533	61.5	ug/l	2025340	4	13.610	1646400	50.0
Naphthalene, 2-...	16.739	49.0	ug/l	1613910	4	13.610	1646400	50.0