

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073535.D
 Acq On : 20 Jul 2022 20:34
 Operator : JC\MD
 Sample : N3779-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-A

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: VN073535.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	rBV	211062	564122	6.12%	1.805%
2	4.228	389	398	407	rBV	71827	205982	2.23%	0.659%
3	7.751	988	997	1008	rBV3	36489	95146	1.03%	0.304%
4	7.951	1015	1031	1036	rBV2	179235	443144	4.81%	1.418%
5	8.016	1036	1042	1054	rVB	336869	767129	8.32%	2.455%
6	8.386	1092	1105	1125	rBV3	384765	1098341	11.92%	3.514%
7	8.904	1183	1193	1208	rBV	474475	972852	10.56%	3.113%
8	10.380	1436	1444	1450	rBV	645641	1200463	13.02%	3.841%
9	10.445	1450	1455	1468	rVB	438518	806329	8.75%	2.580%
10	10.698	1490	1498	1505	rBV	95702	172042	1.87%	0.550%
11	11.086	1556	1564	1570	rBV2	109335	227245	2.47%	0.727%
12	11.163	1570	1577	1594	rVB	703353	1363800	14.80%	4.364%
13	11.686	1657	1666	1670	rBV	657620	1213962	13.17%	3.884%
14	11.727	1670	1673	1679	rVV	237249	400313	4.34%	1.281%
15	11.786	1679	1683	1690	rVV	70658	124611	1.35%	0.399%
16	11.886	1690	1700	1711	rVB	364615	697290	7.57%	2.231%
17	12.027	1717	1724	1737	rVB3	194700	417472	4.53%	1.336%
18	12.221	1751	1757	1766	rVB2	358955	645465	7.00%	2.065%
19	12.463	1792	1798	1803	rVV	132226	258142	2.80%	0.826%
20	12.510	1803	1806	1814	rVB3	64208	108619	1.18%	0.348%
21	12.674	1825	1834	1846	rBV	556785	1005659	10.91%	3.218%
22	12.951	1871	1881	1885	rBV3	136288	332171	3.60%	1.063%
23	12.998	1885	1889	1894	rVB	73675	117190	1.27%	0.375%
24	13.163	1910	1917	1924	rBV2	44247	96672	1.05%	0.309%
25	13.310	1934	1942	1947	rVV2	309102	661328	7.18%	2.116%
26	13.527	1966	1979	1982	rBV6	35882	111288	1.21%	0.356%
27	13.615	1987	1994	2005	rVV2	700754	1412250	15.32%	4.519%
28	13.710	2005	2010	2016	rVB2	64056	108713	1.18%	0.348%
29	13.815	2022	2028	2032	rBV2	70125	129448	1.40%	0.414%
30	13.998	2053	2059	2067	rVB	338297	586903	6.37%	1.878%
31	14.362	2115	2121	2126	rBV2	42009	95732	1.04%	0.306%
32	14.521	2144	2148	2161	rVB3	46565	101688	1.10%	0.325%
33	14.857	2199	2205	2213	rBV3	61018	140565	1.53%	0.450%
34	15.015	2226	2232	2242	rBV2	63499	132500	1.44%	0.424%
35	15.433	2291	2303	2313	rBV	4852615	9216851	100.00%	29.491%
36	15.533	2314	2320	2328	rVB	160870	315860	3.43%	1.011%

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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	16.527	2481	2489	2504	rVB	1232019	2757349	29.92%	8.823%
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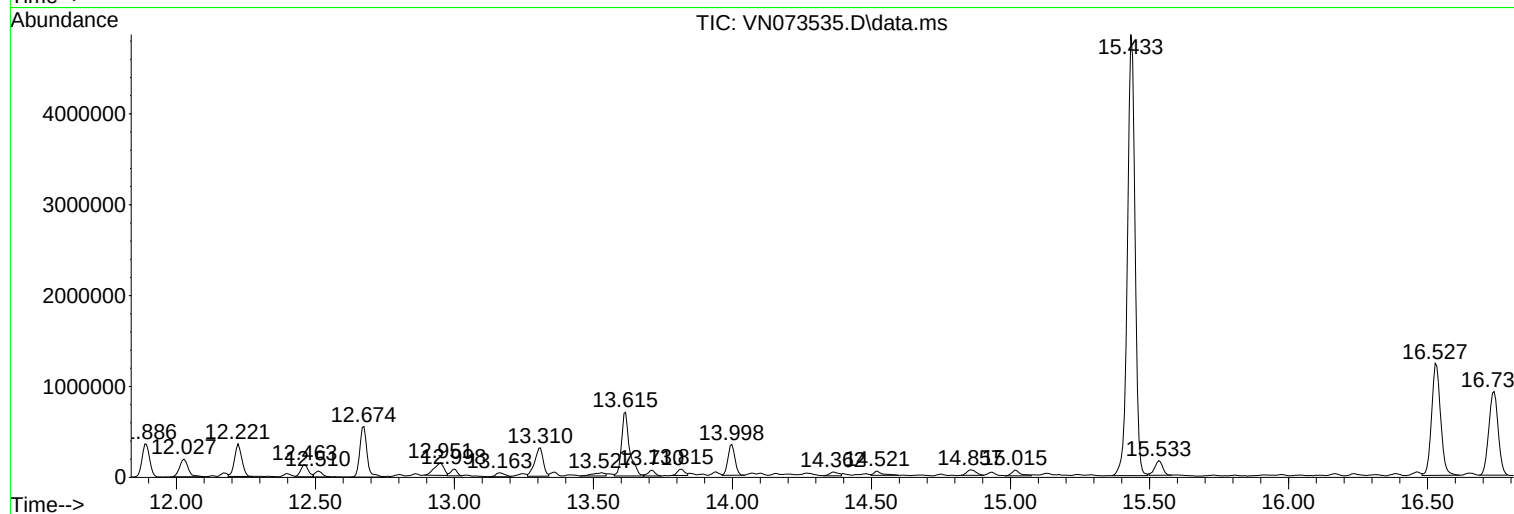
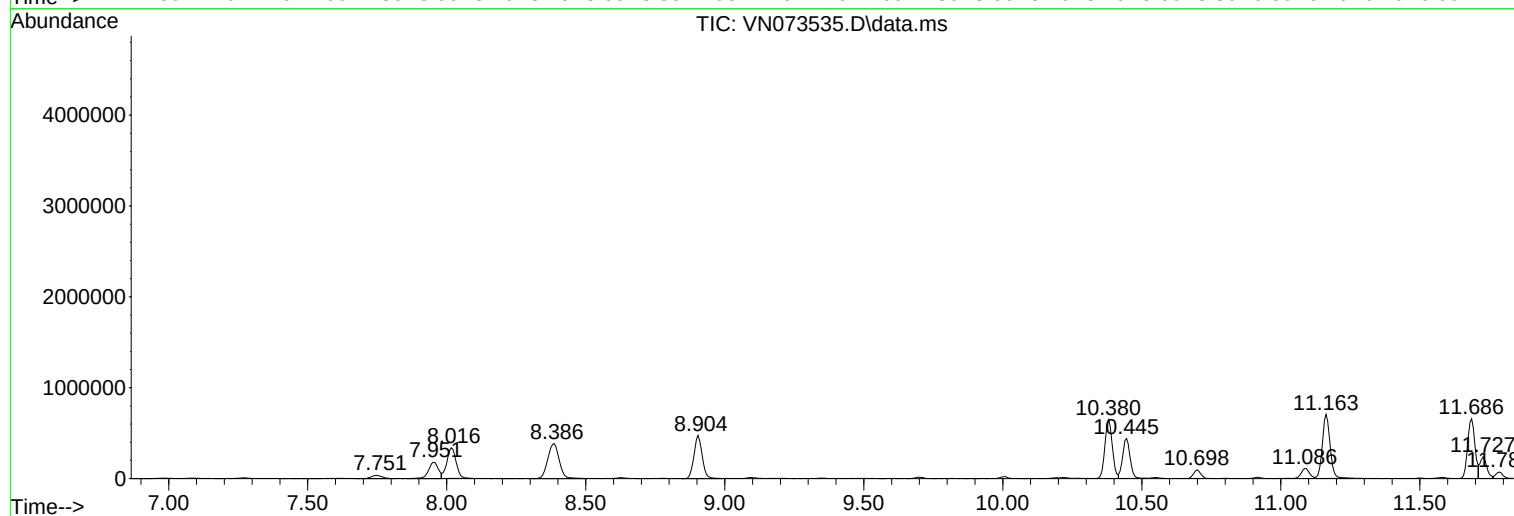
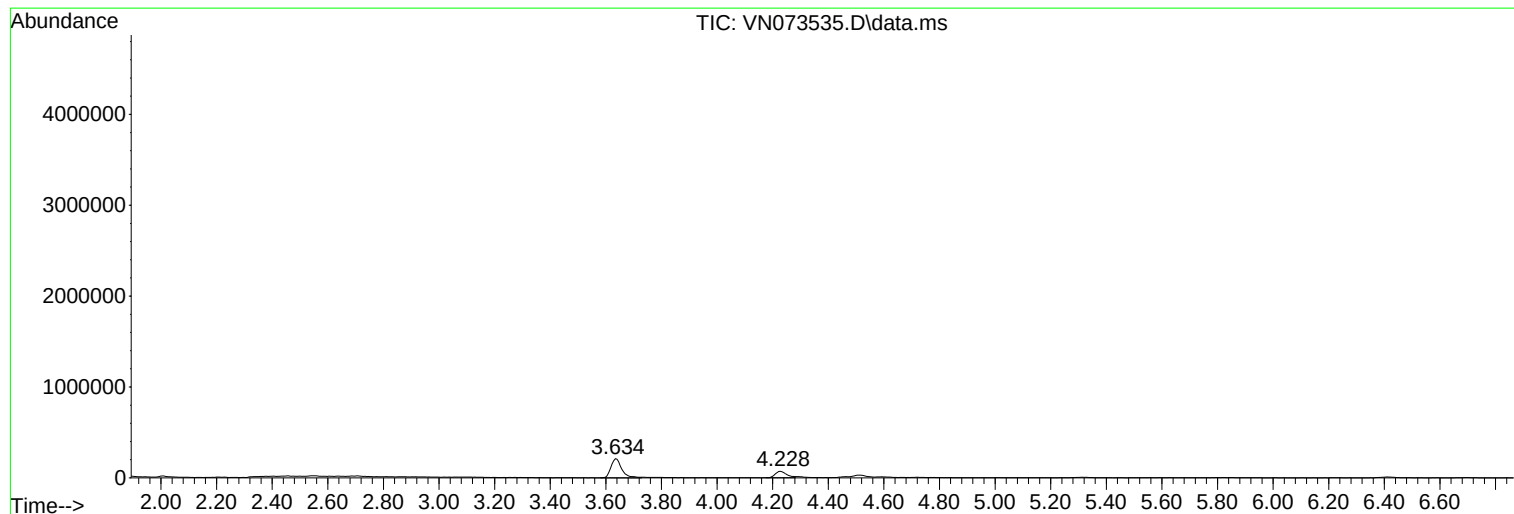
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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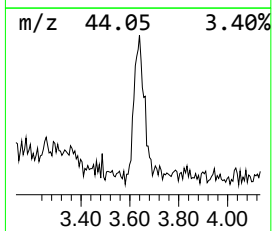
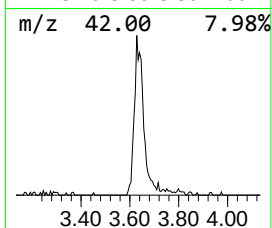
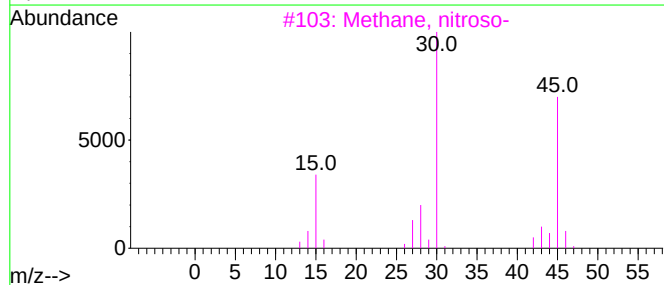
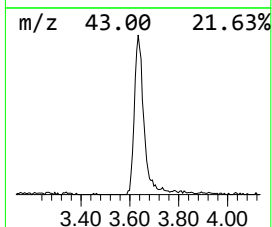
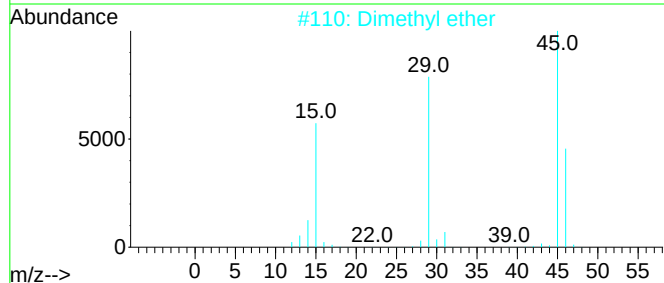
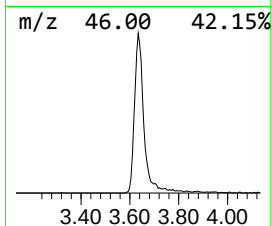
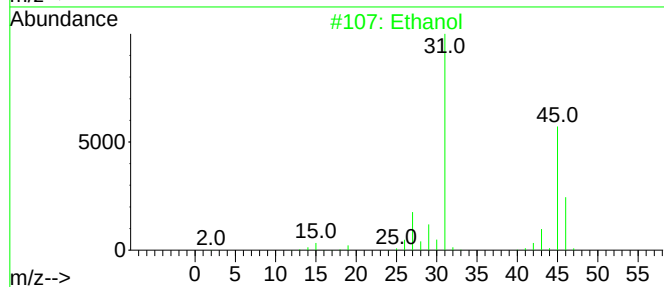
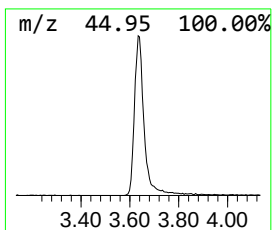
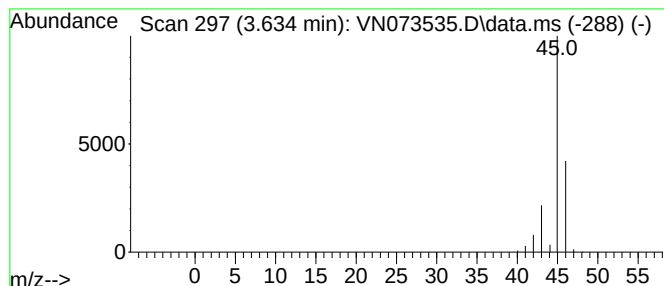
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	36.77 ug/l	564122	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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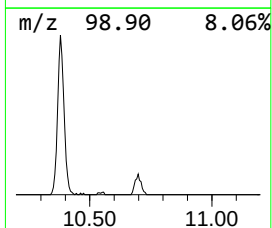
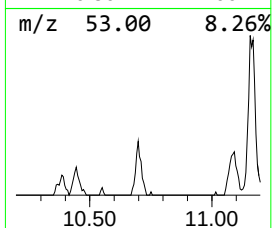
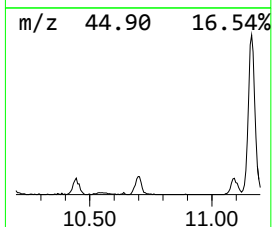
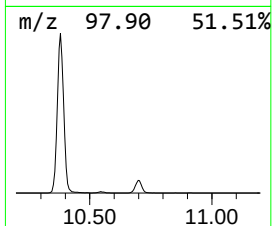
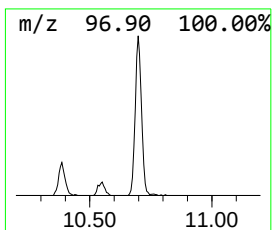
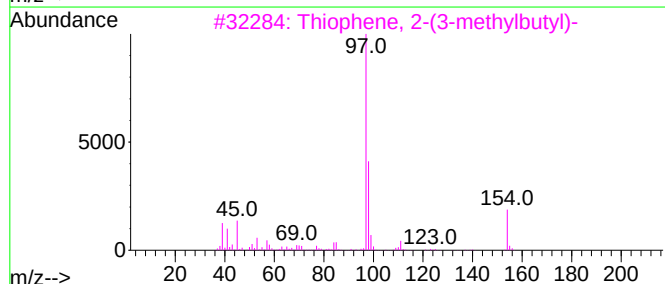
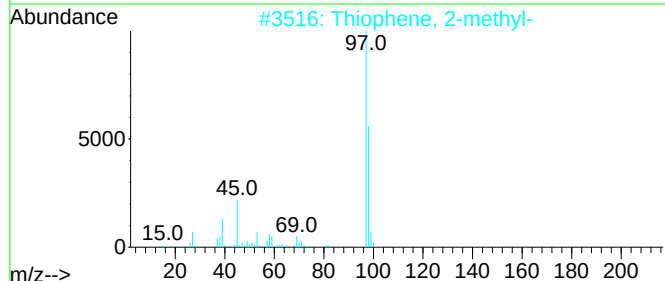
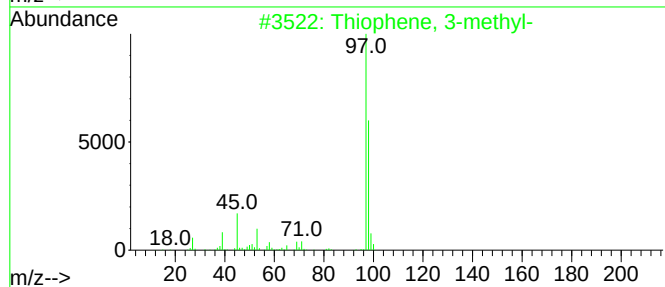
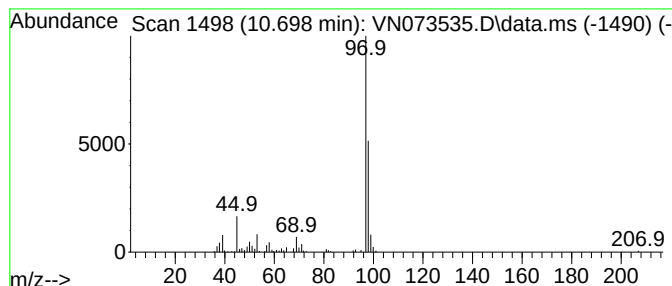
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Peak Number 2 Thiophene, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.698	7.09 ug/l	172042	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	94
3			Thiophene, 2-(3-methylbutyl)-	154	C9H14S	026963-33-7	78
4			3-Thiopheneacetamide	141	C6H7NOS	013781-66-3	64
5			Thiophene, 2-(2-ethylbutyl)-	168	C10H16S	005682-00-8	64



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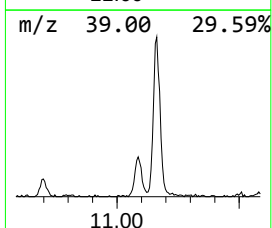
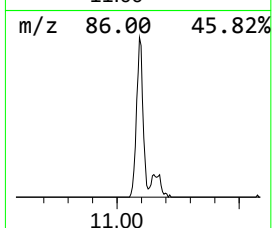
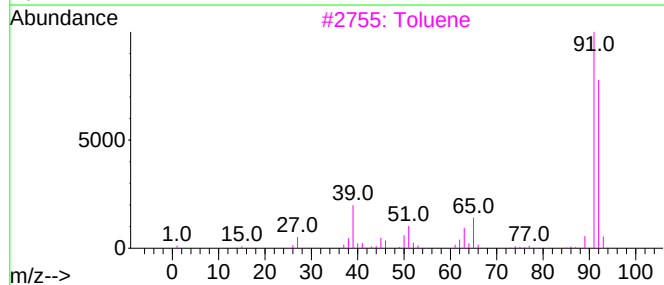
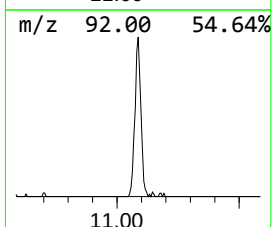
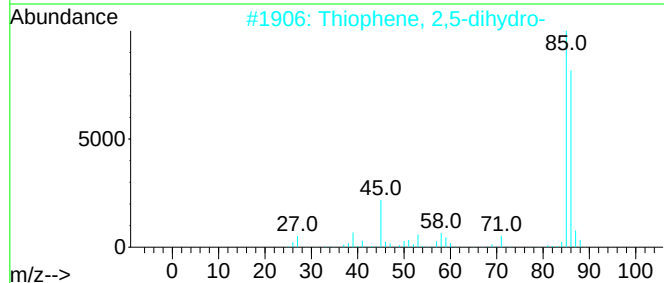
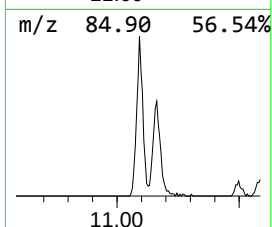
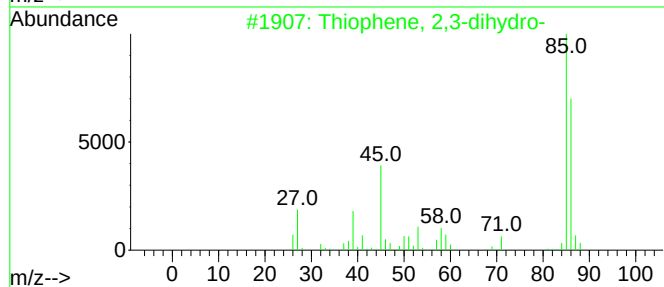
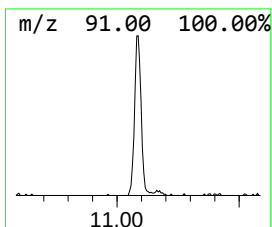
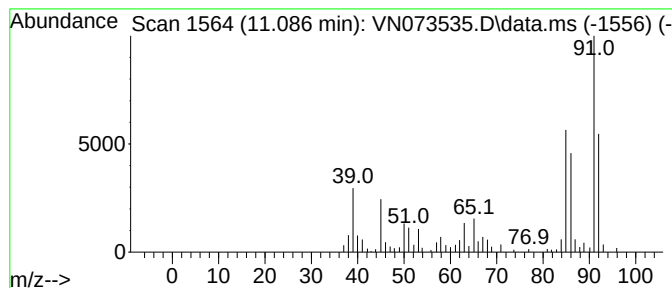
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Quant Title : SW846 8260

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

Peak Number 3 Thiophene, 2,3-dihydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.086	9.36 ug/l	227245	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2,3-dihydro-	86	C4H6S	001120-59-8	53
2			Thiophene, 2,5-dihydro-	86	C4H6S	001708-32-3	46
3			Toluene	92	C7H8	000108-88-3	42
4			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	38
5			Divinyl sulfide	86	C4H6S	000627-51-0	32



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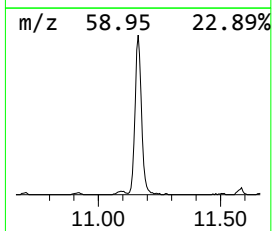
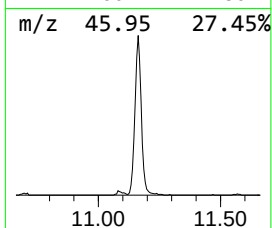
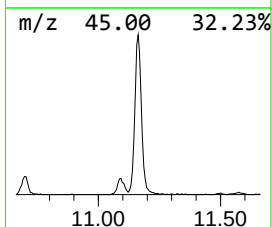
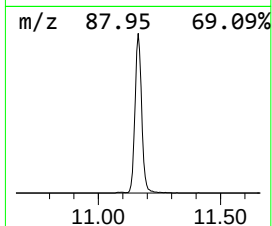
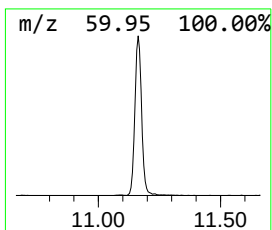
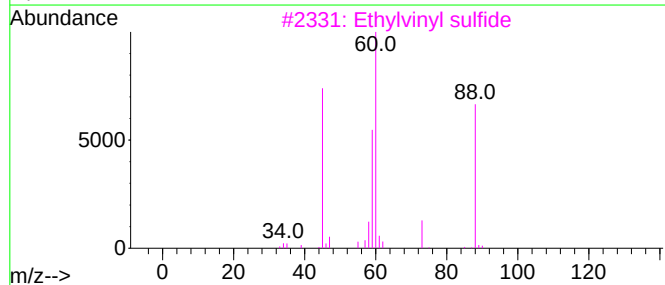
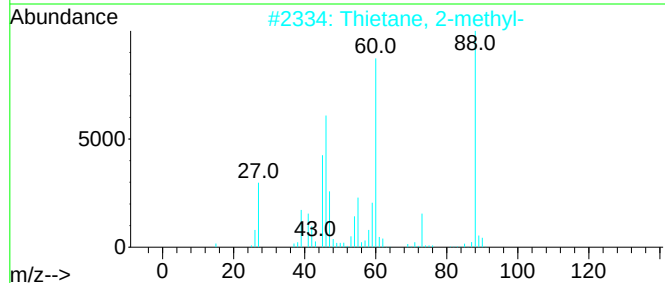
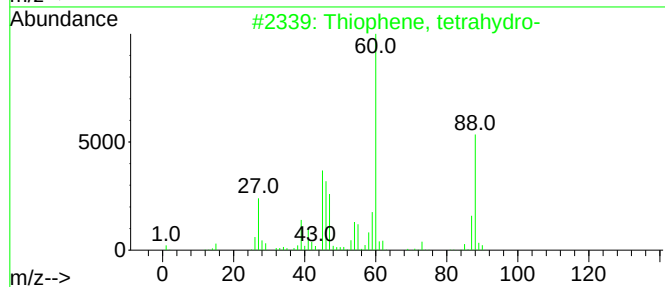
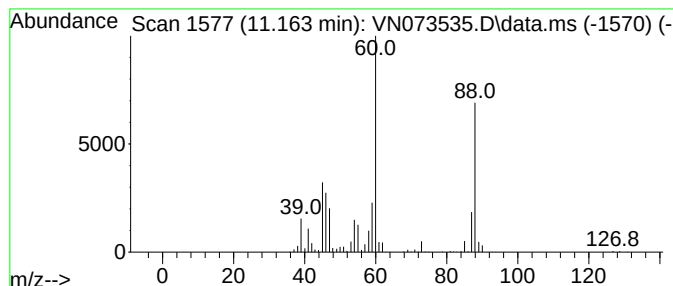
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	56.17 ug/l	1363800	Chlorobenzene-d5	11.686

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	46
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4			Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	37
5			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33



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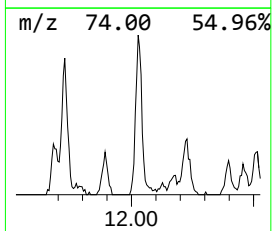
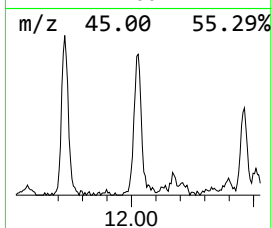
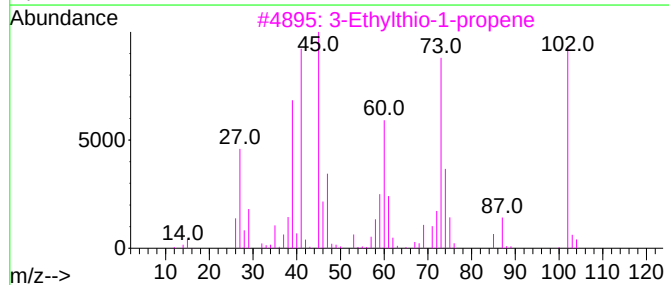
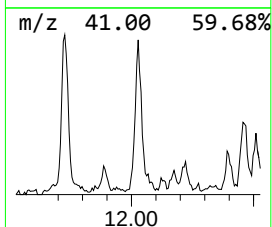
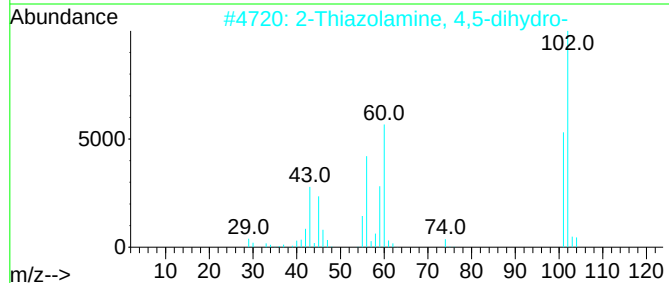
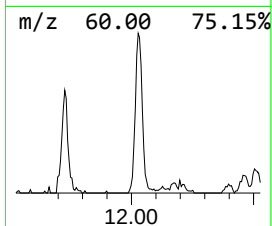
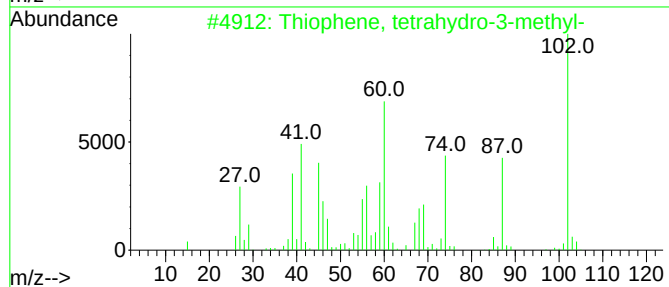
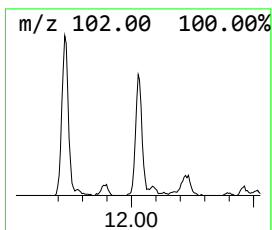
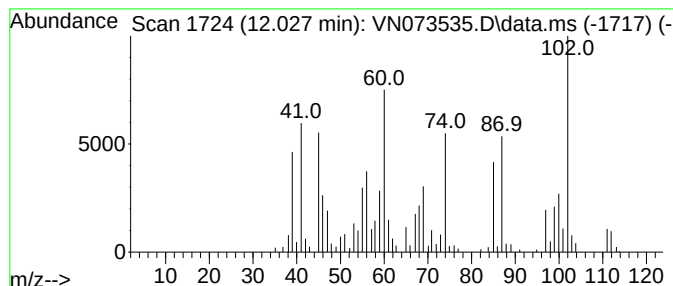
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Thiophene, tetrahydro-3-met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.027	17.19 ug/l	417472	Chlorobenzene-d5	11.686	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	93
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	38
3	3-Ethylthio-1-propene	102	C5H10S	005296-62-8	38
4	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	27
5	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073535.D
Acq On : 20 Jul 2022 20:34
Operator : JC\MD
Sample : N3779-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-A

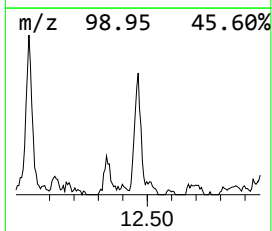
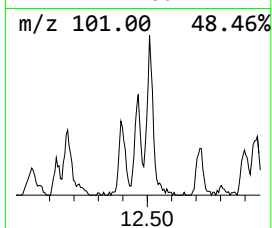
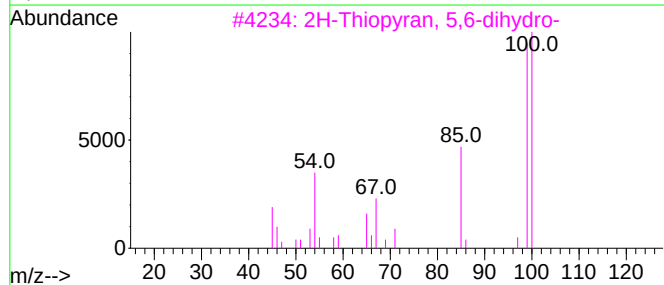
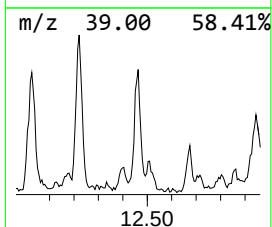
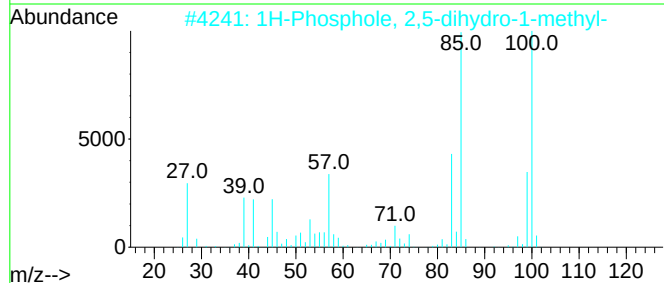
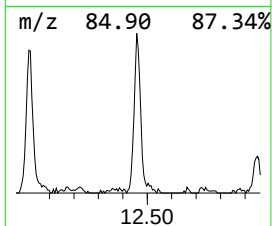
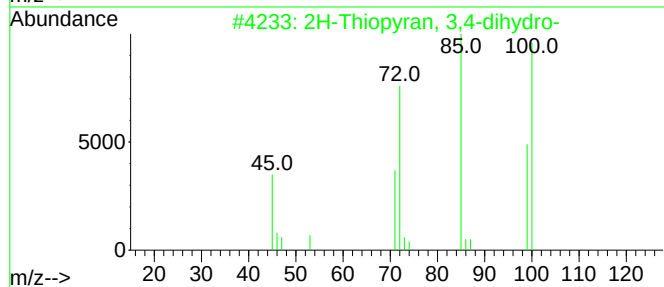
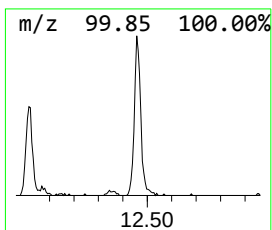
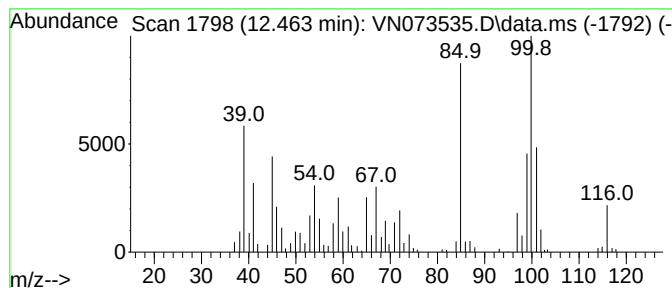
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Quant Title : SW846 8260

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

Peak Number 6 2H-Thiopyran, 3,4-dihydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	10.63 ug/l	258142	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Thiopyran, 3,4-dihydro-	100	C5H8S	013042-80-3	52
2			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	43
3			2H-Thiopyran, 5,6-dihydro-	100	C5H8S	040697-99-2	38
4			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	38
5			Pentadecane-2,4-dione	240	C15H28O2	053759-23-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073535.D
Acq On : 20 Jul 2022 20:34
Operator : JC\MD
Sample : N3779-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-A

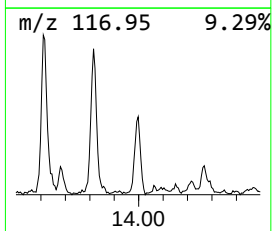
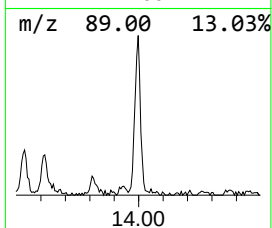
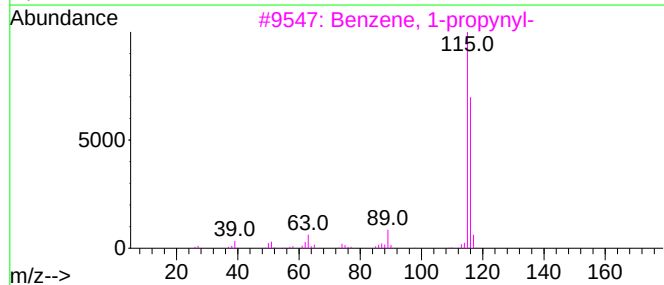
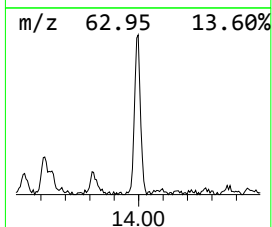
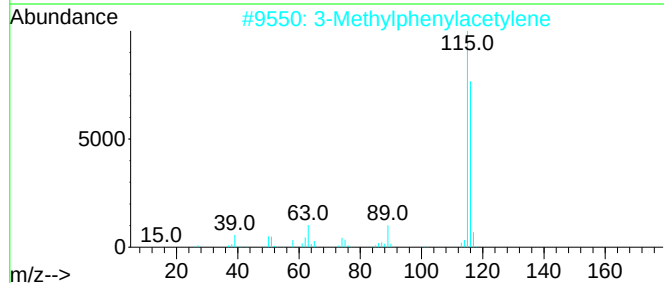
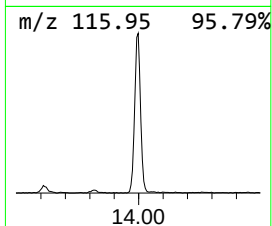
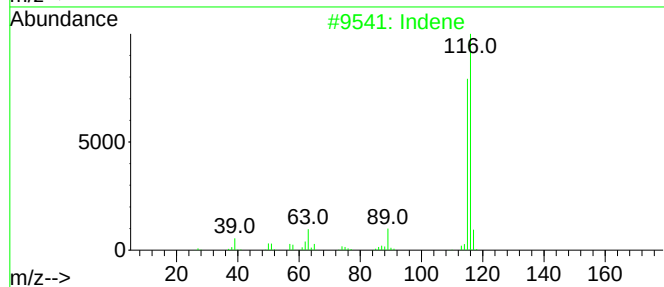
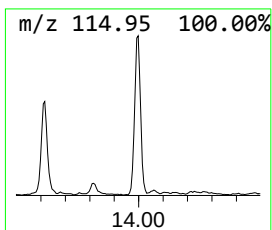
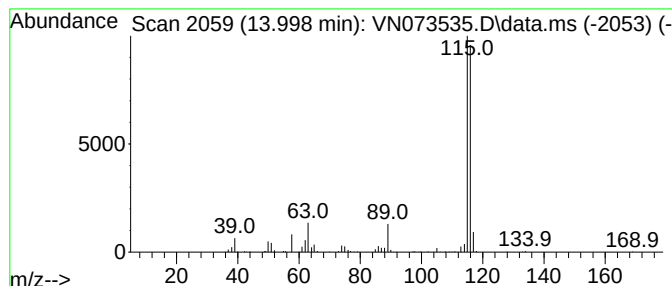
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Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	20.78 ug/l	586903	1,4-Dichlorobenzene-d4	13.615

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			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073535.D
Acq On : 20 Jul 2022 20:34
Operator : JC\MD
Sample : N3779-03
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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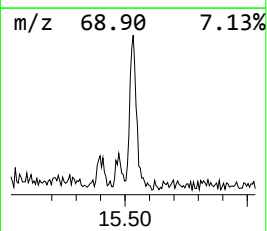
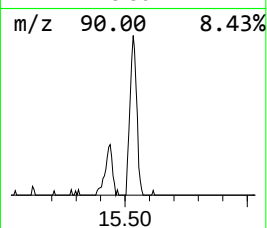
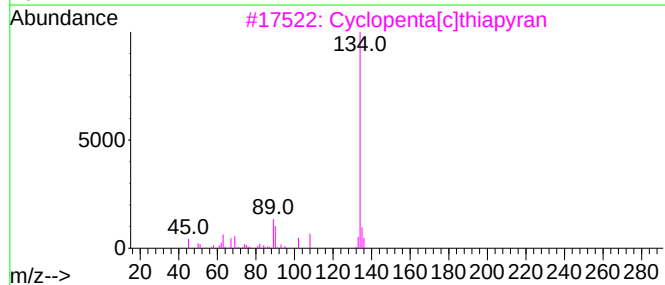
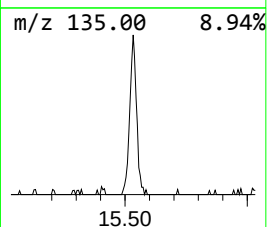
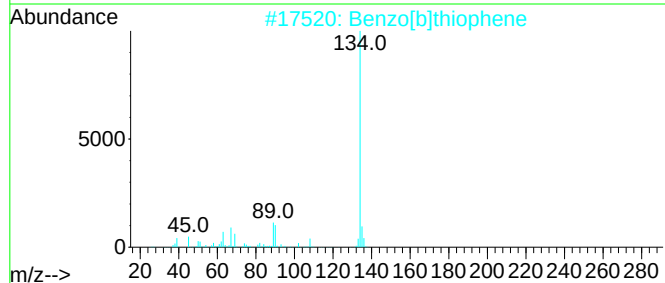
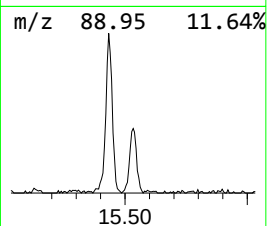
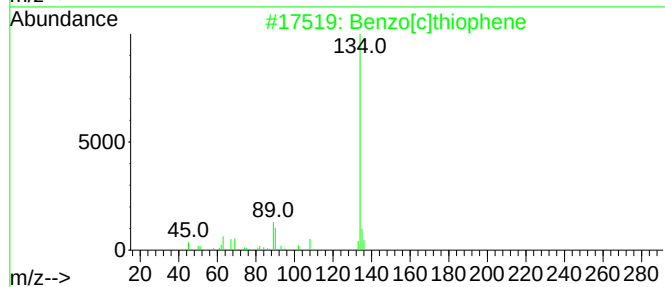
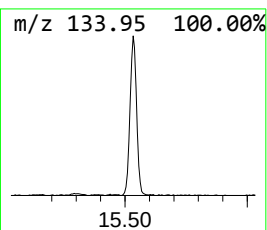
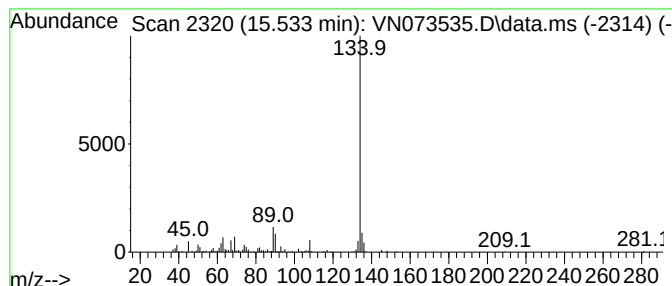
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[c]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	11.18 ug/l	315860	1,4-Dichlorobenzene-d4	13.615

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	90
4			5-Benzylidene-3-(2,5-dimethylani...	338	C19H18N2O2S	302955-01-7	64
5			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073535.D
Acq On : 20 Jul 2022 20:34
Operator : JC\MD
Sample : N3779-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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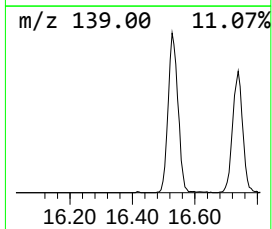
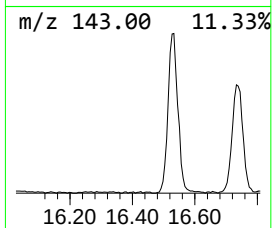
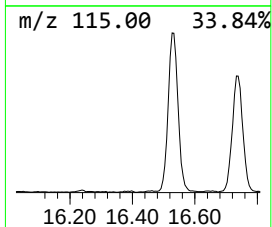
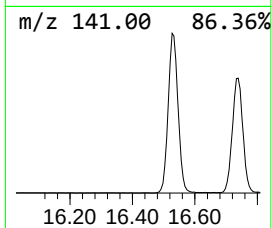
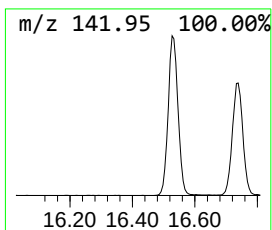
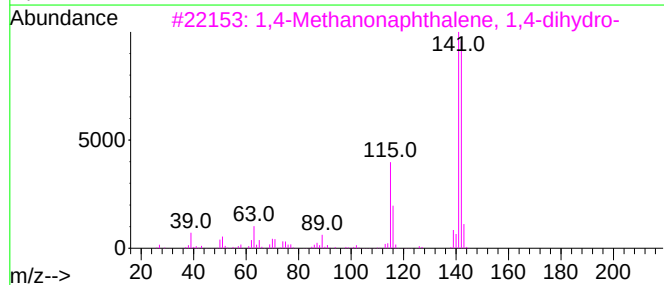
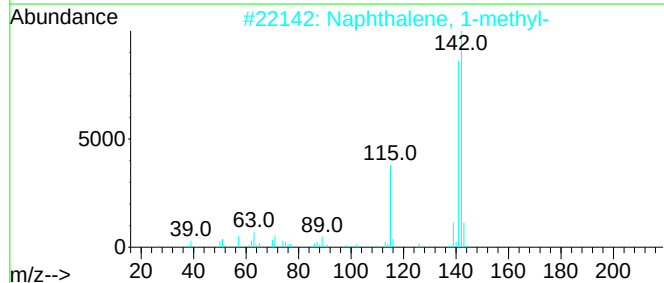
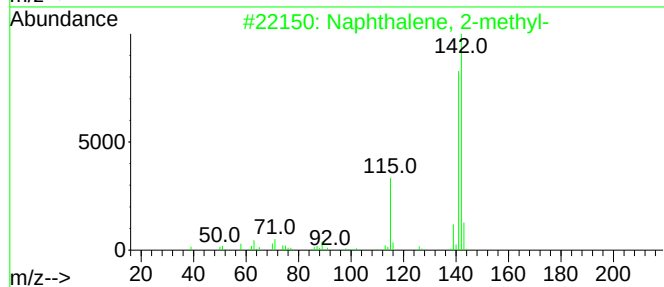
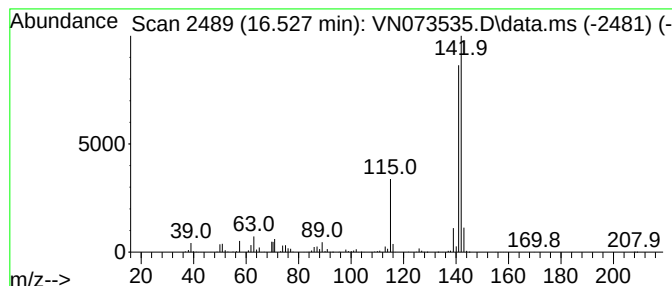
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	97.62 ug/l	2757350	1,4-Dichlorobenzene-d4	13.615

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	90
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indole-6-carbonitrile	142	C9H6N2	015861-36-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073535.D
Acq On : 20 Jul 2022 20:34
Operator : JC\MD
Sample : N3779-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-A

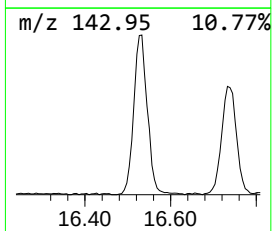
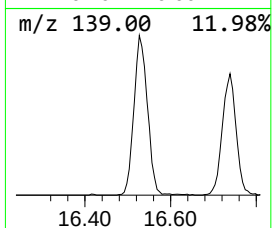
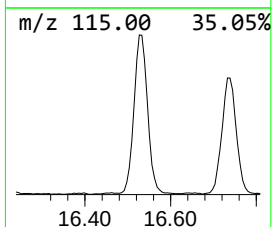
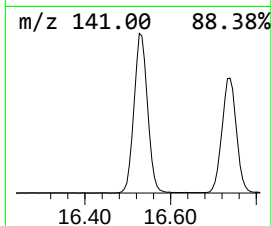
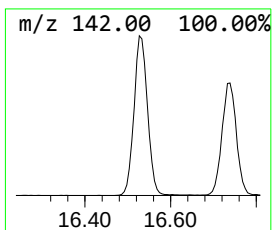
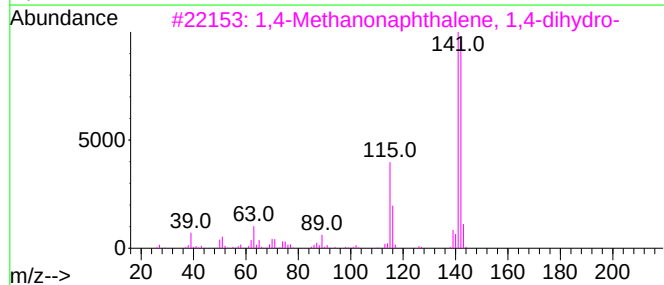
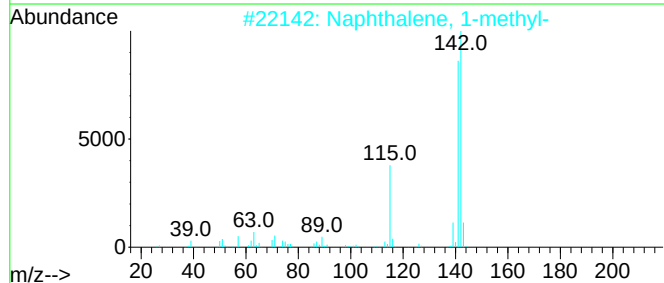
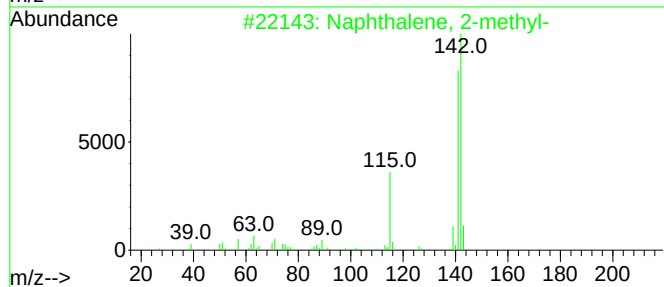
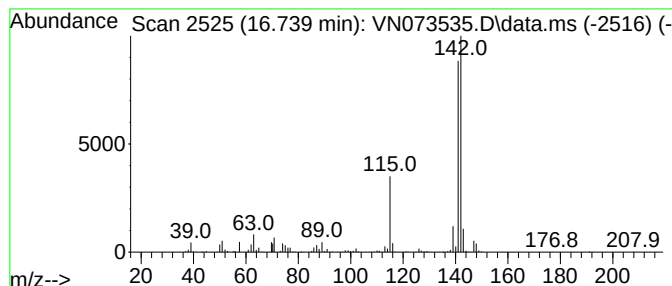
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	76.06 ug/l	2148400	1,4-Dichlorobenzene-d4	13.615

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	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073535.D
Acq On : 20 Jul 2022 20:34
Operator : JC\MD
Sample : N3779-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-A

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

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					#	RT	Resp	Conc
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Thiophene, 3-me...	10.698	7.1	ug/l	172042	3	11.686	1213960	50.0
Thiophene, 2,3-...	11.086	9.4	ug/l	227245	3	11.686	1213960	50.0
Thiophene, tetr...	11.163	56.2	ug/l	1363800	3	11.686	1213960	50.0
Thiophene, tetr...	12.027	17.2	ug/l	417472	3	11.686	1213960	50.0
2H-Thiopyran, 3...	12.463	10.6	ug/l	258142	3	11.686	1213960	50.0
Indene	13.998	20.8	ug/l	586903	4	13.615	1412250	50.0
Benzo[c]thiophene	15.533	11.2	ug/l	315860	4	13.615	1412250	50.0
Naphthalene, 2-...	16.527	97.6	ug/l	2757350	4	13.615	1412250	50.0
Naphthalene, 1-...	16.739	76.1	ug/l	2148400	4	13.615	1412250	50.0