

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073537.D
 Acq On : 20 Jul 2022 21:24
 Operator : JC\MD
 Sample : N3779-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-C

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: VN073537.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.005	14	20	28	rVB2	67804	106587	1.08%	0.303%
2	4.228	390	398	405	rBV	42168	119478	1.21%	0.339%
3	7.745	987	996	1011	rBV3	41772	117196	1.19%	0.333%
4	7.951	1021	1031	1036	rBV2	191224	457485	4.63%	1.300%
5	8.016	1036	1042	1058	rVB	360739	831979	8.42%	2.364%
6	8.387	1094	1105	1123	rBV3	425255	1216726	12.32%	3.457%
7	8.904	1183	1193	1207	rBV	494678	1038411	10.51%	2.951%
8	10.381	1436	1444	1450	rBV	694562	1274802	12.91%	3.622%
9	10.445	1450	1455	1466	rVB	527242	956343	9.68%	2.717%
10	11.092	1557	1565	1570	rBV2	50300	103087	1.04%	0.293%
11	11.163	1570	1577	1587	rVV	639827	1201165	12.16%	3.413%
12	11.686	1658	1666	1670	rBV	749527	1364551	13.81%	3.877%
13	11.728	1670	1673	1679	rVV	348573	612429	6.20%	1.740%
14	11.786	1679	1683	1693	rVV	98127	199210	2.02%	0.566%
15	11.892	1693	1701	1712	rVB	399114	762503	7.72%	2.167%
16	12.022	1712	1723	1736	rBV4	253737	595174	6.03%	1.691%
17	12.222	1752	1757	1768	rVB2	389603	703339	7.12%	1.998%
18	12.463	1792	1798	1803	rVV2	156527	291915	2.96%	0.829%
19	12.510	1803	1806	1814	rVB3	77837	139030	1.41%	0.395%
20	12.675	1824	1834	1847	rBV	656294	1229991	12.45%	3.495%
21	12.951	1868	1881	1886	rBV2	239968	572923	5.80%	1.628%
22	12.998	1886	1889	1893	rVB	77331	104240	1.06%	0.296%
23	13.157	1914	1916	1924	rVB2	58073	110401	1.12%	0.314%
24	13.245	1925	1931	1934	rVV3	70292	126197	1.28%	0.359%
25	13.304	1934	1941	1947	rVV2	366230	849617	8.60%	2.414%
26	13.498	1958	1974	1986	rVV5	160138	800747	8.11%	2.275%
27	13.616	1987	1994	2006	rVV2	921890	1971134	19.95%	5.601%
28	13.810	2022	2027	2032	rBV3	71665	139298	1.41%	0.396%
29	13.939	2045	2049	2053	rBV3	69949	123058	1.25%	0.350%
30	13.998	2053	2059	2066	rVV2	362202	671653	6.80%	1.908%
31	14.663	2168	2172	2182	rVB2	37156	105863	1.07%	0.301%
32	14.857	2198	2205	2214	rBV3	80968	225788	2.29%	0.642%
33	15.021	2227	2233	2237	rBV4	61393	131979	1.34%	0.375%
34	15.433	2290	2303	2313	rBV	5093382	9878069	100.00%	28.068%
35	15.533	2314	2320	2329	rVB	161326	317921	3.22%	0.903%
36	16.463	2471	2478	2482	rBV4	47568	108074	1.09%	0.307%

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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

37	16.533	2482	2490	2504	rVB	1466597	3239829	32.80%	9.206%
38	16.739	2516	2525	2533	rBV	1046273	2395737	24.25%	6.807%

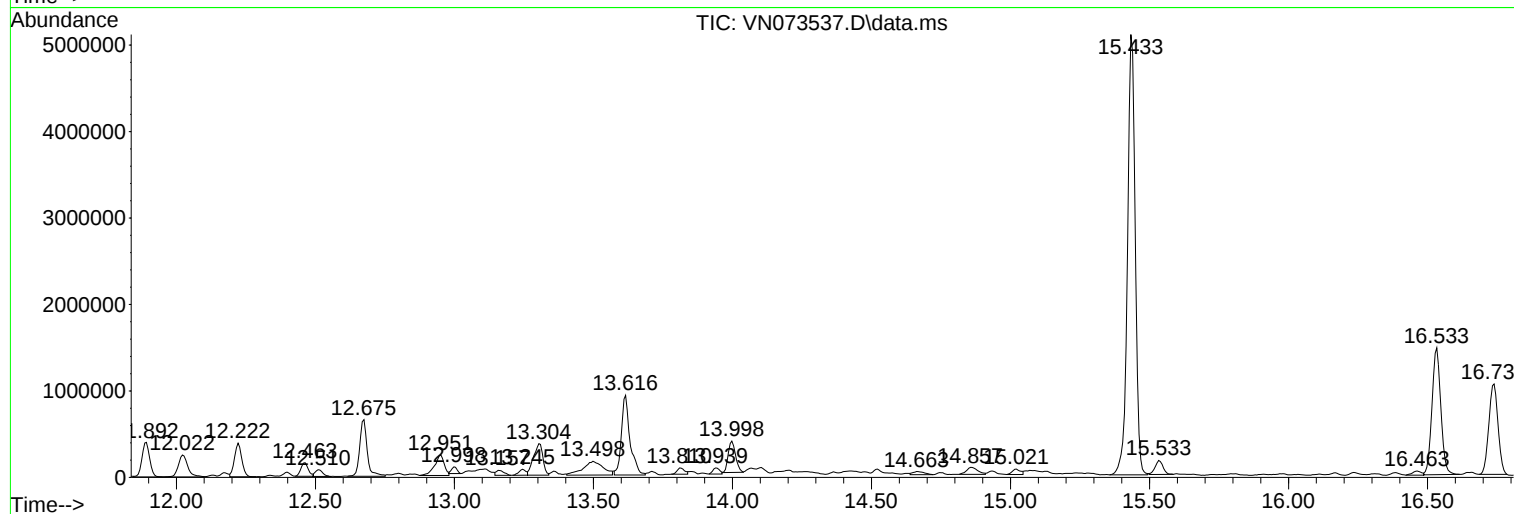
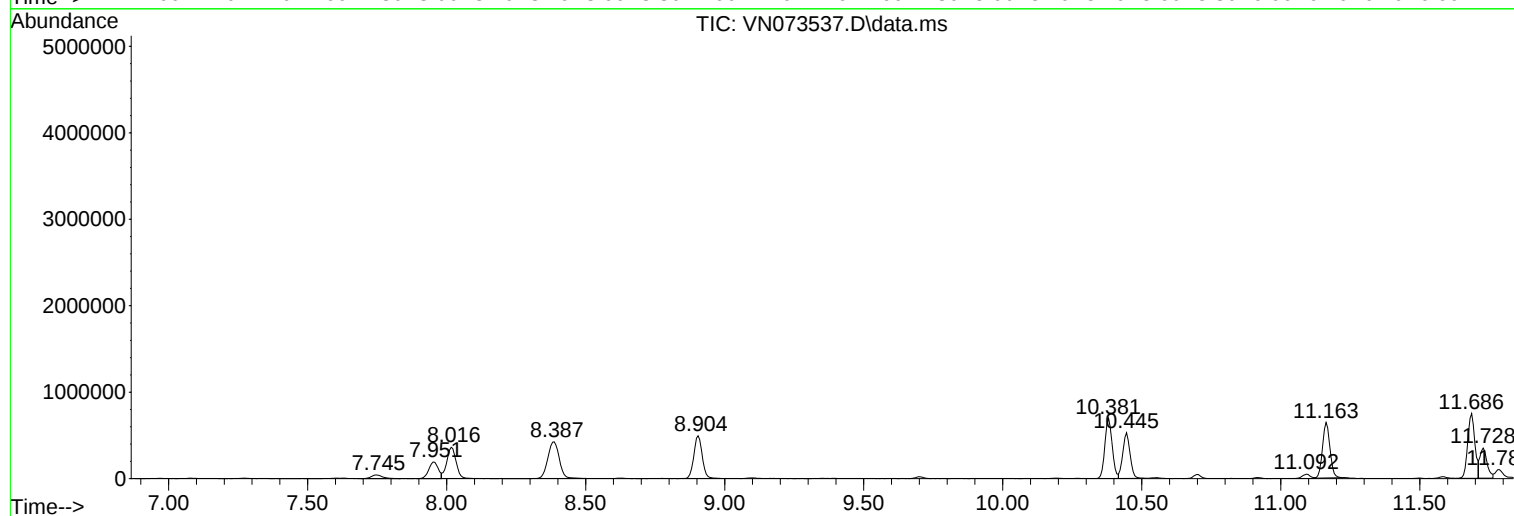
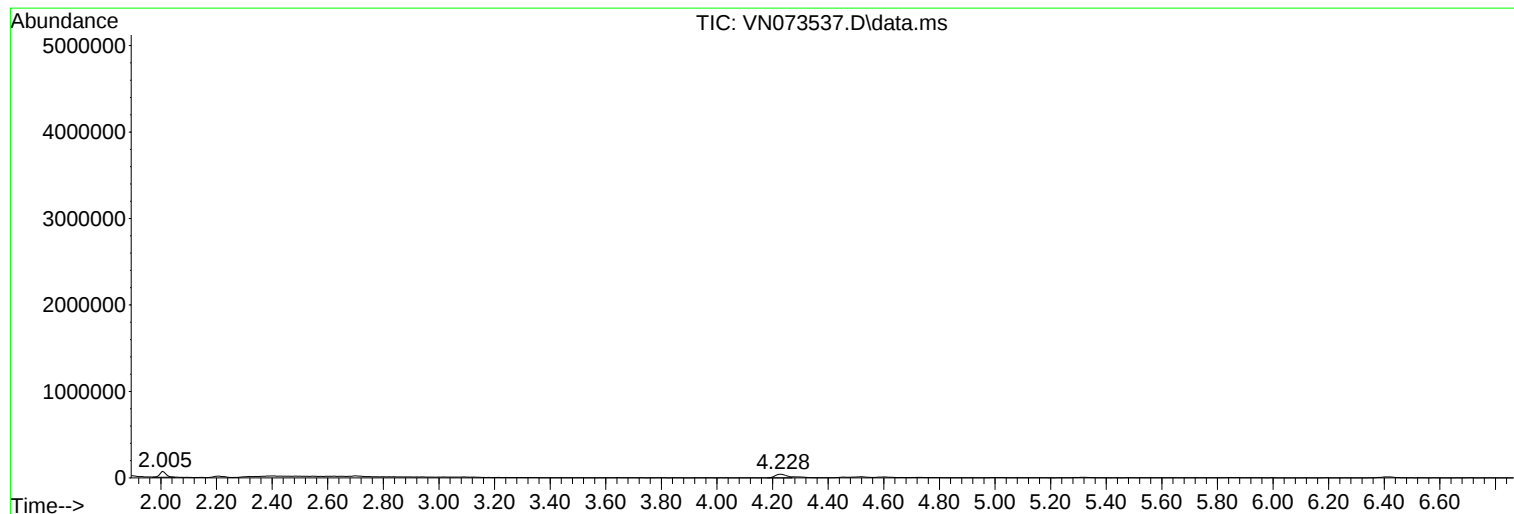
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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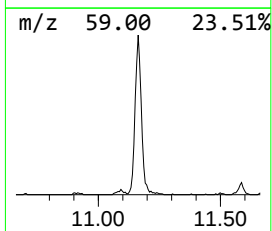
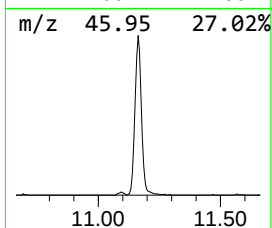
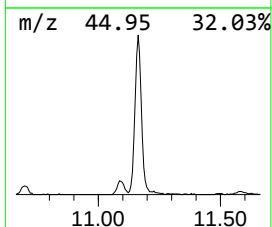
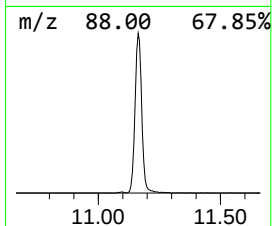
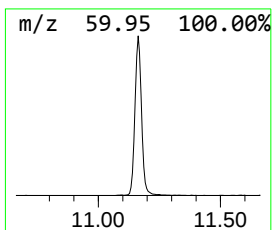
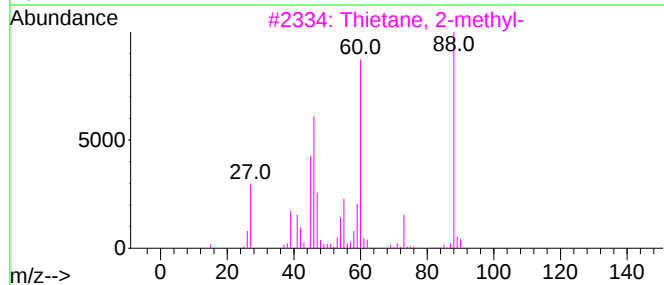
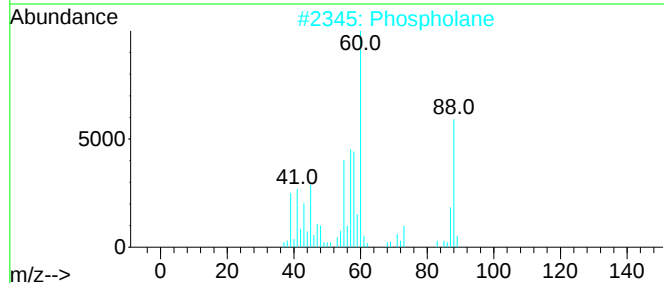
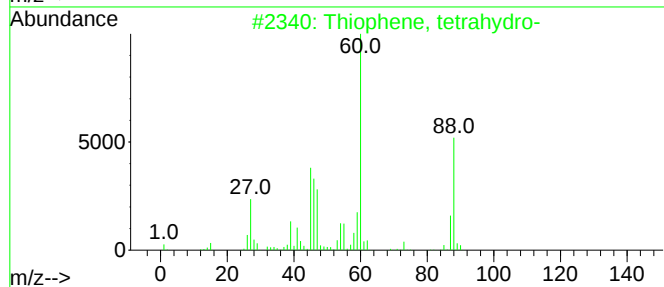
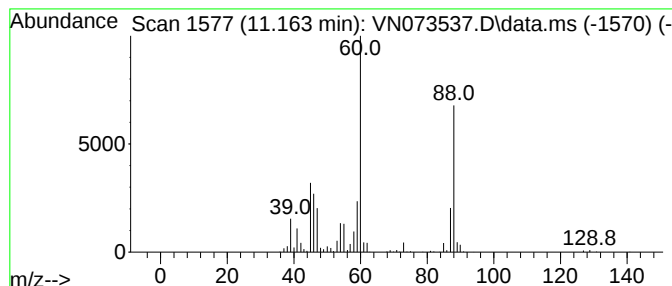
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	44.01 ug/l	1201170	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	96
2			Phospholane	88	C4H9P	003466-00-0	64
3			Thietane, 2-methyl-	88	C4H8S	017837-41-1	49
4			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
5			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33



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Instrument :
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ClientSampleId :
070622-C

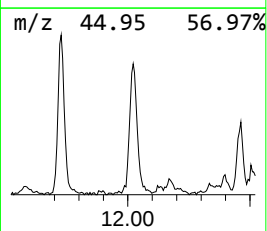
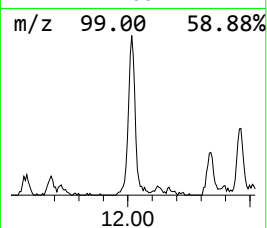
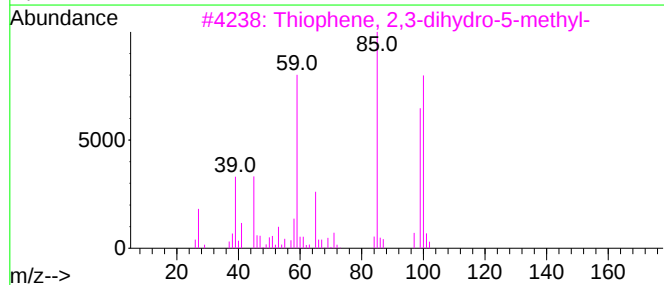
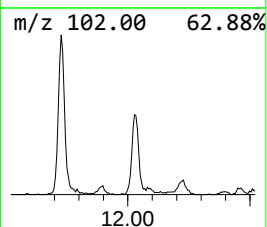
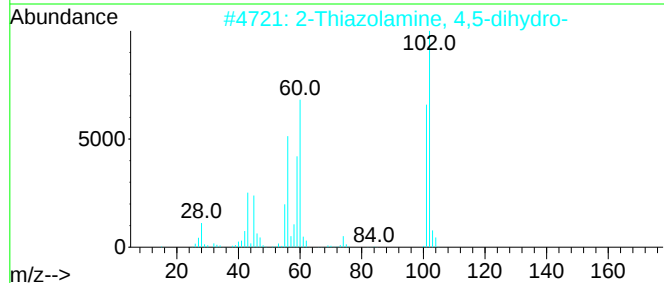
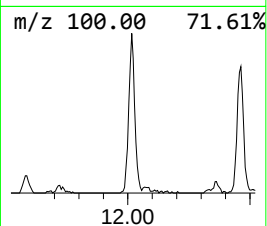
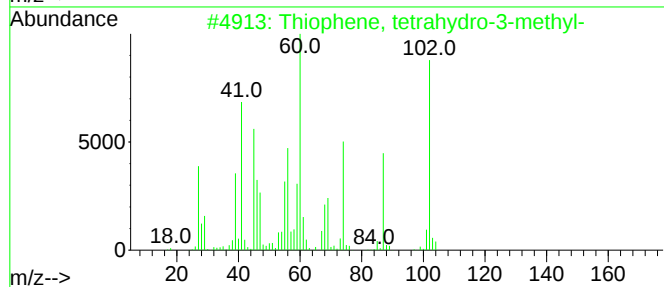
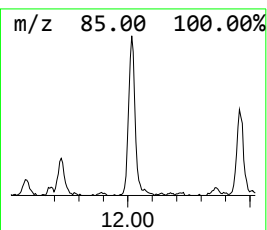
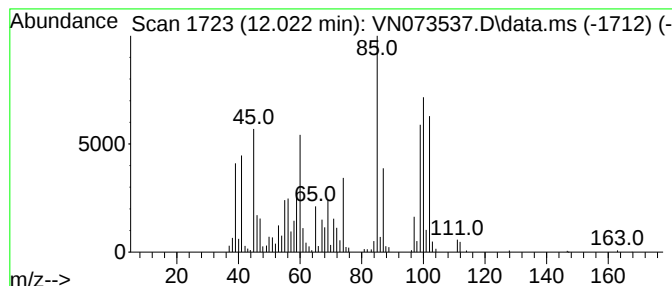
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	21.81 ug/l	595174	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	83
2			2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	46
3			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	46
4			Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	27
5			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	27



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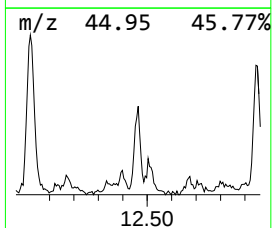
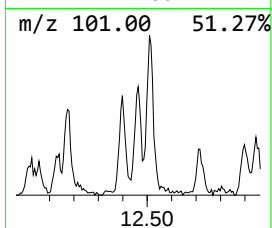
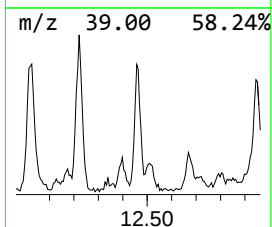
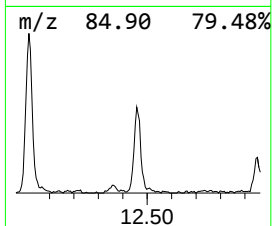
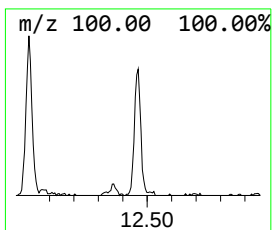
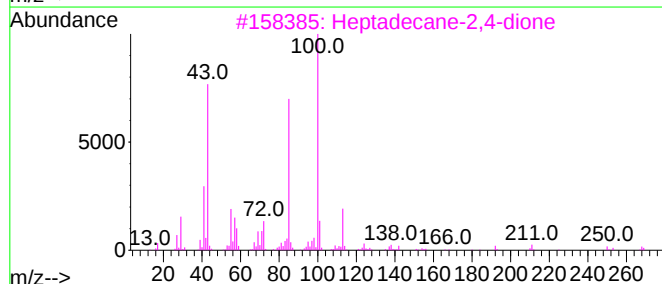
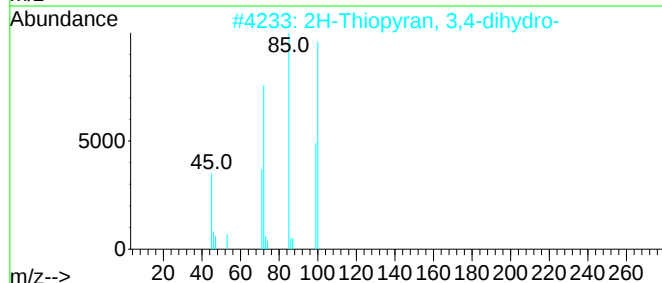
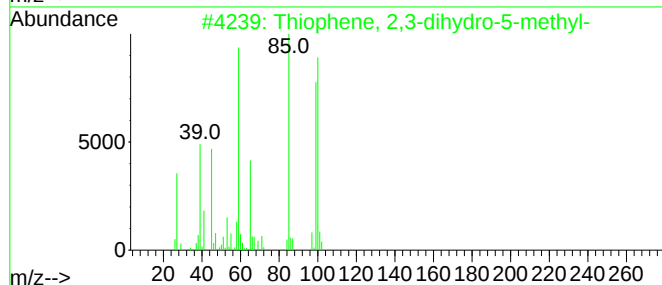
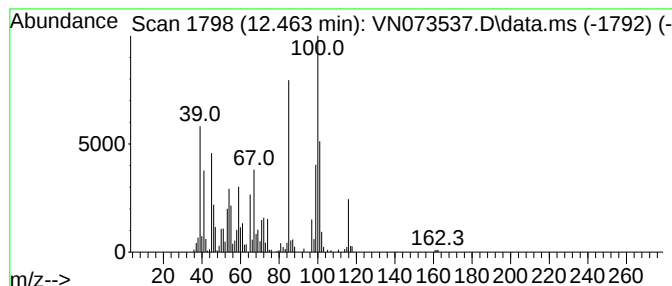
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.463 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	10.70 ug/l	291915	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			2H-Thiopyran, 3,4-dihydro-	100	C5H8S	013042-80-3	43
3			Heptadecane-2,4-dione	268	C17H32O2	064042-18-8	27
4			Nonadecane-2,4-dione	296	C19H36O2	016577-69-8	16
5			Pentadecane-2,4-dione	240	C15H28O2	053759-23-2	16



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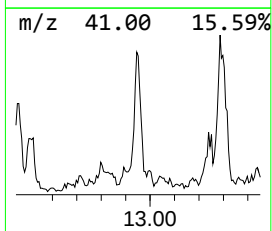
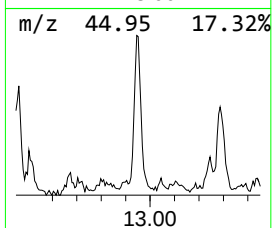
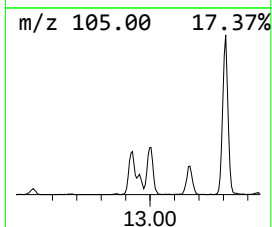
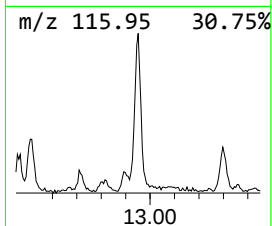
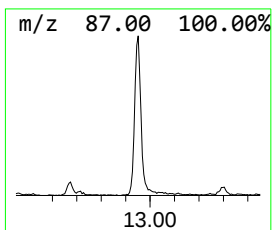
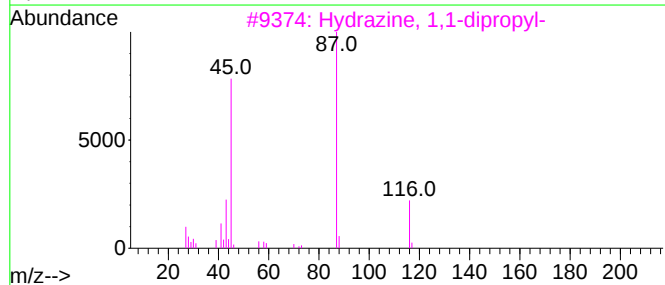
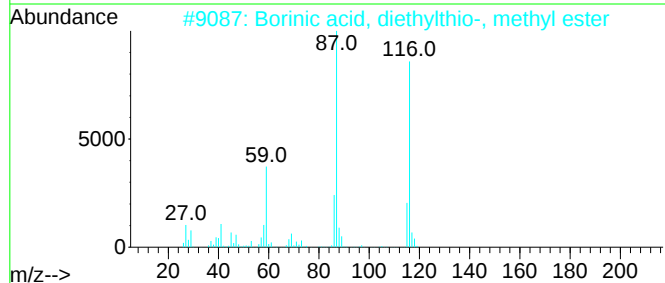
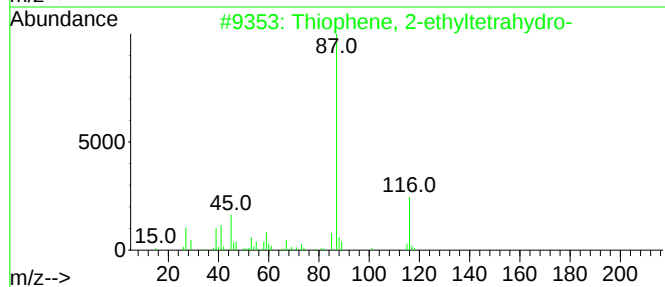
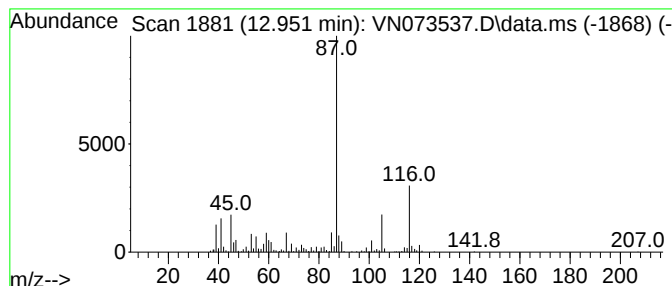
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 5 Thiophene, 2-ethyltetrahydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	14.53 ug/l	572923	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	93
2			Borinic acid, diethylthio-, meth...	116	C5H13BS	092276-84-1	59
3			Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	53
4			Thiophane, propyl-	130	C7H14S	001551-34-4	50
5			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	47



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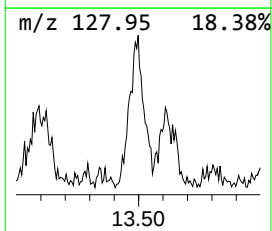
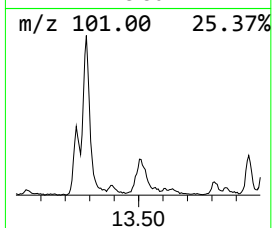
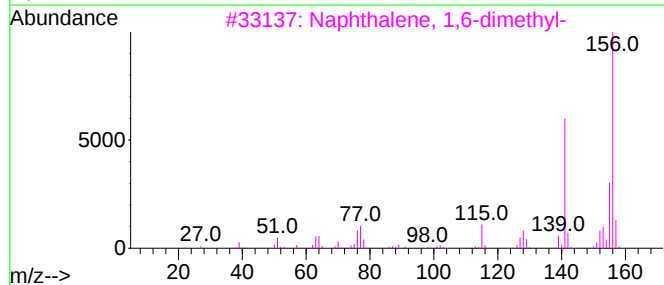
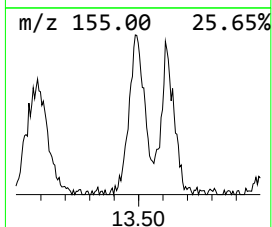
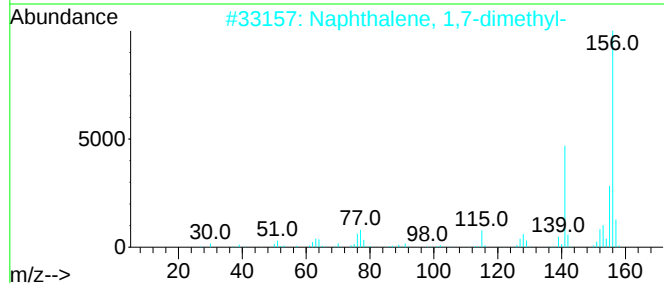
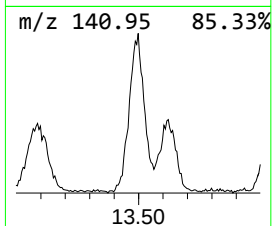
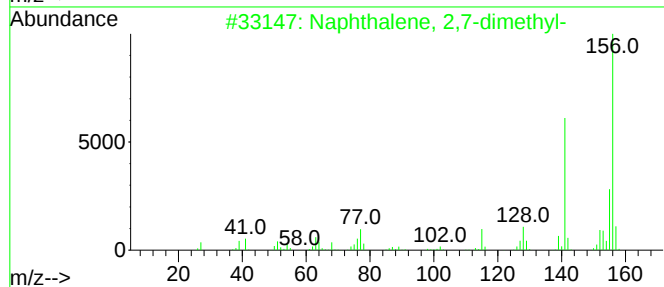
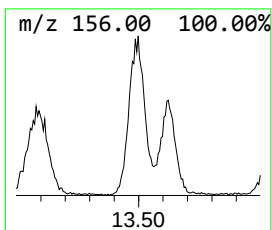
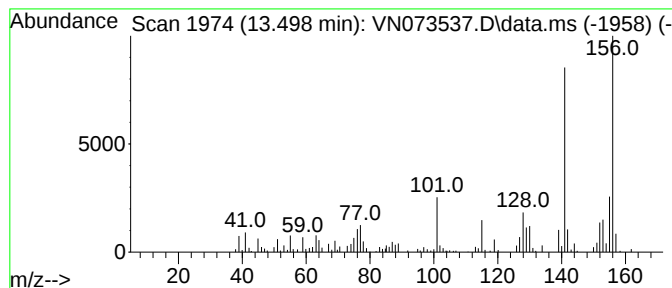
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	20.31 ug/l	800747	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	93
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073537.D
Acq On : 20 Jul 2022 21:24
Operator : JC\MD
Sample : N3779-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

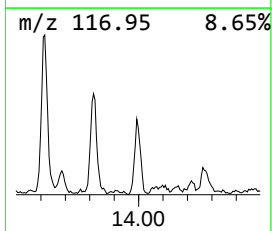
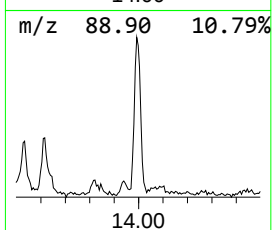
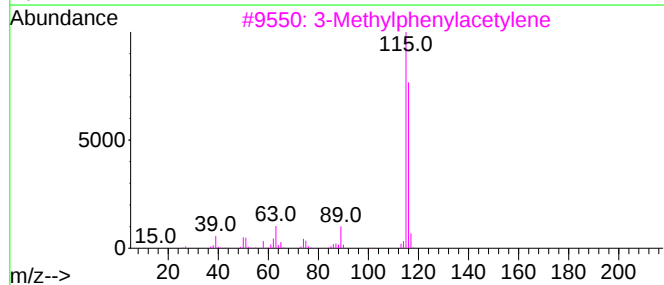
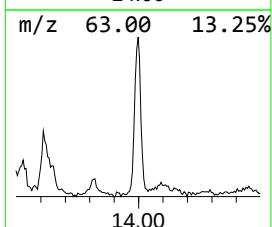
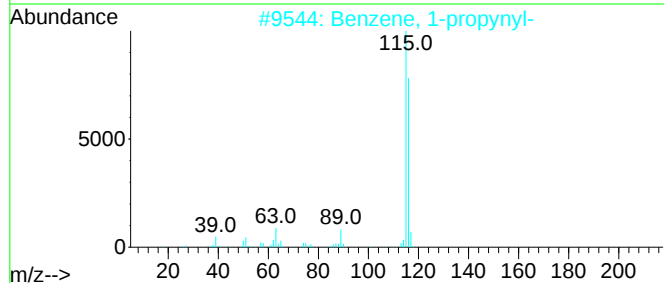
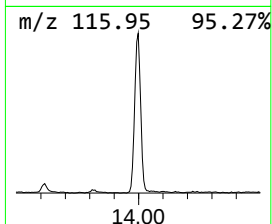
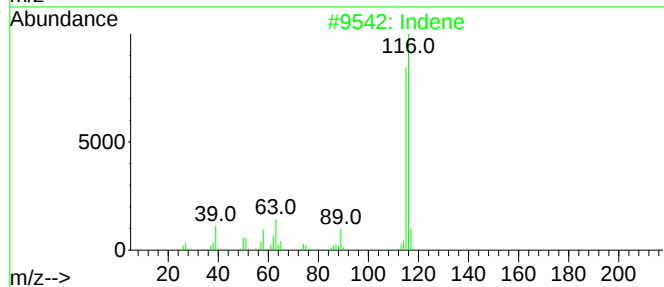
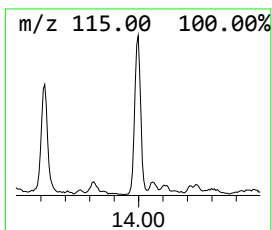
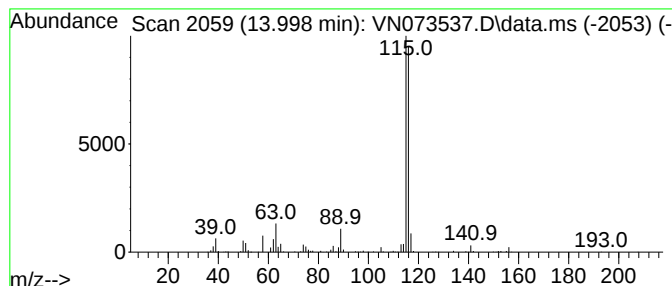
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ClientSampleId :
070622-C

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

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

Peak Number 7 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.998	17.04 ug/l	671653	1,4-Dichlorobenzene-d4			13.616
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	91
3	3-Methylphenylacetylene		116	C9H8	000766-82-5	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 : VN073537.D
Acq On : 20 Jul 2022 21:24
Operator : JC\MD
Sample : N3779-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-C

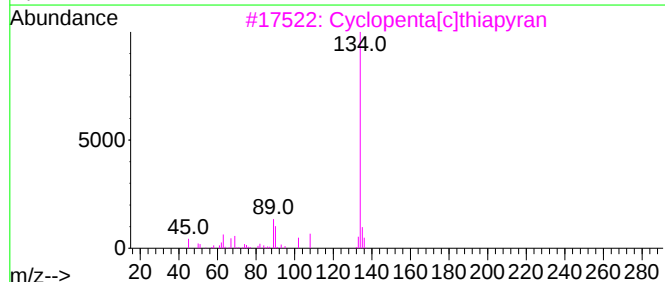
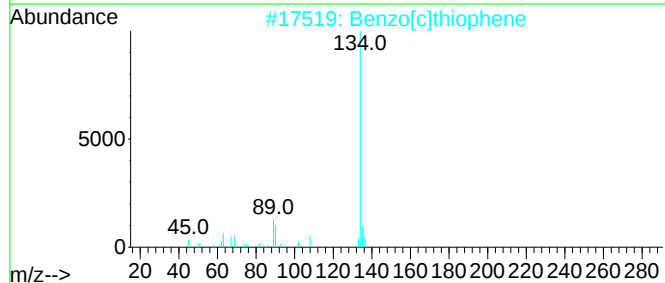
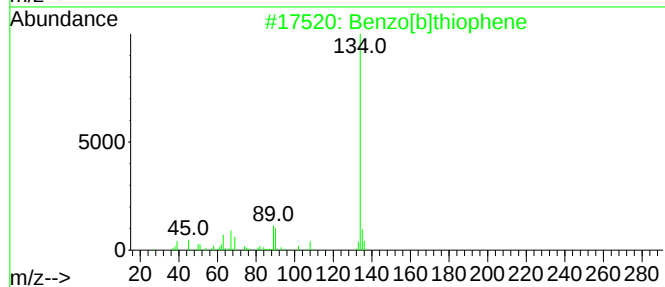
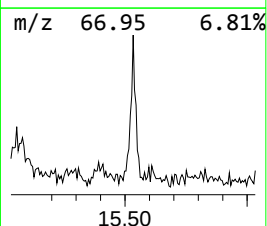
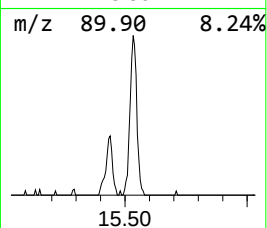
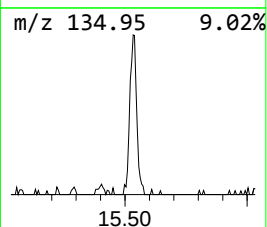
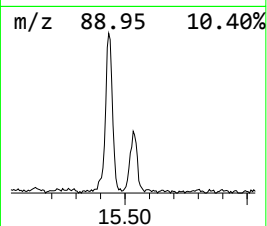
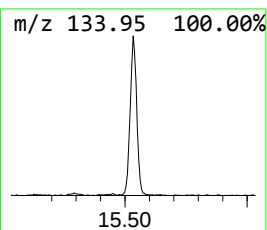
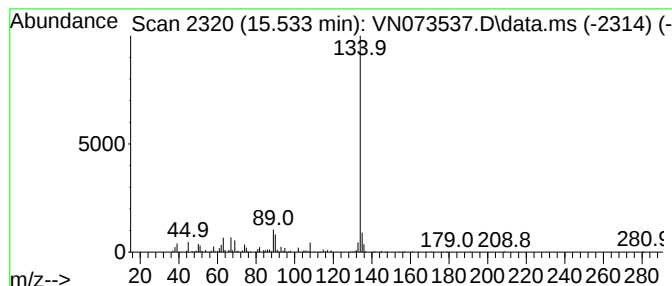
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[b]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	8.06 ug/l	317921	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	97
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	87
4			(5E)-(E)-5-Benzylidene-2-thioxot...	221	C10H7NOS2	1000497-38-8	83
5			Thiepino[3,2-e]isobenzofuran-1,3...	260	C14H12O3S	055044-57-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073537.D
Acq On : 20 Jul 2022 21:24
Operator : JC\MD
Sample : N3779-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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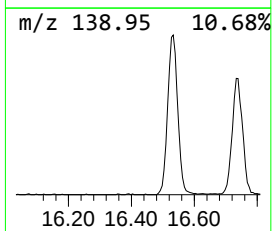
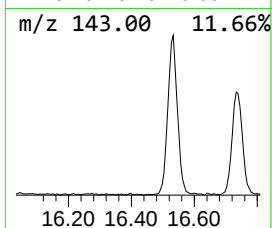
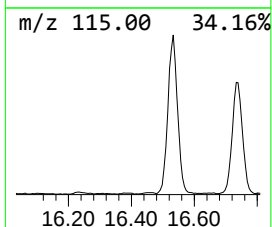
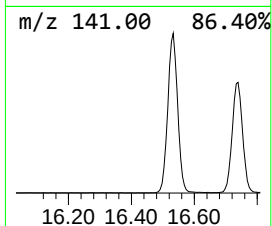
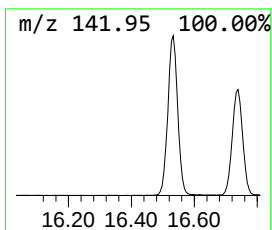
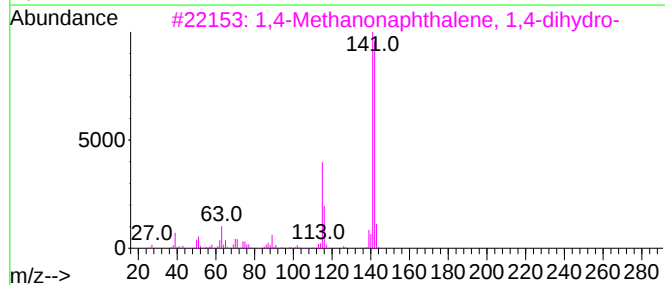
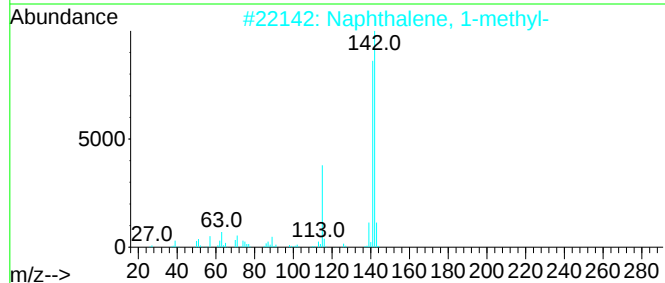
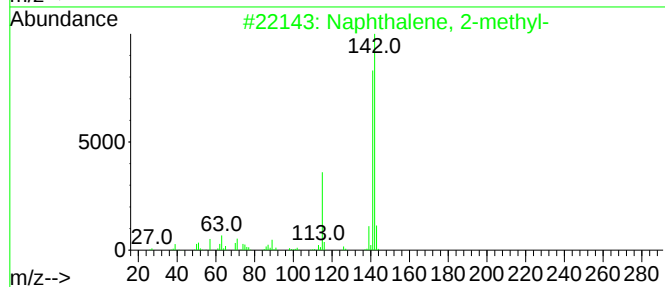
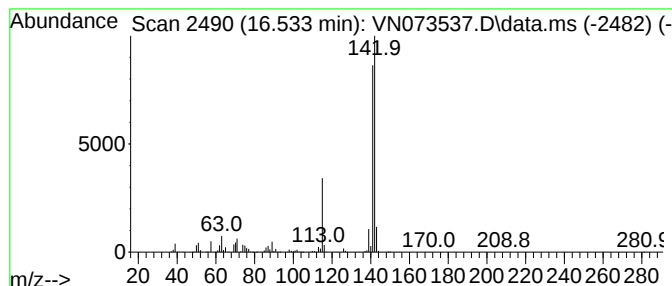
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Quant Title : SW846 8260

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	82.18 ug/l	3239830	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073537.D
Acq On : 20 Jul 2022 21:24
Operator : JC\MD
Sample : N3779-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

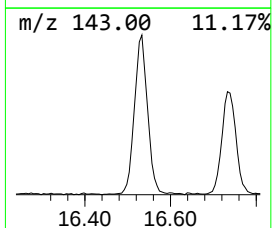
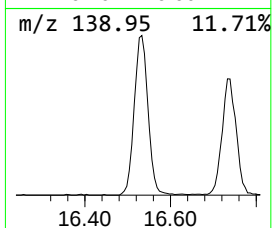
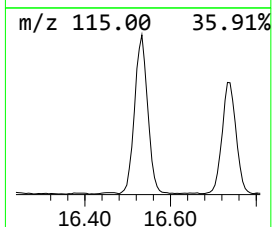
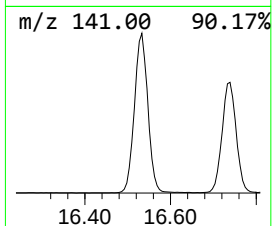
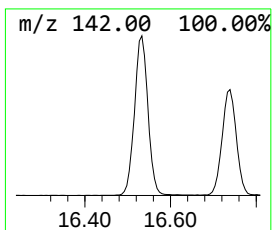
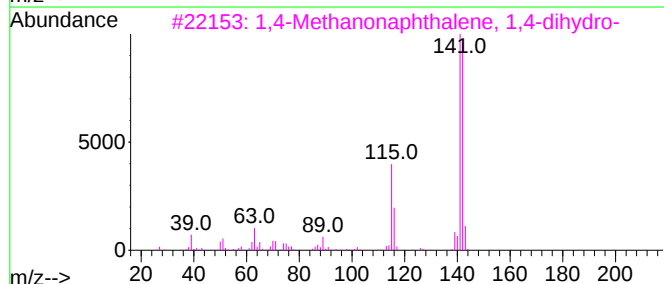
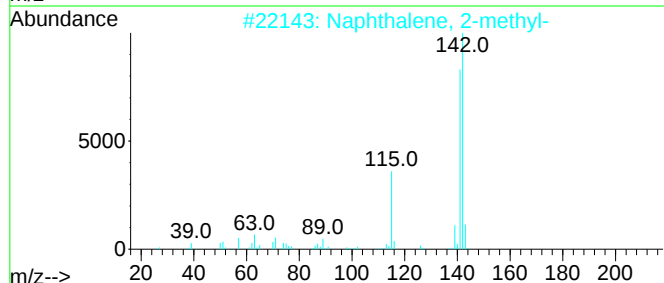
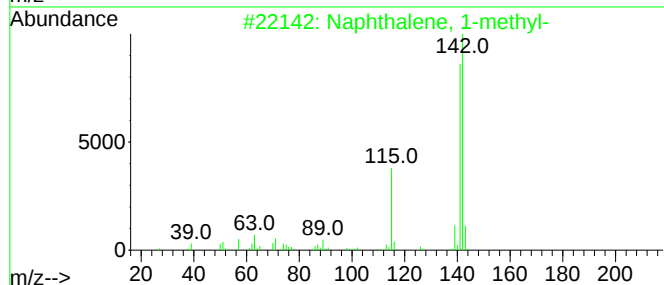
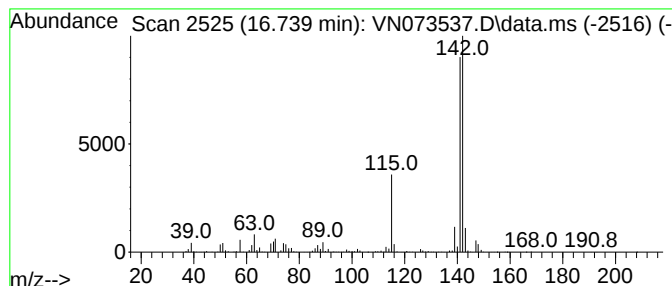
Instrument :
MSVOA_N
ClientSampleId :
070622-C

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 10 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.739	60.77 ug/l	2395740	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	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073537.D
Acq On : 20 Jul 2022 21:24
Operator : JC\MD
Sample : N3779-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-C

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...	12.022	21.8	ug/l	595174	3	11.686	1364550	50.0
unknown12.463	12.463	10.7	ug/l	291915	3	11.686	1364550	50.0
Thiophene, 2-et...	12.951	14.5	ug/l	572923	4	13.616	1971130	50.0
Naphthalene, 2,...	13.498	20.3	ug/l	800747	4	13.616	1971130	50.0
Indene	13.998	17.0	ug/l	671653	4	13.616	1971130	50.0
Benzo[b]thiophene	15.533	8.1	ug/l	317921	4	13.616	1971130	50.0
Naphthalene, 2-...	16.533	82.2	ug/l	3239830	4	13.616	1971130	50.0
Naphthalene, 1-...	16.739	60.8	ug/l	2395740	4	13.616	1971130	50.0