

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073536.D
 Acq On : 20 Jul 2022 20:59
 Operator : JC\MD
 Sample : N3779-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-B

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: VN073536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.228	385	398	407	rBV	41928	124936	1.35%	0.404%
2	4.516	427	447	459	rBV2	27440	105887	1.14%	0.342%
3	7.745	987	996	1008	rBV2	44218	110951	1.20%	0.359%
4	7.951	1021	1031	1036	rBV	188439	448174	4.85%	1.448%
5	8.016	1036	1042	1059	rVB	342450	792034	8.56%	2.559%
6	8.386	1090	1105	1122	rBV3	383765	1098120	11.87%	3.548%
7	8.904	1183	1193	1208	rBV	492611	1004709	10.86%	3.246%
8	10.380	1436	1444	1450	rBV	670468	1226004	13.26%	3.962%
9	10.445	1450	1455	1465	rVB	414962	759556	8.21%	2.454%
10	10.698	1490	1498	1506	rBV	112977	200784	2.17%	0.649%
11	11.163	1570	1577	1589	rVB	447396	834960	9.03%	2.698%
12	11.686	1655	1666	1670	rBV	702496	1275895	13.80%	4.123%
13	11.727	1670	1673	1679	rVV	244510	440834	4.77%	1.424%
14	11.786	1679	1683	1691	rVV	85675	170891	1.85%	0.552%
15	11.892	1691	1701	1712	rVB	375819	725083	7.84%	2.343%
16	12.027	1717	1724	1737	rBV4	118339	239672	2.59%	0.774%
17	12.221	1751	1757	1765	rVB2	358572	636759	6.88%	2.058%
18	12.463	1792	1798	1803	rVV2	109161	207301	2.24%	0.670%
19	12.510	1803	1806	1812	rVB3	54268	97645	1.06%	0.316%
20	12.674	1820	1834	1845	rBV	602728	1129893	12.22%	3.651%
21	12.951	1869	1881	1886	rBV2	163711	409354	4.43%	1.323%
22	12.998	1886	1889	1894	rVB	70525	101089	1.09%	0.327%
23	13.163	1913	1917	1925	rVB2	52904	111318	1.20%	0.360%
24	13.304	1934	1941	1947	rVB2	303033	644383	6.97%	2.082%
25	13.498	1959	1974	1986	rBV7	122202	583765	6.31%	1.886%
26	13.615	1987	1994	2006	rVV2	814246	1719753	18.59%	5.557%
27	13.815	2022	2028	2032	rBV2	68895	132471	1.43%	0.428%
28	13.998	2053	2059	2066	rBV	293734	524133	5.67%	1.694%
29	14.857	2199	2205	2213	rBV3	69056	172757	1.87%	0.558%
30	15.015	2227	2232	2236	rBV2	54760	101213	1.09%	0.327%
31	15.433	2291	2303	2313	rBV	4789542	9248668	100.00%	29.885%
32	15.533	2314	2320	2328	rVB	153848	299403	3.24%	0.967%
33	16.462	2470	2478	2481	rBV3	43561	94765	1.02%	0.306%
34	16.533	2481	2490	2504	rVV	1324050	2984335	32.27%	9.643%
35	16.739	2516	2525	2533	rBV	965735	2190063	23.68%	7.077%

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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

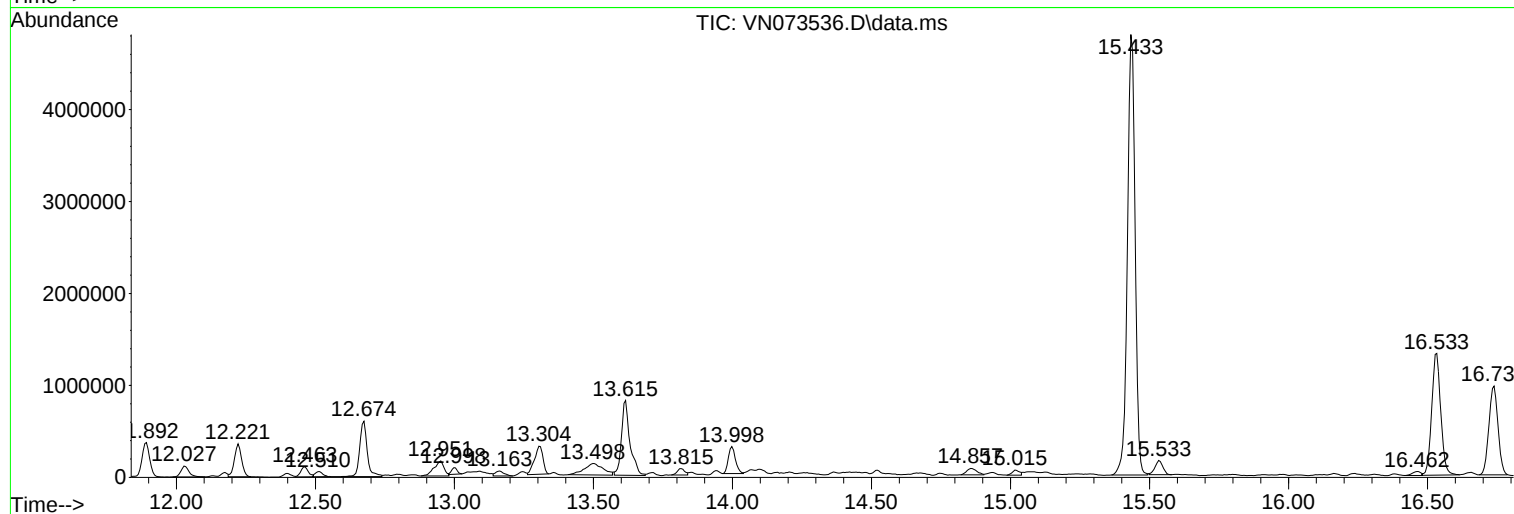
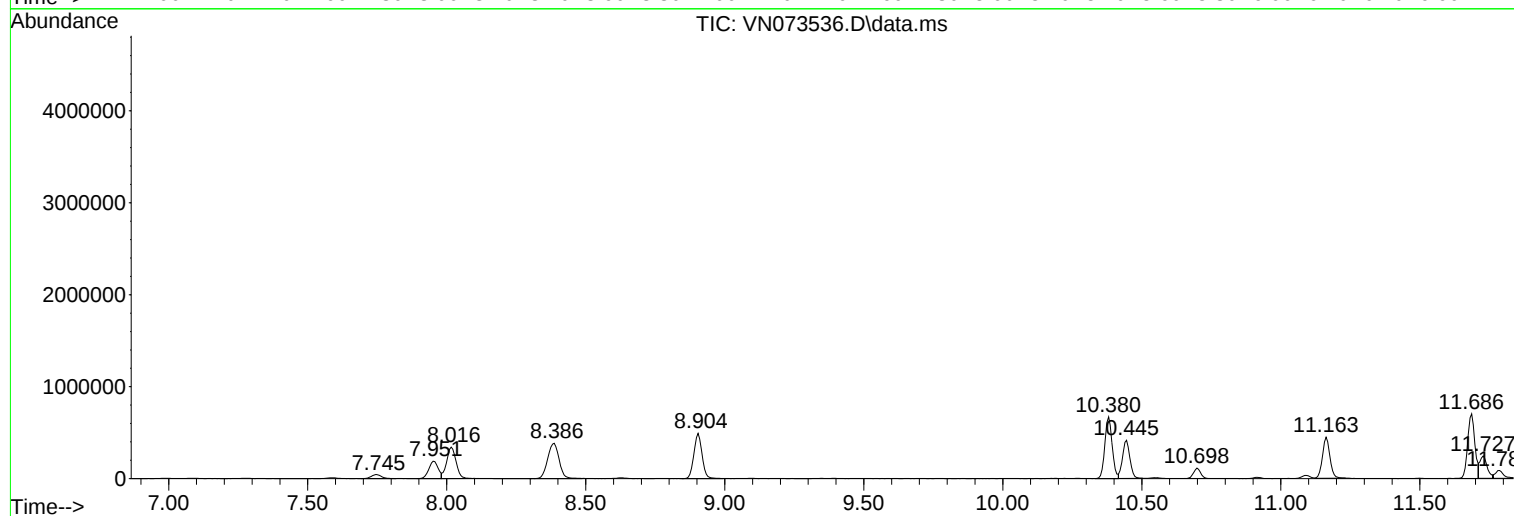
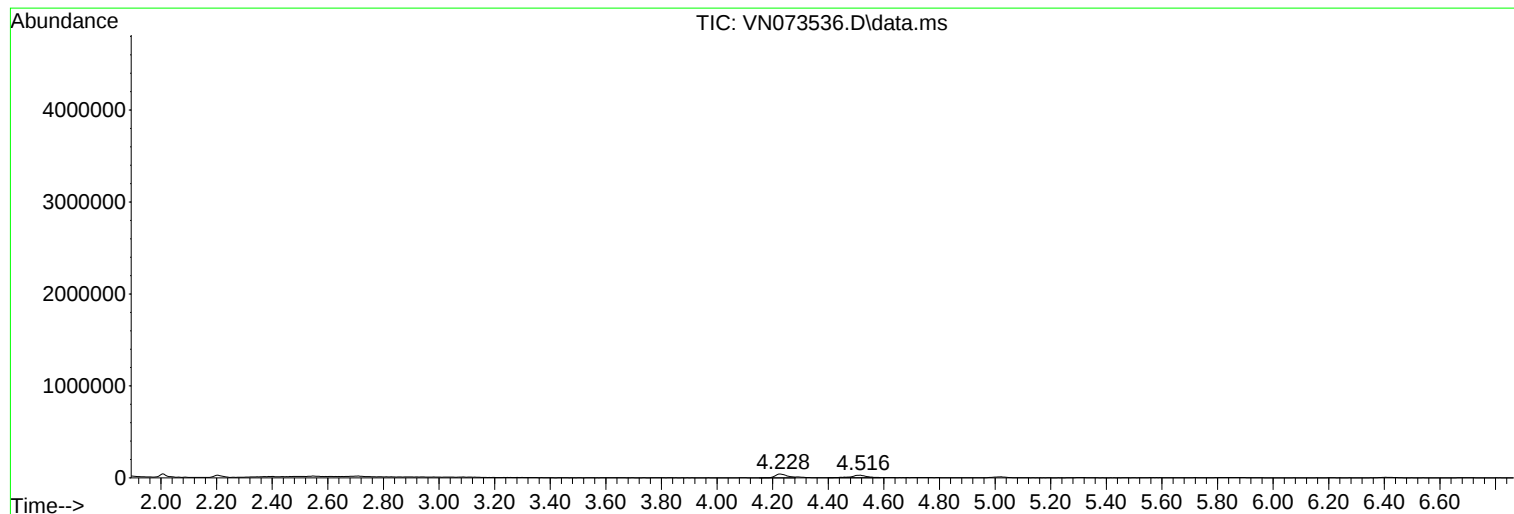
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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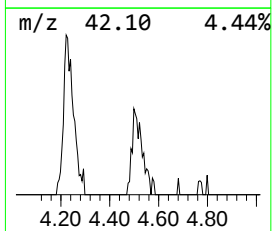
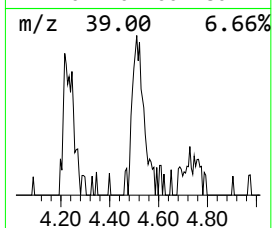
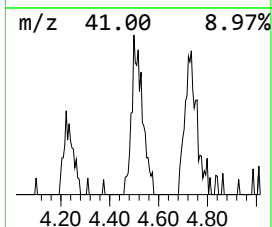
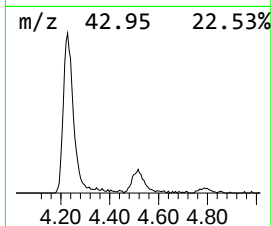
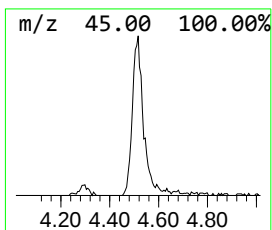
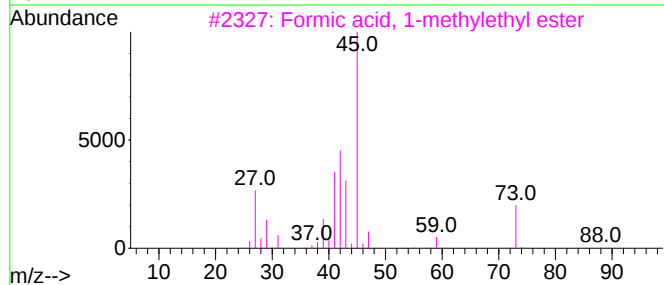
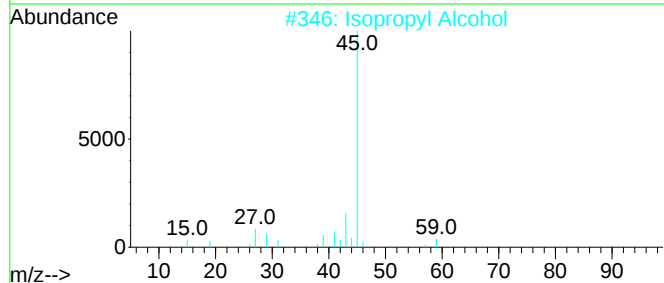
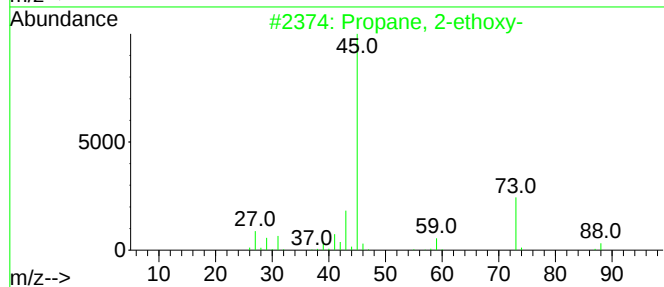
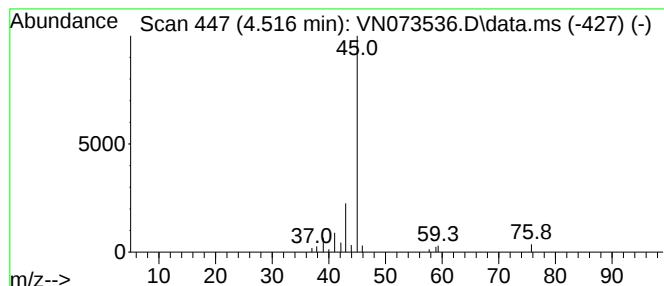
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane, 2-ethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.516	6.68 ug/l	105887	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4			2-Pentanol	88	C5H12O	006032-29-7	9
5			Ethanol, 2-methoxy-, carbonate (...)	178	C7H14O5	000626-84-6	9



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Instrument :
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ClientSampleId :
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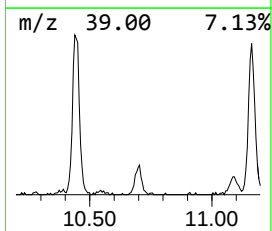
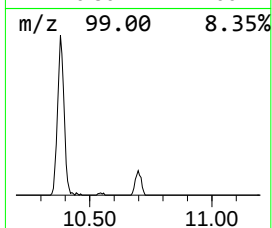
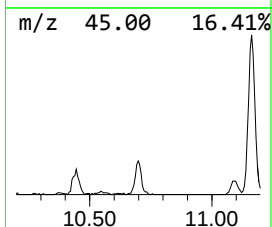
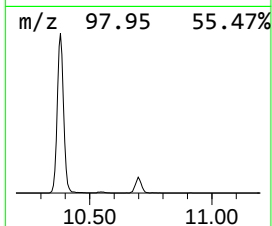
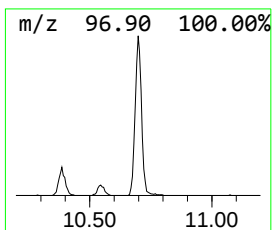
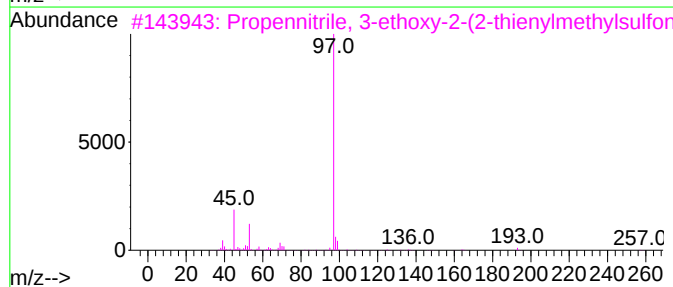
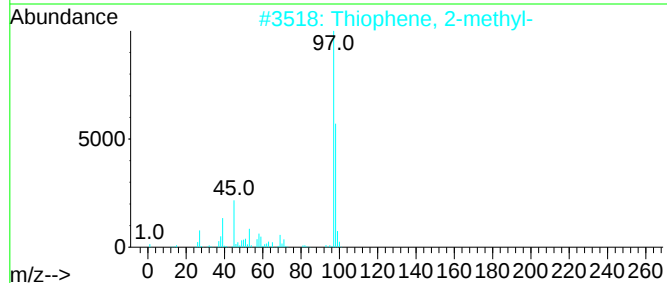
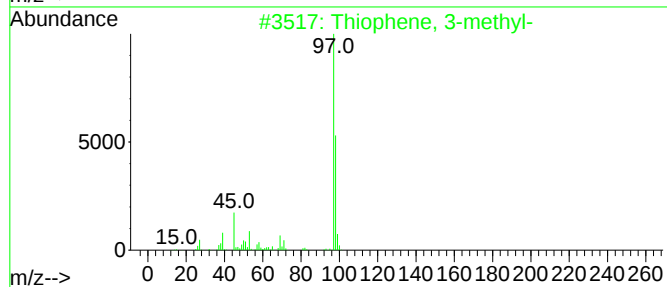
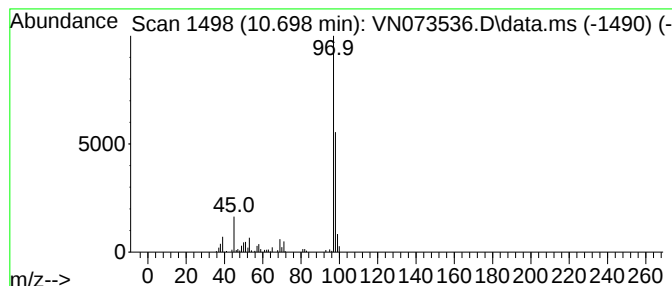
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Peak Number 2 Thiophene, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.698	7.87 ug/l	200784	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	97
2			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
3			Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11NO3S2	1000267-97-5	53
4			2-Fluoropyridine	97	C5H4FN	000372-48-5	47
5			Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	47



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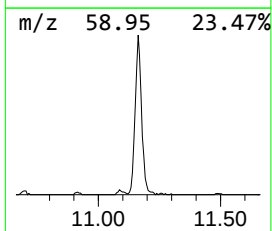
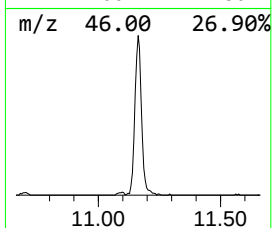
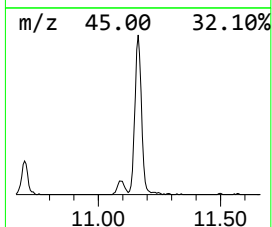
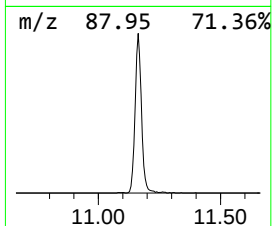
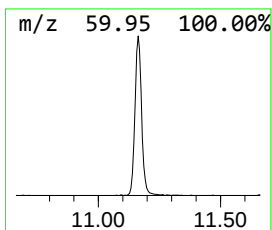
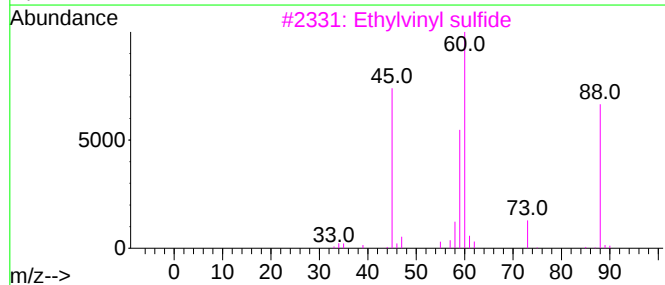
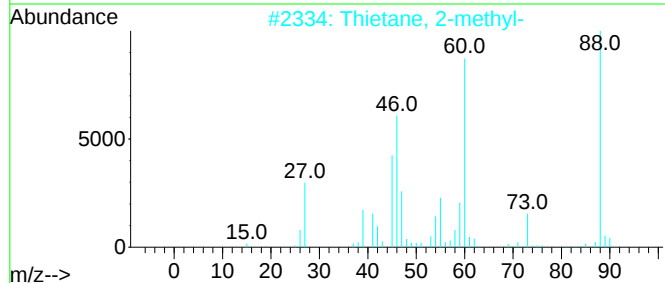
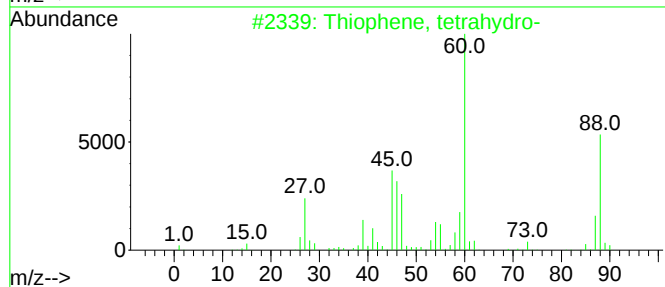
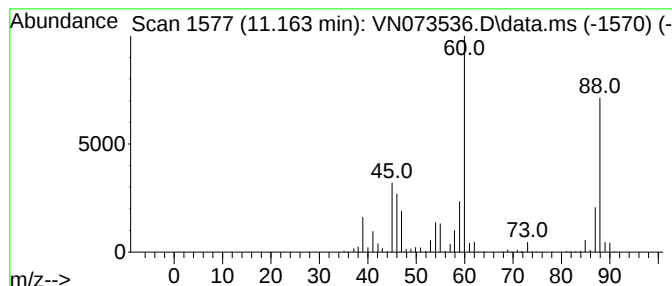
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Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	32.72 ug/l	834960	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	74
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5			Acetic acid, nitro-, ethyl ester	133	C4H7NO4	000626-35-7	27



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ALS Vial : 14 Sample Multiplier: 1

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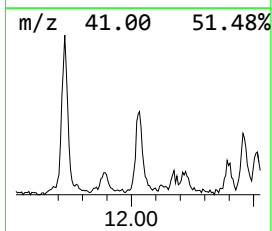
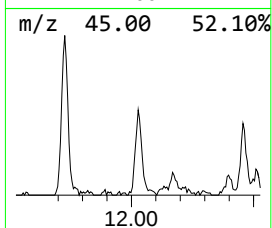
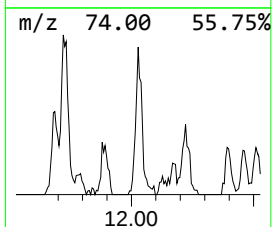
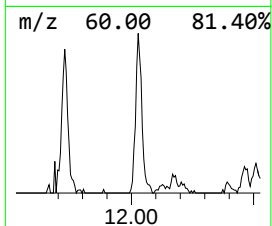
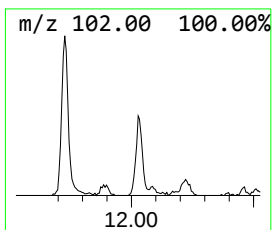
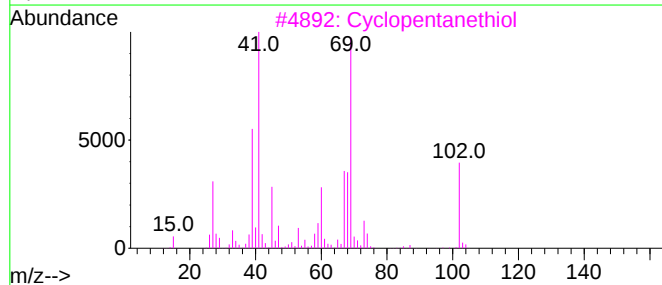
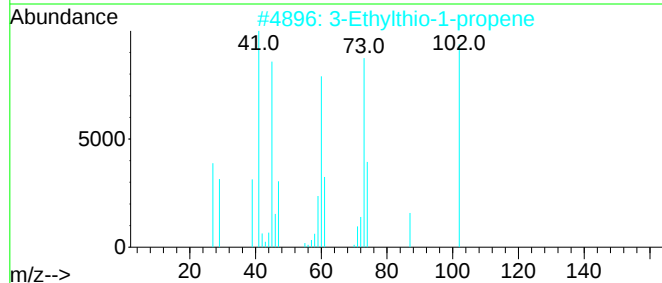
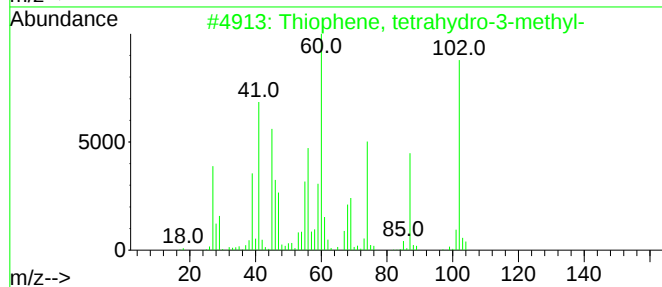
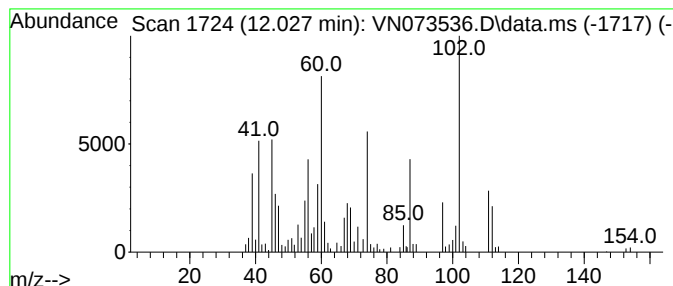
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophene, tetrahydro-3-met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.027	9.39 ug/l	239672	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	98
2			3-Ethylthio-1-propene	102	C5H10S	005296-62-8	52
3			Cyclopentanethiol	102	C5H10S	001679-07-8	43
4			Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	32
5			2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	25



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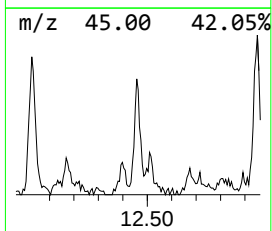
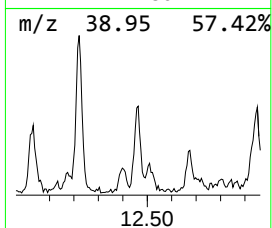
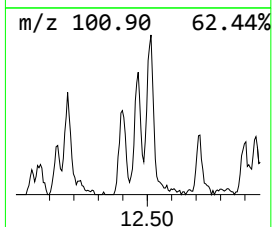
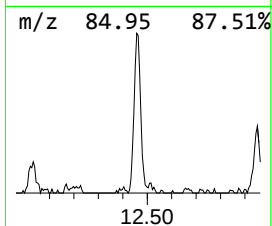
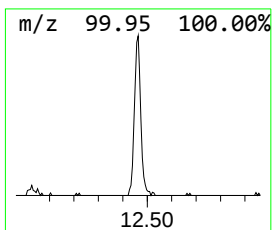
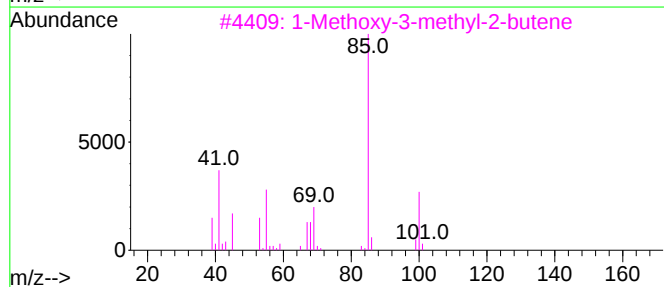
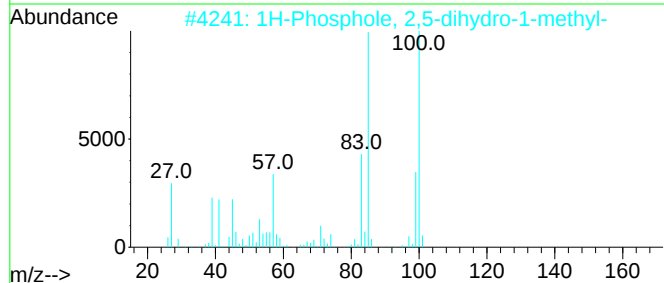
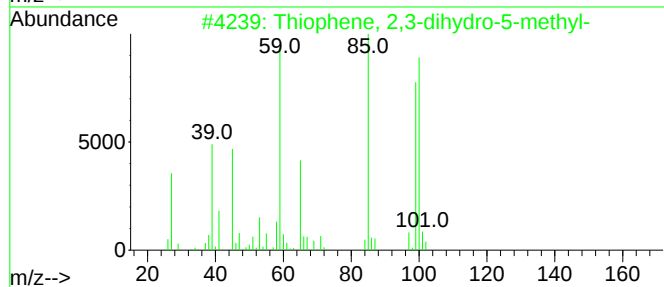
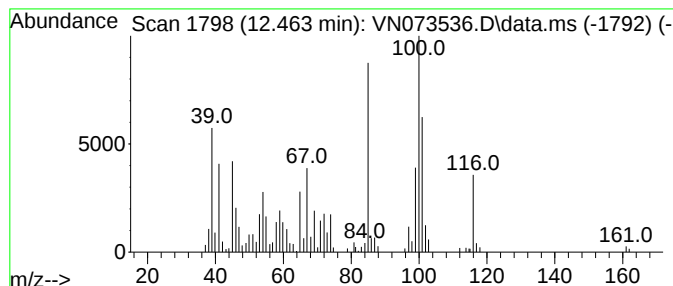
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown12.463 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	8.12 ug/l	207301	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	49
2			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	43
3			1-Methoxy-3-methyl-2-butene	100	C6H12O	022093-99-8	43
4			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	35
5			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073536.D
Acq On : 20 Jul 2022 20:59
Operator : JC\MD
Sample : N3779-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-B

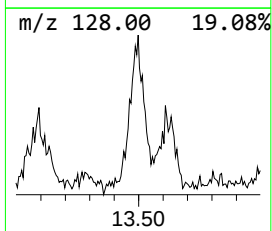
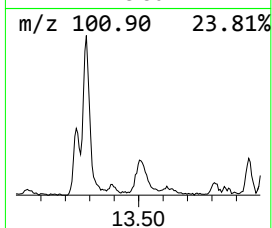
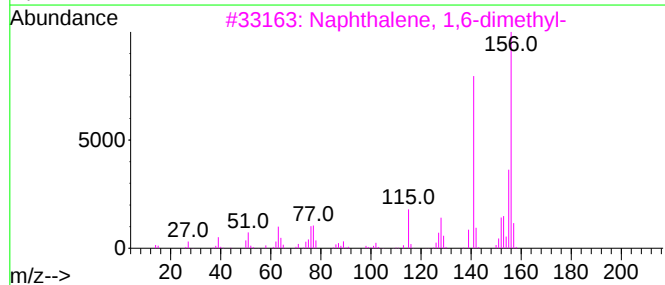
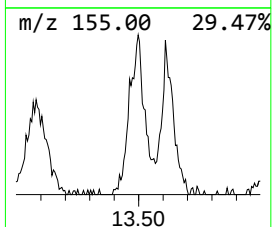
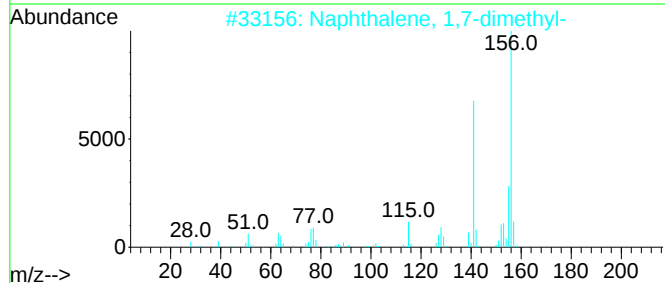
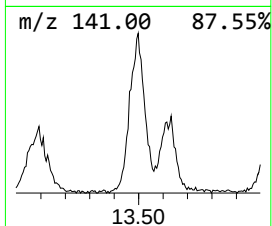
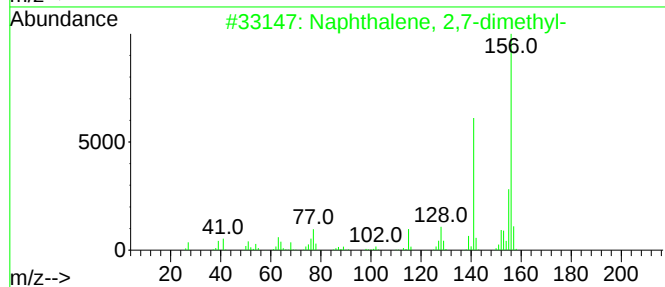
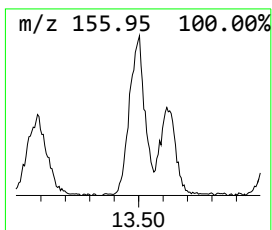
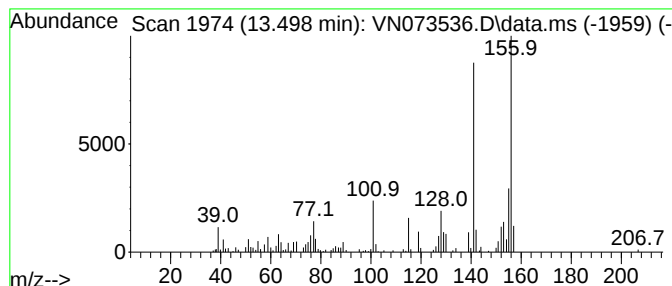
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	16.97 ug/l	583765	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073536.D
Acq On : 20 Jul 2022 20:59
Operator : JC\MD
Sample : N3779-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-B

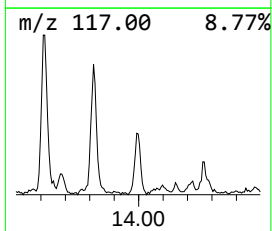
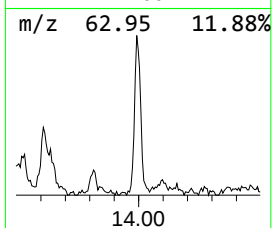
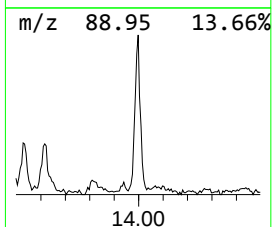
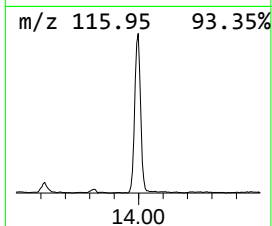
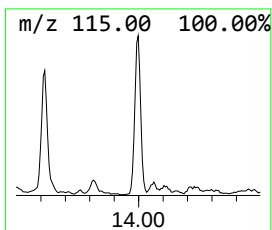
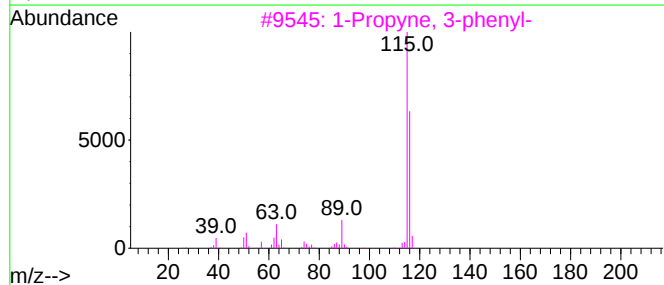
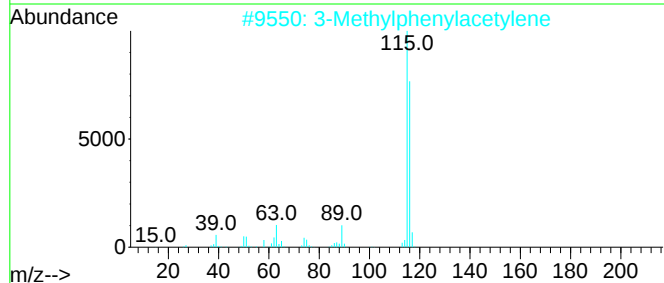
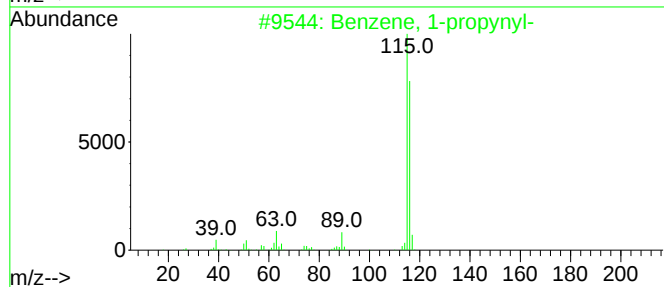
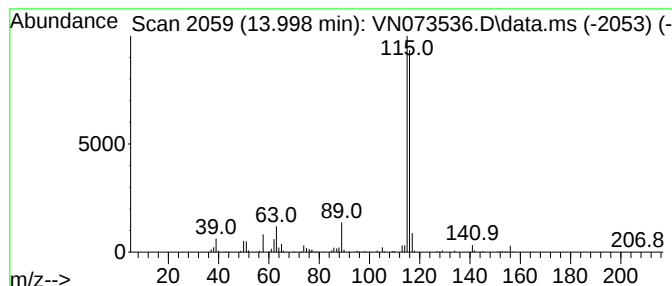
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-propynyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	15.24 ug/l	524133	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	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 : VN073536.D
Acq On : 20 Jul 2022 20:59
Operator : JC\MD
Sample : N3779-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-B

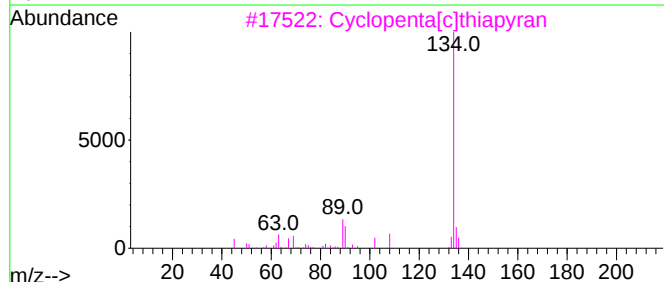
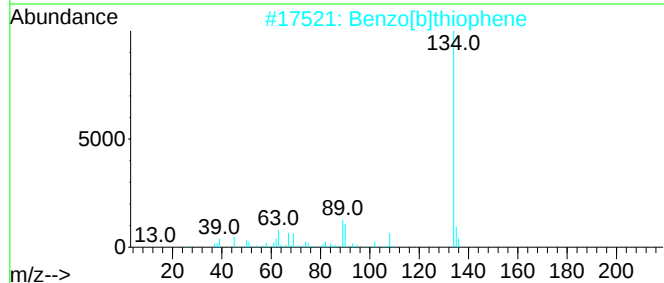
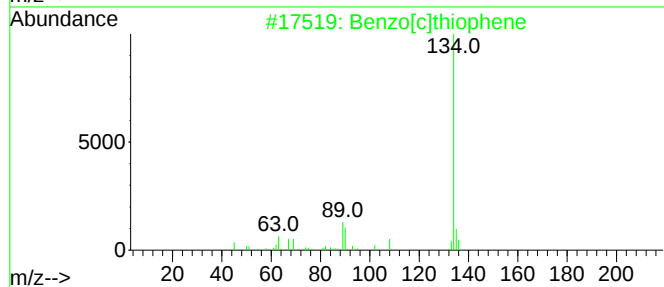
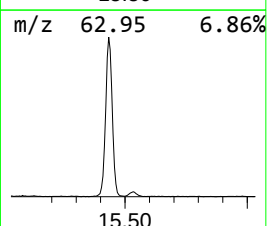
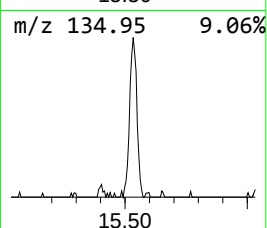
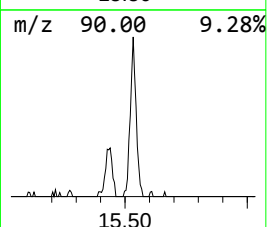
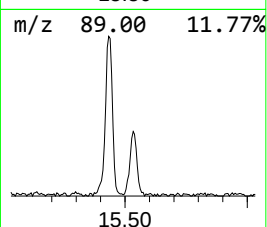
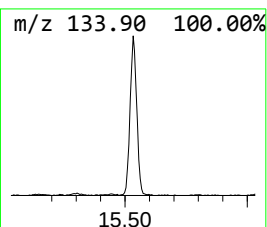
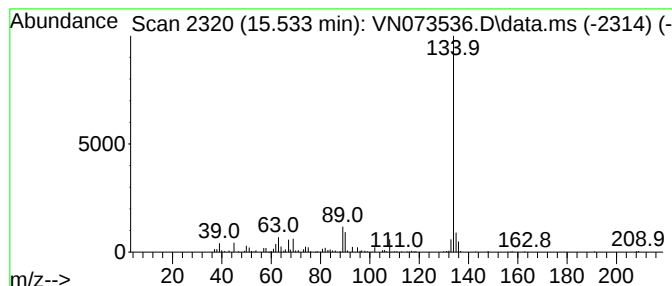
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Quant Title : SW846 8260

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	8.70 ug/l	299403	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			3-Deazaadenine	134	C6H6N4	006811-77-4	59
5			6-Phenyl-[1,3]thiazine-2,4-dione	205	C10H7N02S	1000300-90-1	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073536.D
Acq On : 20 Jul 2022 20:59
Operator : JC\MD
Sample : N3779-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-B

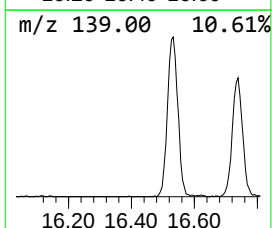
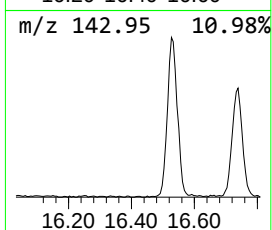
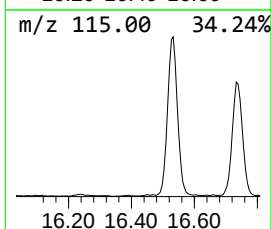
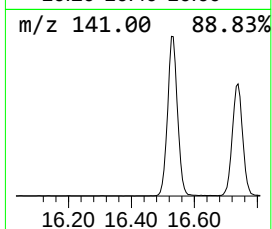
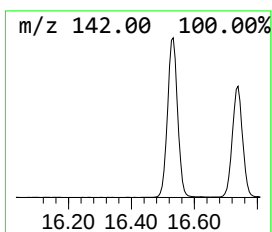
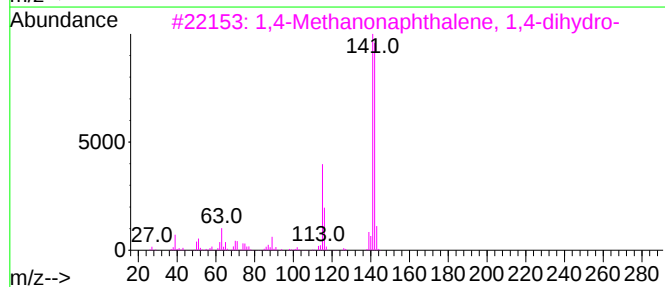
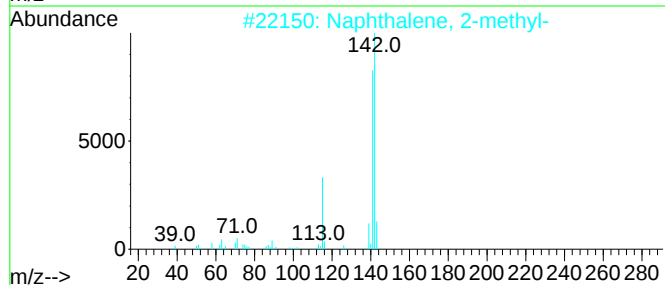
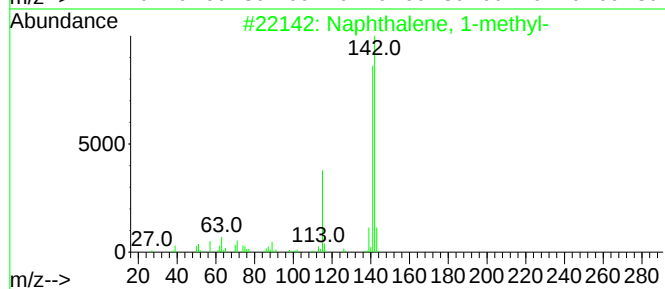
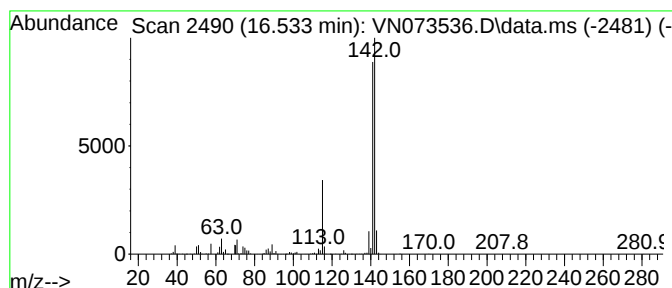
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.533	86.77 ug/l	2984340	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	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	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073536.D
Acq On : 20 Jul 2022 20:59
Operator : JC\MD
Sample : N3779-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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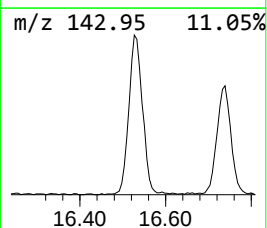
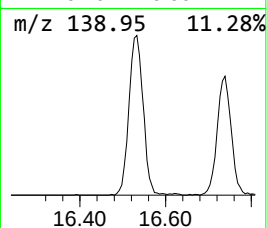
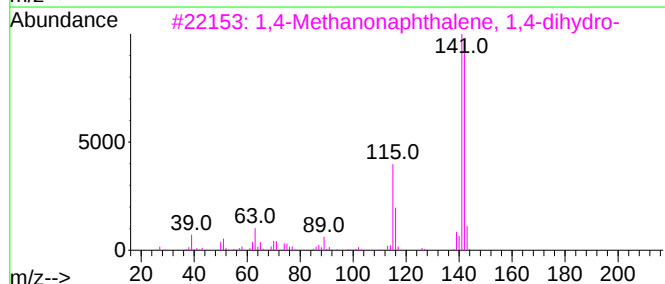
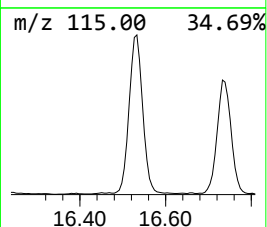
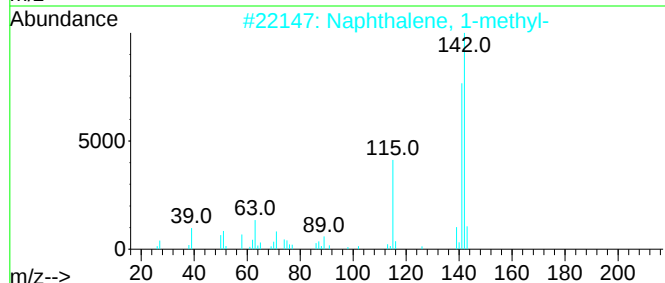
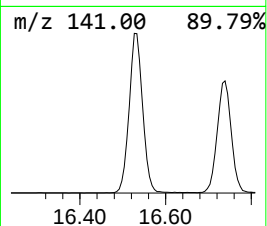
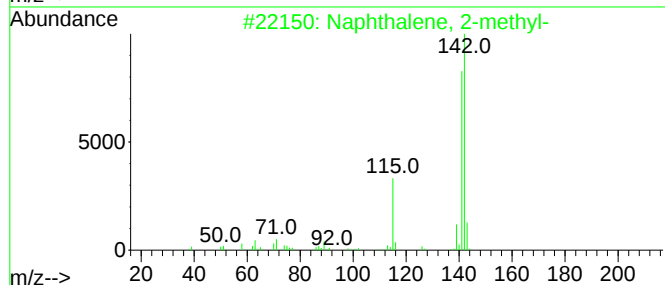
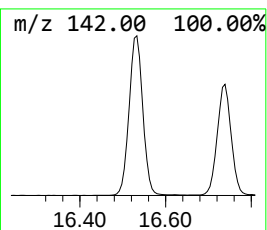
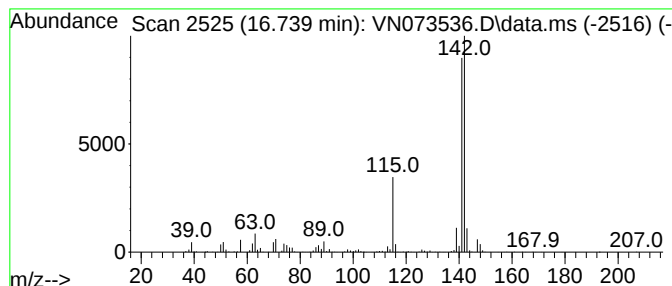
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	63.67 ug/l	2190060	1,4-Dichlorobenzene-d4	13.616

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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073536.D
Acq On : 20 Jul 2022 20:59
Operator : JC\MD
Sample : N3779-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 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

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					#	RT	Resp	Conc
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Thiophene, 3-me...	10.698	7.9	ug/l	200784	3	11.686	1275900	50.0
Thiophene, tetr...	11.163	32.7	ug/l	834960	3	11.686	1275900	50.0
Thiophene, tetr...	12.027	9.4	ug/l	239672	3	11.686	1275900	50.0
unknown12.463	12.463	8.1	ug/l	207301	3	11.686	1275900	50.0
Naphthalene, 2,...	13.498	17.0	ug/l	583765	4	13.616	1719750	50.0
Benzene, 1-prop...	13.998	15.2	ug/l	524133	4	13.616	1719750	50.0
Benzo[c]thiophene	15.533	8.7	ug/l	299403	4	13.616	1719750	50.0
Naphthalene, 1-...	16.533	86.8	ug/l	2984340	4	13.616	1719750	50.0
Naphthalene, 2-...	16.739	63.7	ug/l	2190060	4	13.616	1719750	50.0