

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073538.D
 Acq On : 20 Jul 2022 21:48
 Operator : JC\MD
 Sample : N3779-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-D

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: VN073538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.004	15	20	29	rVB	245458	360243	3.43%	0.951%
2	7.745	987	996	1011	rBV2	40252	115082	1.10%	0.304%
3	7.951	1020	1031	1036	rBV	193428	462373	4.41%	1.221%
4	8.016	1036	1042	1058	rVB	355687	827882	7.89%	2.186%
5	8.386	1093	1105	1124	rBV3	520122	1436399	13.69%	3.794%
6	8.904	1184	1193	1208	rBV	504276	1042626	9.94%	2.754%
7	10.380	1435	1444	1450	rBV	696931	1288407	12.28%	3.403%
8	10.445	1450	1455	1467	rVB	668383	1227057	11.69%	3.241%
9	11.092	1558	1565	1570	rBV2	51486	110390	1.05%	0.292%
10	11.163	1570	1577	1586	rVV	812185	1506529	14.36%	3.979%
11	11.686	1657	1666	1670	rVV	760410	1389839	13.25%	3.671%
12	11.727	1670	1673	1679	rVV	453266	782840	7.46%	2.068%
13	11.786	1679	1683	1691	rVV	126585	246538	2.35%	0.651%
14	11.892	1693	1701	1710	rVB	489958	917756	8.75%	2.424%
15	12.021	1714	1723	1737	rVV4	315724	729462	6.95%	1.927%
16	12.221	1752	1757	1769	rVB3	496590	934118	8.90%	2.467%
17	12.463	1792	1798	1802	rVV2	191920	346749	3.30%	0.916%
18	12.510	1802	1806	1815	rVB2	104485	198698	1.89%	0.525%
19	12.674	1824	1834	1845	rBV	647272	1234450	11.76%	3.260%
20	12.951	1868	1881	1886	rBV2	294736	711019	6.78%	1.878%
21	12.998	1886	1889	1894	rVB	84333	108832	1.04%	0.287%
22	13.163	1913	1917	1924	rVB	71404	161680	1.54%	0.427%
23	13.245	1924	1931	1934	rBV2	86165	164995	1.57%	0.436%
24	13.304	1934	1941	1947	rVV2	431671	977848	9.32%	2.583%
25	13.504	1965	1975	1986	rBV6	132523	496289	4.73%	1.311%
26	13.615	1987	1994	2005	rVB2	909860	1901567	18.12%	5.022%
27	13.815	2016	2028	2032	rBV3	107399	228693	2.18%	0.604%
28	13.939	2044	2049	2053	rBV2	85412	147770	1.41%	0.390%
29	13.998	2053	2059	2066	rVV	516388	907128	8.65%	2.396%
30	14.857	2197	2205	2213	rBV5	90447	261896	2.50%	0.692%
31	15.015	2228	2232	2236	rBV2	66129	119938	1.14%	0.317%
32	15.433	2291	2303	2314	rBV	5262359	10492588	100.00%	27.711%
33	15.533	2314	2320	2328	rVB	163955	316986	3.02%	0.837%
34	16.462	2471	2478	2482	rVV3	55013	112345	1.07%	0.297%
35	16.533	2482	2490	2505	rVV	1384702	3162221	30.14%	8.352%
36	16.739	2516	2525	2533	rVB	1065776	2434456	23.20%	6.430%

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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
Title : SW846 8260

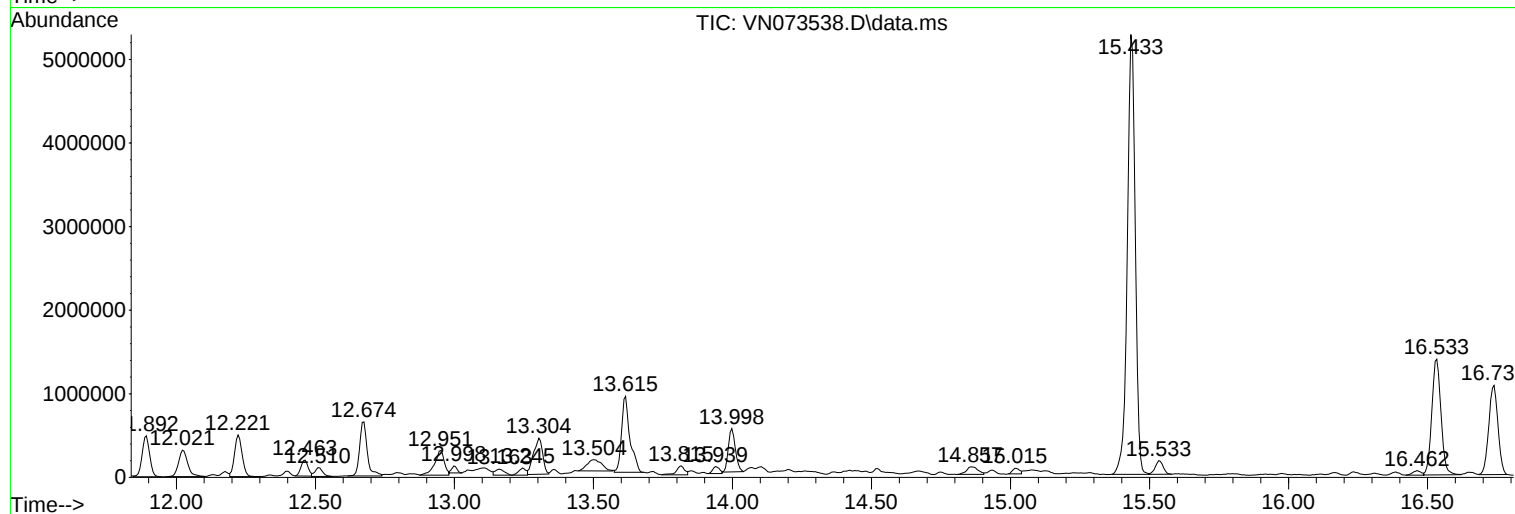
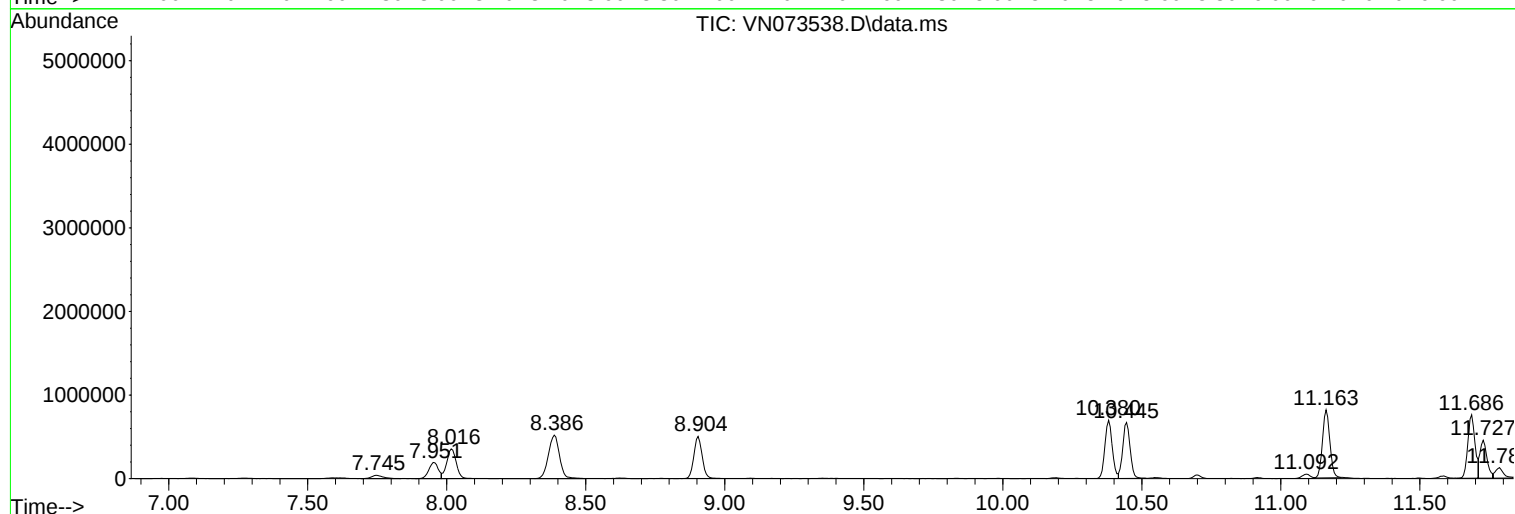
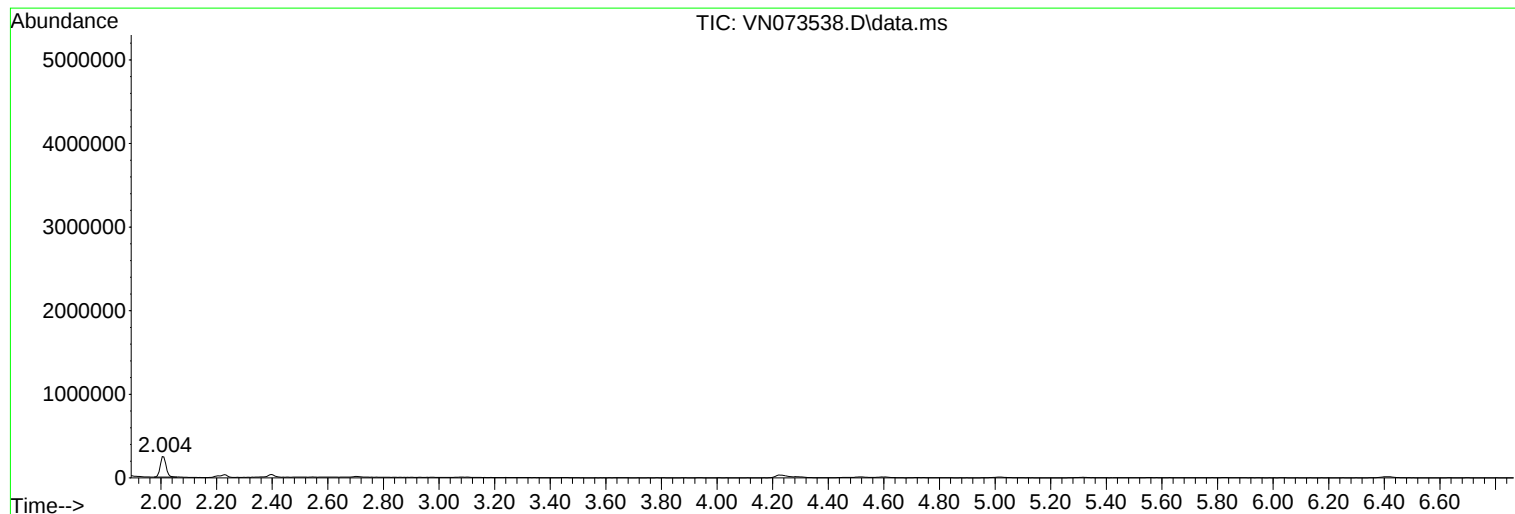
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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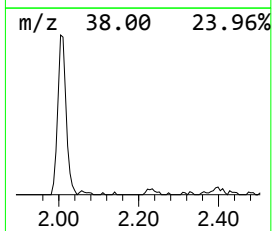
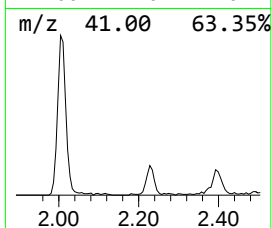
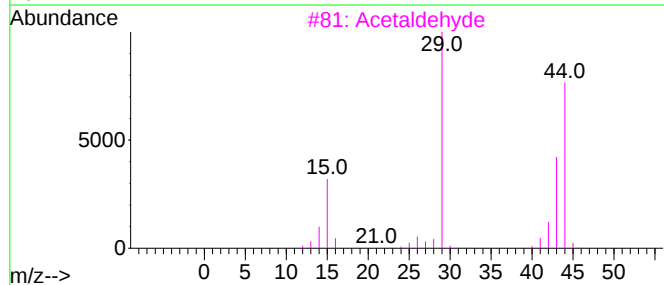
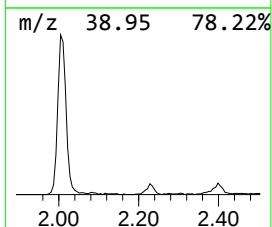
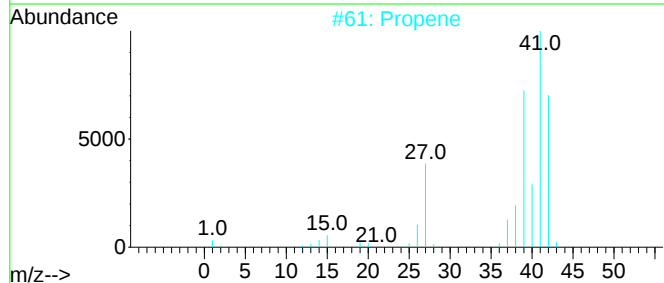
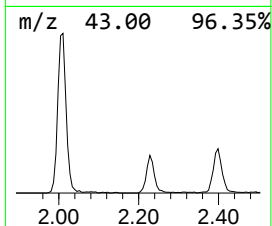
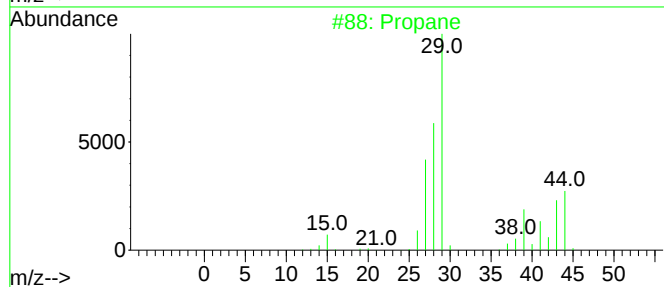
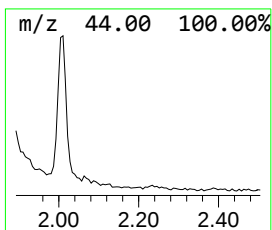
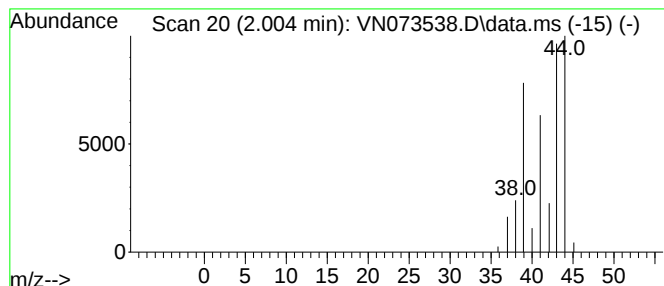
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.004	21.76 ug/l	360243	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propene	42	C3H6	000115-07-1	9
3			Acetaldehyde	44	C2H4O	000075-07-0	5
4			Cyclopropene	40	C3H4	002781-85-3	4
5			1-(Methylamino)propan-2-ol	89	C4H11NO	1000486-79-1	2



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Instrument :
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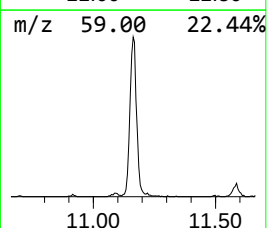
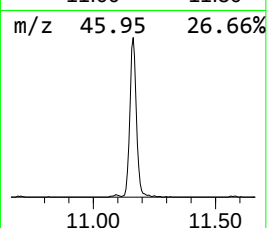
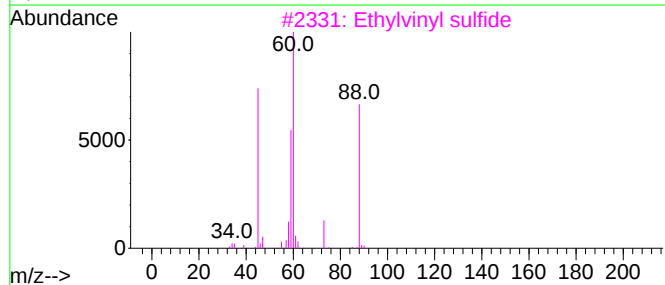
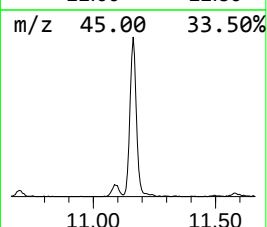
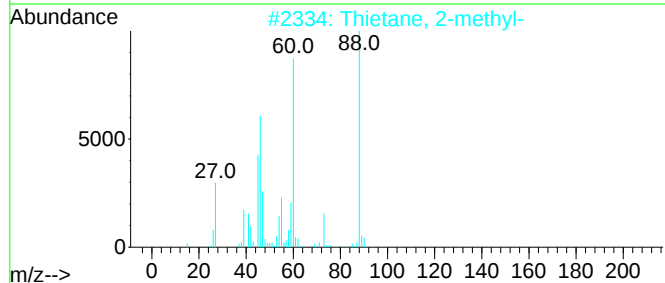
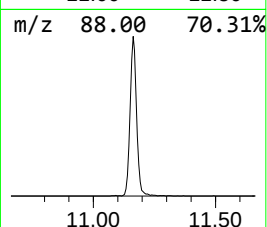
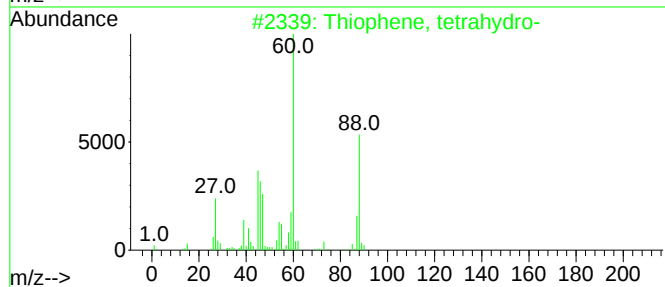
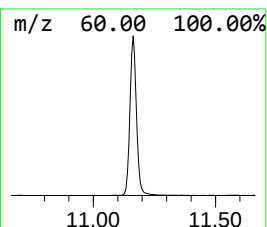
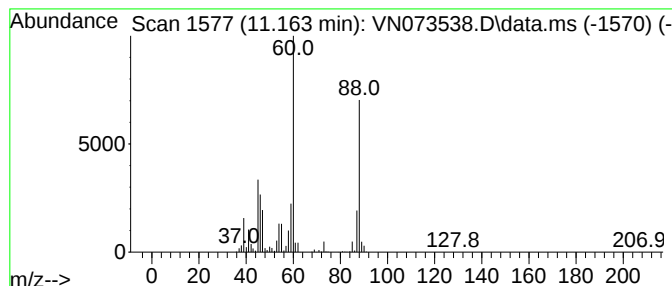
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Peak Number 2 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	54.20 ug/l	1506530	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	49
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	23



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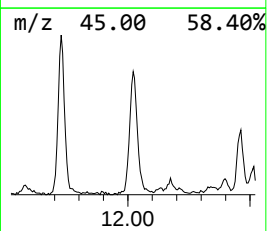
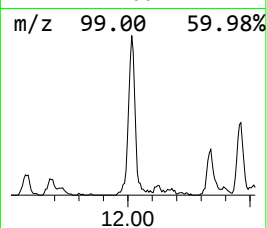
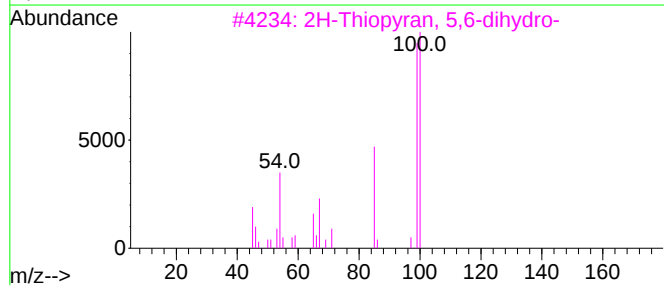
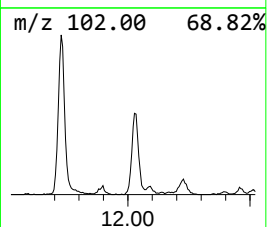
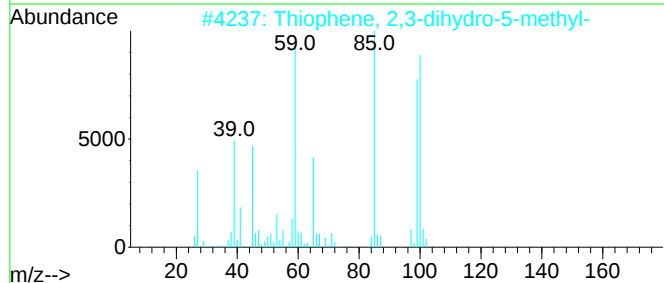
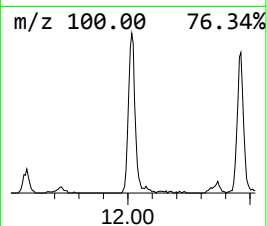
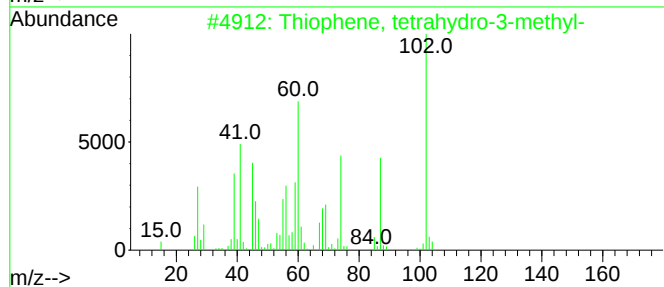
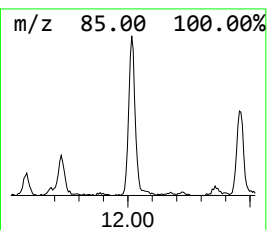
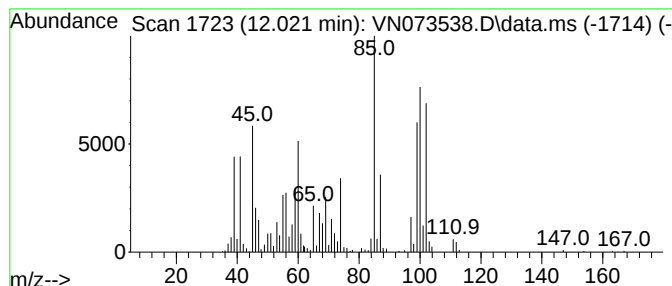
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.022	26.24 ug/l	729462	Chlorobenzene-d5	11.686	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	86
2	Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	49
3	2H-Thiopyran, 5,6-dihydro-	100	C5H8S	040697-99-2	43
4	1-Methoxy-2-methyl-2-butene	100	C6H12O	1000279-59-7	38
5	1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	38



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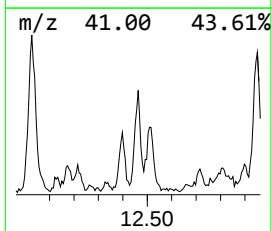
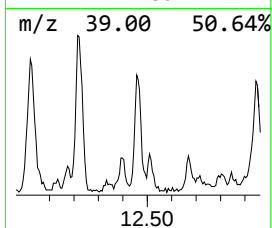
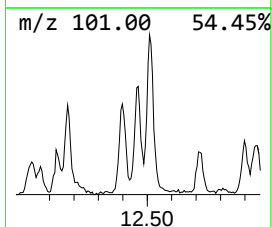
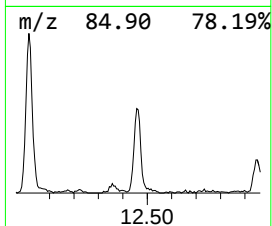
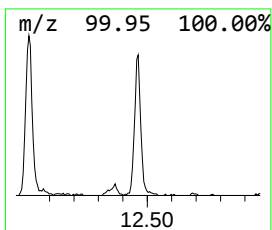
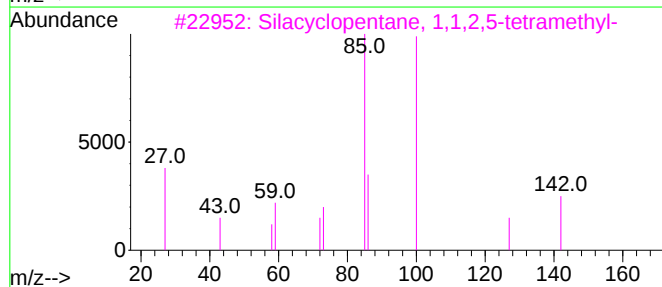
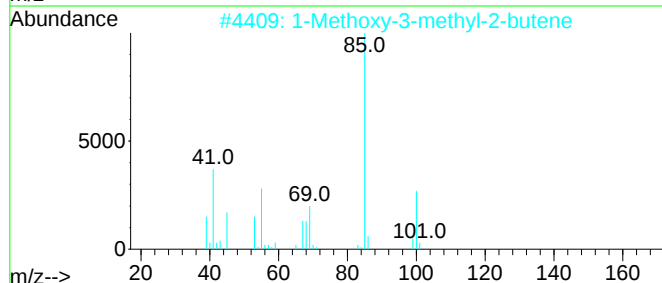
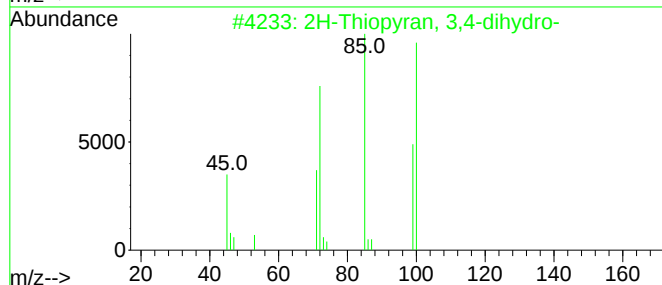
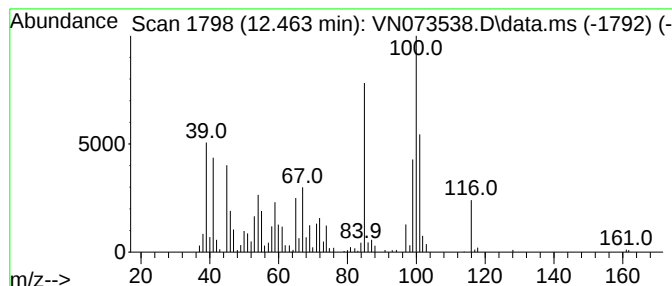
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	12.47 ug/l	346749	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Thiopyran, 3,4-dihydro-	100	C5H8S	013042-80-3	58
2			1-Methoxy-3-methyl-2-butene	100	C6H12O	022093-99-8	47
3			Silacyclopentane, 1,1,2,5-tetram...	142	C8H18Si	055956-01-9	32
4			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	30
5			2H-Thiopyran, 5,6-dihydro-	100	C5H8S	040697-99-2	27



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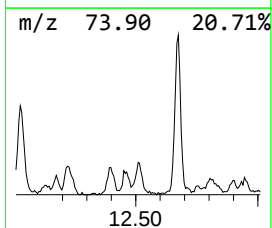
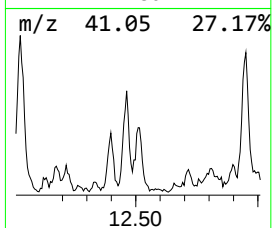
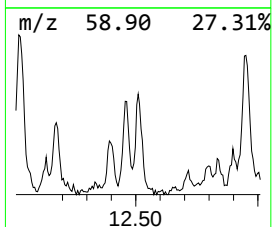
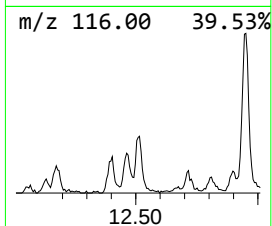
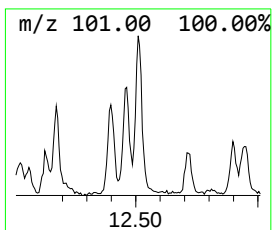
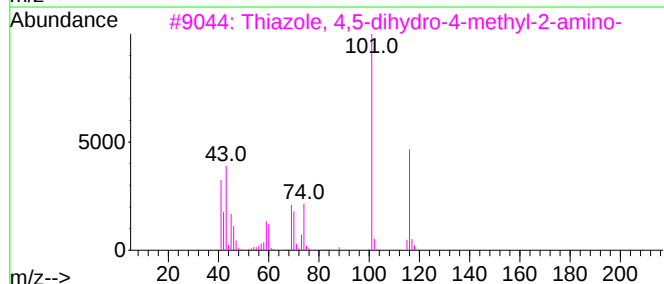
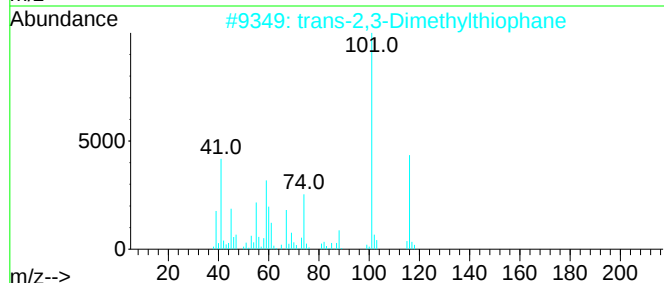
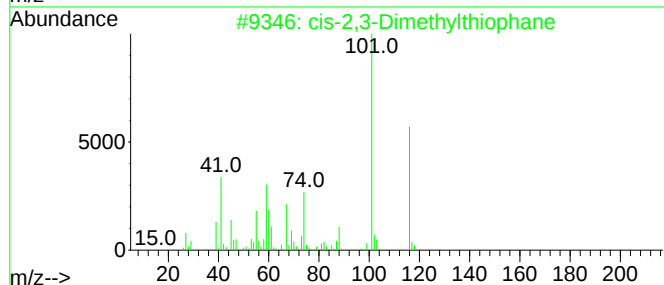
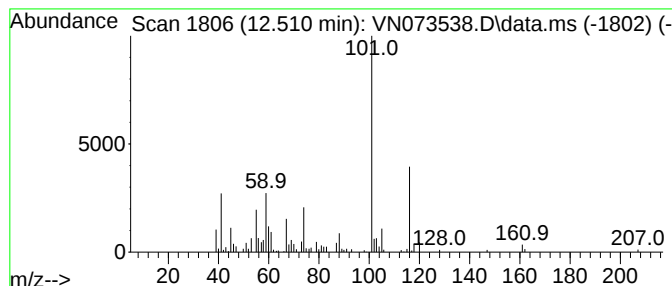
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 cis-2,3-Dimethylthiophane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	7.15 ug/l	198698	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	94
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	83
3			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	72
4			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	72
5			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073538.D
Acq On : 20 Jul 2022 21:48
Operator : JC\MD
Sample : N3779-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-D

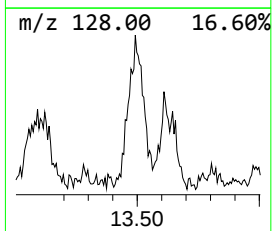
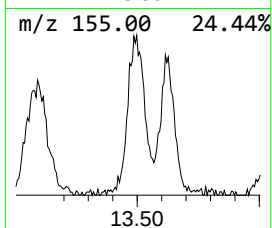
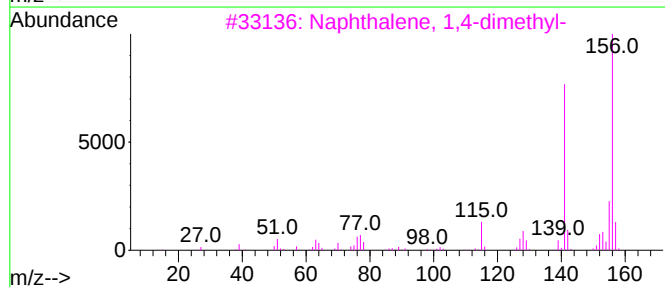
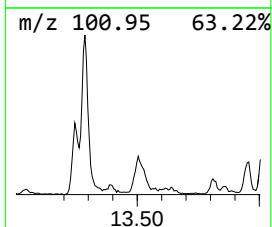
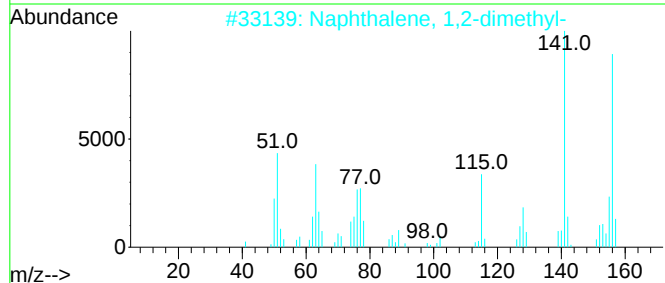
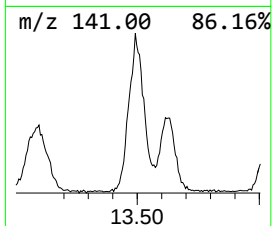
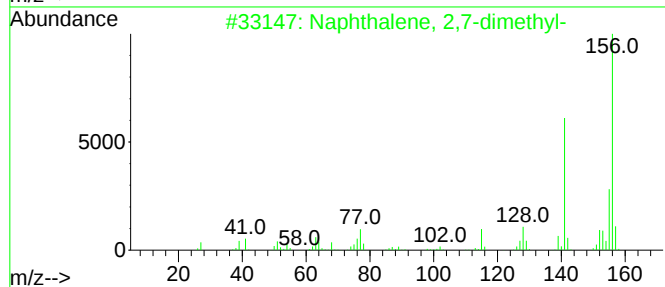
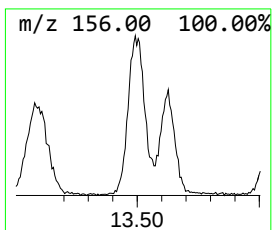
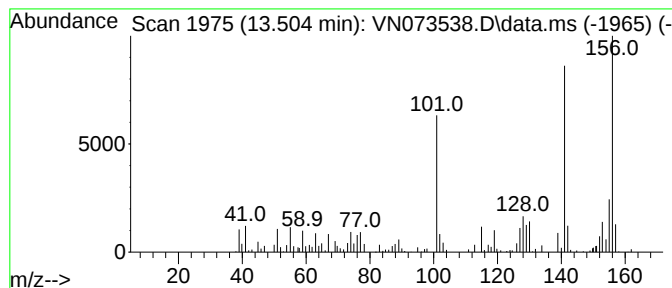
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	13.05 ug/l	496289	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	95
2			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	94
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	94
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073538.D
Acq On : 20 Jul 2022 21:48
Operator : JC\MD
Sample : N3779-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-D

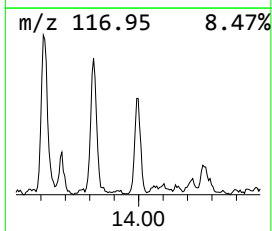
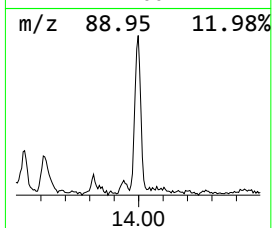
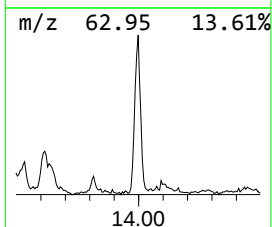
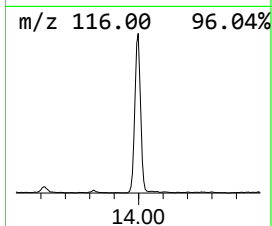
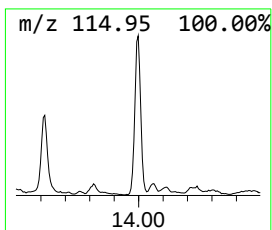
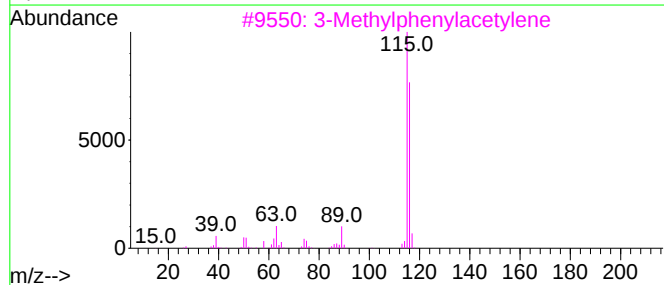
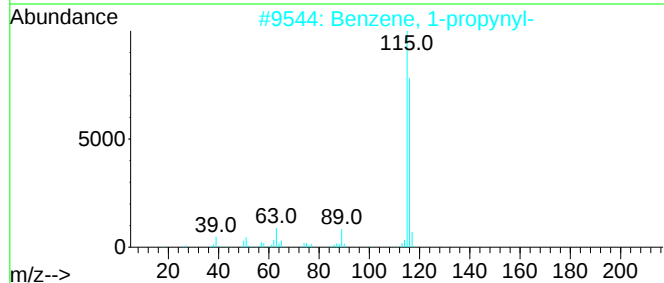
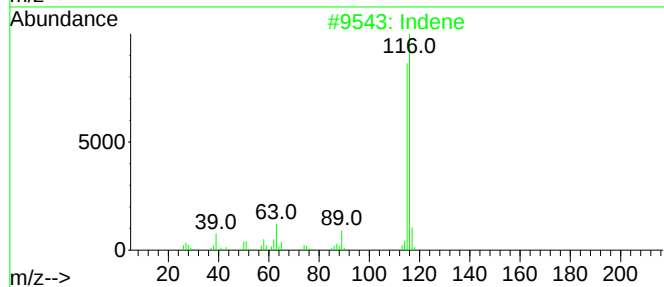
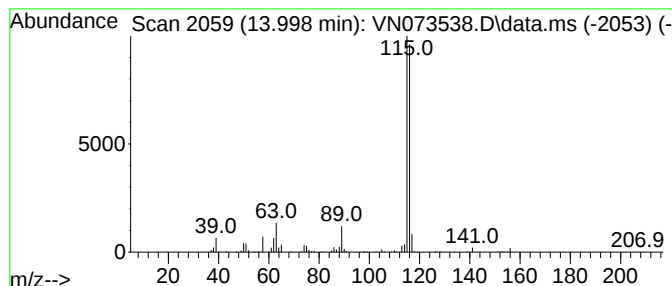
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Quant Title : SW846 8260

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	23.85 ug/l	907128	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	94
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			2-Methylphenylacetylene	116	C9H8	000766-47-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073538.D
Acq On : 20 Jul 2022 21:48
Operator : JC\MD
Sample : N3779-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-D

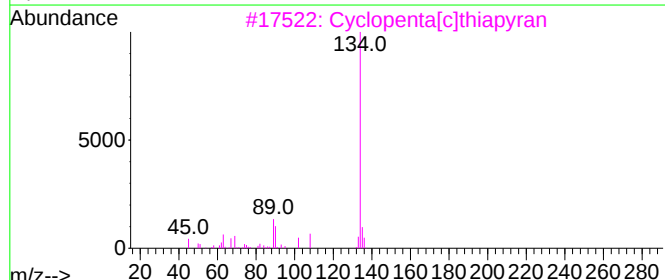
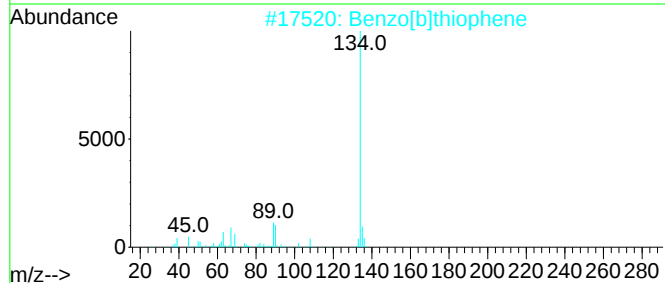
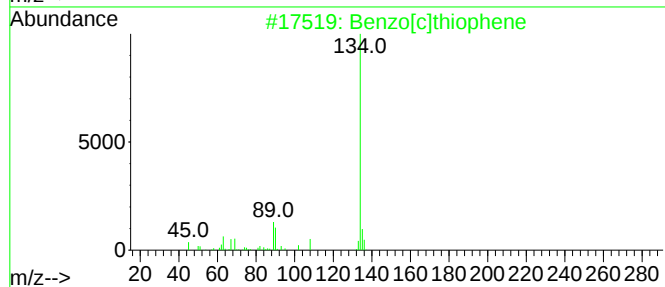
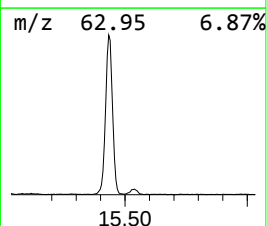
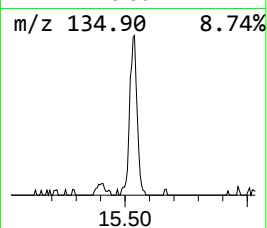
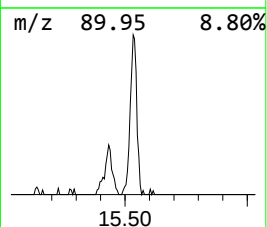
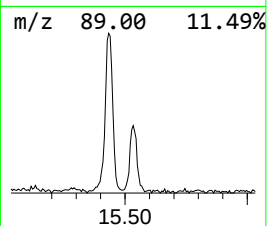
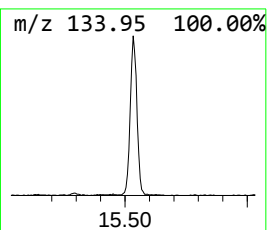
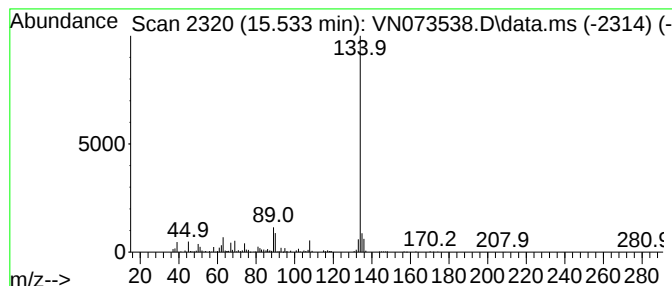
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[c]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	8.33 ug/l	316986	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	93
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	93
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	93
4			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50
5			4-Cyano-2-fluorobenzyl bromide	213	C8H5BrFN	105942-09-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073538.D
Acq On : 20 Jul 2022 21:48
Operator : JC\MD
Sample : N3779-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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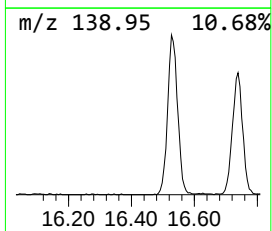
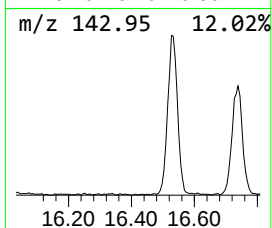
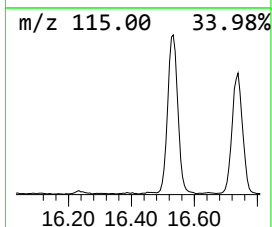
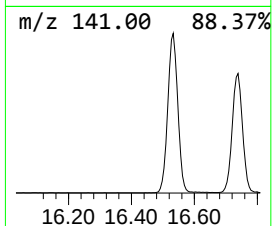
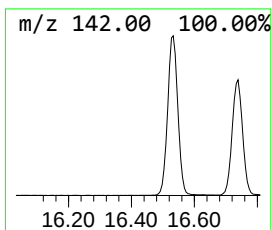
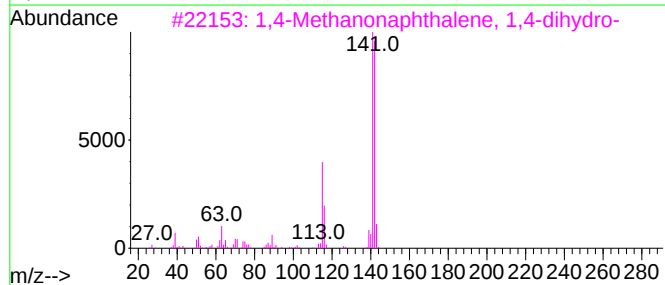
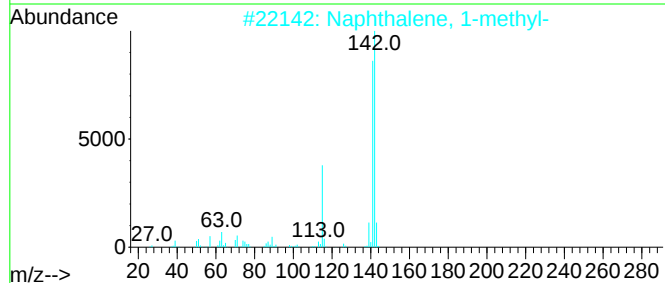
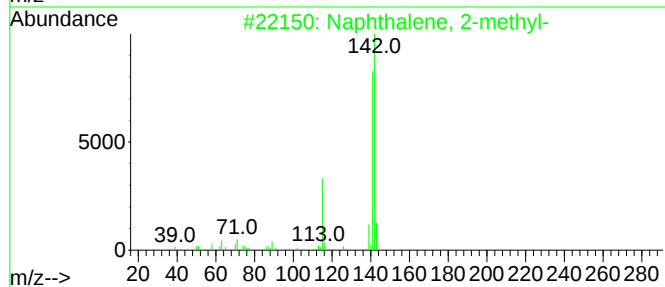
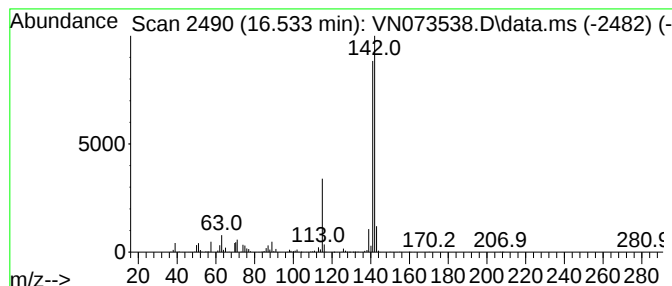
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Quant Title : SW846 8260

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.
16.533	83.15 ug/l	3162220	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073538.D
Acq On : 20 Jul 2022 21:48
Operator : JC\MD
Sample : N3779-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
070622-D

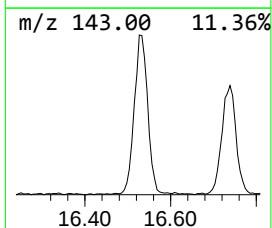
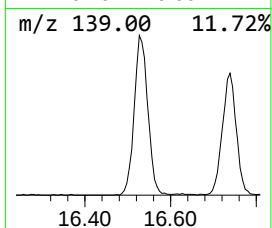
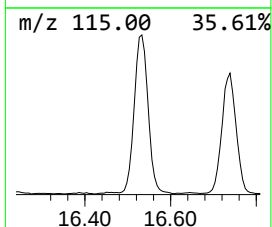
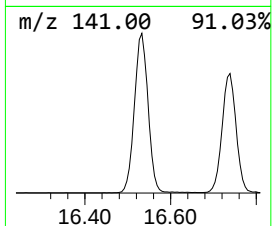
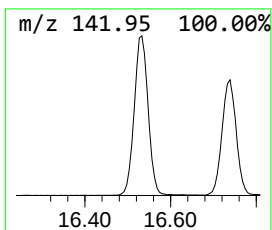
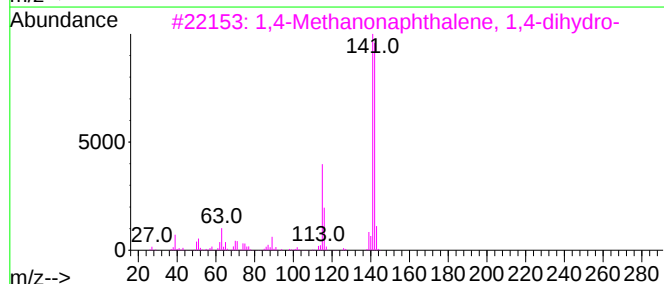
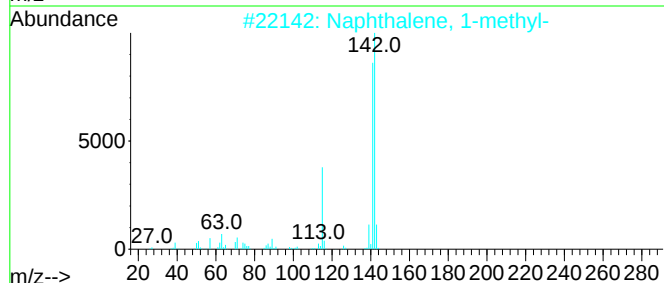
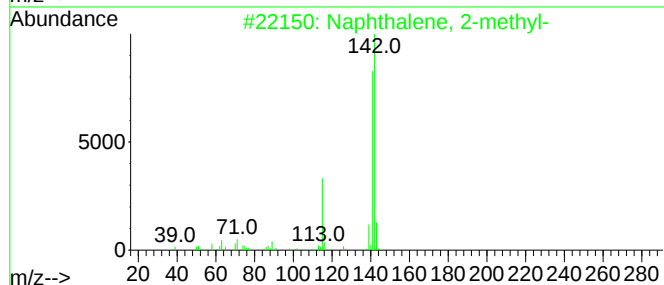
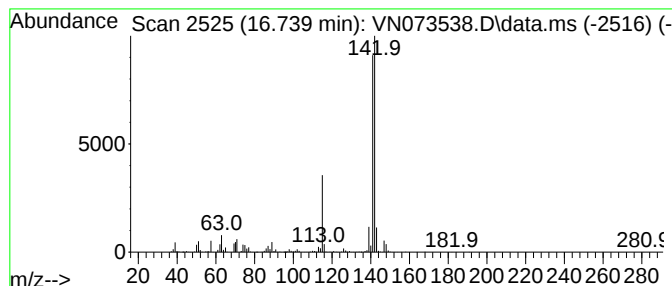
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Quant Title : SW846 8260

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	64.01 ug/l	2434460	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073538.D
Acq On : 20 Jul 2022 21:48
Operator : JC\MD
Sample : N3779-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-D

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, tetr...	11.163	54.2	ug/l	1506530	3	11.686	1389840	50.0
Thiophene, tetr...	12.022	26.2	ug/l	729462	3	11.686	1389840	50.0
2H-Thiopyran, 3...	12.463	12.5	ug/l	346749	3	11.686	1389840	50.0
cis-2,3-Dimethy...	12.510	7.2	ug/l	198698	3	11.686	1389840	50.0
Naphthalene, 2,...	13.504	13.1	ug/l	496289	4	13.616	1901570	50.0
Indene	13.998	23.9	ug/l	907128	4	13.616	1901570	50.0
Benzo[c]thiophene	15.533	8.3	ug/l	316986	4	13.616	1901570	50.0
Naphthalene, 2-...	16.533	83.2	ug/l	3162220	4	13.616	1901570	50.0
Naphthalene, 1-...	16.739	64.0	ug/l	2434460	4	13.616	1901570	50.0