

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
 Data File : VN073541.D
 Acq On : 20 Jul 2022 23:02
 Operator : JC\MD
 Sample : N3779-09
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 070622-G

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: VN073541.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.551	107	113	120	rVB	85857	147767	1.49%	0.409%
2	7.745	987	996	1008	rBV2	40067	106791	1.08%	0.296%
3	7.951	1016	1031	1036	rBV	205881	495409	5.00%	1.372%
4	8.016	1036	1042	1053	rVB	366785	868061	8.76%	2.404%
5	8.386	1092	1105	1122	rBV3	409910	1198819	12.09%	3.320%
6	8.904	1184	1193	1207	rBV2	519394	1101125	11.11%	3.049%
7	10.380	1434	1444	1450	rBV	755599	1369767	13.82%	3.793%
8	10.445	1450	1455	1467	rVB	484414	872756	8.80%	2.417%
9	10.698	1491	1498	1508	rBV	78040	143017	1.44%	0.396%
10	11.086	1556	1564	1570	rBV4	93355	187948	1.90%	0.520%
11	11.163	1570	1577	1592	rVB	625926	1189977	12.00%	3.295%
12	11.686	1654	1666	1670	rBV	802965	1459120	14.72%	4.040%
13	11.727	1670	1673	1679	rVV	341961	613103	6.18%	1.698%
14	11.786	1679	1683	1693	rVV	111153	245184	2.47%	0.679%
15	11.886	1694	1700	1710	rVB	410944	780665	7.87%	2.162%
16	12.027	1717	1724	1736	rVB5	184928	409210	4.13%	1.133%
17	12.221	1752	1757	1766	rVB3	373291	671144	6.77%	1.858%
18	12.457	1792	1797	1802	rVV3	146446	276982	2.79%	0.767%
19	12.510	1802	1806	1813	rVB3	73363	139163	1.40%	0.385%
20	12.674	1821	1834	1845	rBV	676703	1299380	13.11%	3.598%
21	12.951	1869	1881	1886	rBV2	210932	478393	4.83%	1.325%
22	13.163	1914	1917	1924	rVB2	68283	131522	1.33%	0.364%
23	13.245	1924	1931	1934	rBV3	62914	124163	1.25%	0.344%
24	13.304	1934	1941	1947	rVV2	355993	828463	8.36%	2.294%
25	13.498	1959	1974	1985	rVV6	197156	968658	9.77%	2.682%
26	13.615	1987	1994	2006	rVV2	974729	2133187	21.52%	5.907%
27	13.815	2022	2028	2032	rBV2	80077	149568	1.51%	0.414%
28	13.939	2044	2049	2053	rBV2	66682	120137	1.21%	0.333%
29	13.998	2053	2059	2066	rVV2	388753	722254	7.29%	2.000%
30	14.068	2067	2071	2074	rVV5	56633	126188	1.27%	0.349%
31	14.098	2074	2076	2084	rVB5	74657	136236	1.37%	0.377%
32	14.662	2168	2172	2182	rVB5	44711	137448	1.39%	0.381%
33	14.862	2199	2206	2213	rBV4	73639	197407	1.99%	0.547%
34	15.015	2227	2232	2236	rBV2	63534	121604	1.23%	0.337%
35	15.433	2290	2303	2313	rBV	5045423	9914191	100.00%	27.452%
36	15.533	2314	2320	2328	rVB	165510	331389	3.34%	0.918%

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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	16.462	2470	2478	2482	rBV3	53536	122802	1.24%	0.340%
38	16.527	2482	2489	2504	rVV	1466184	3323085	33.52%	9.202%
39	16.739	2516	2525	2533	rVV	1092542	2472187	24.94%	6.845%

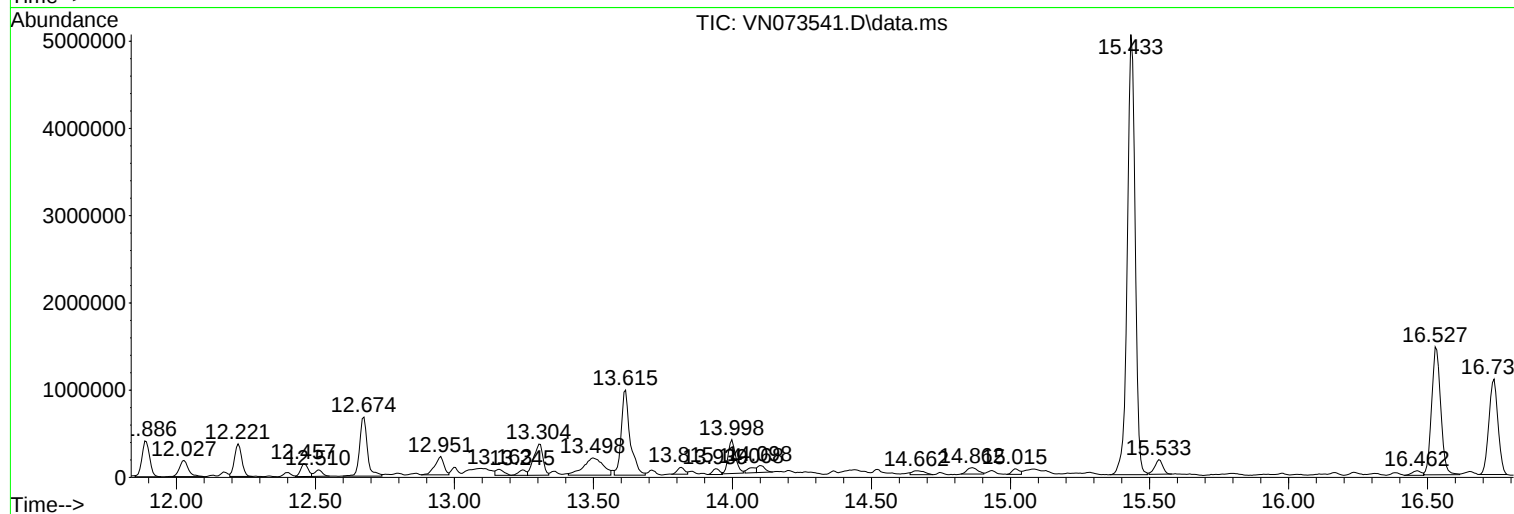
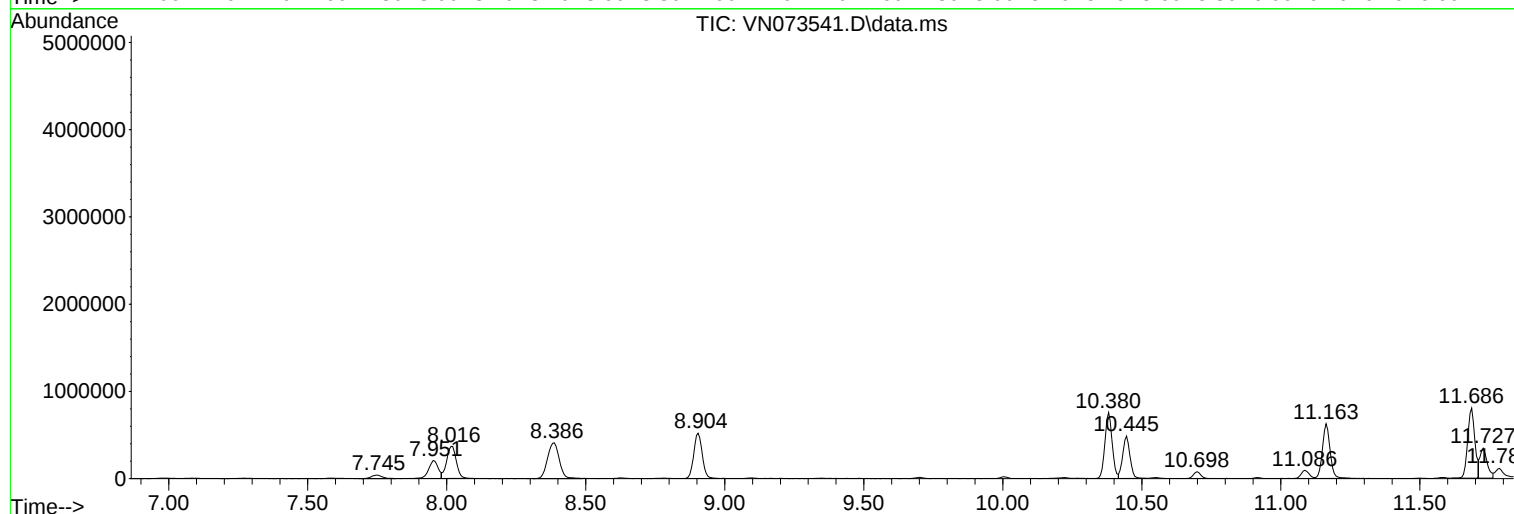
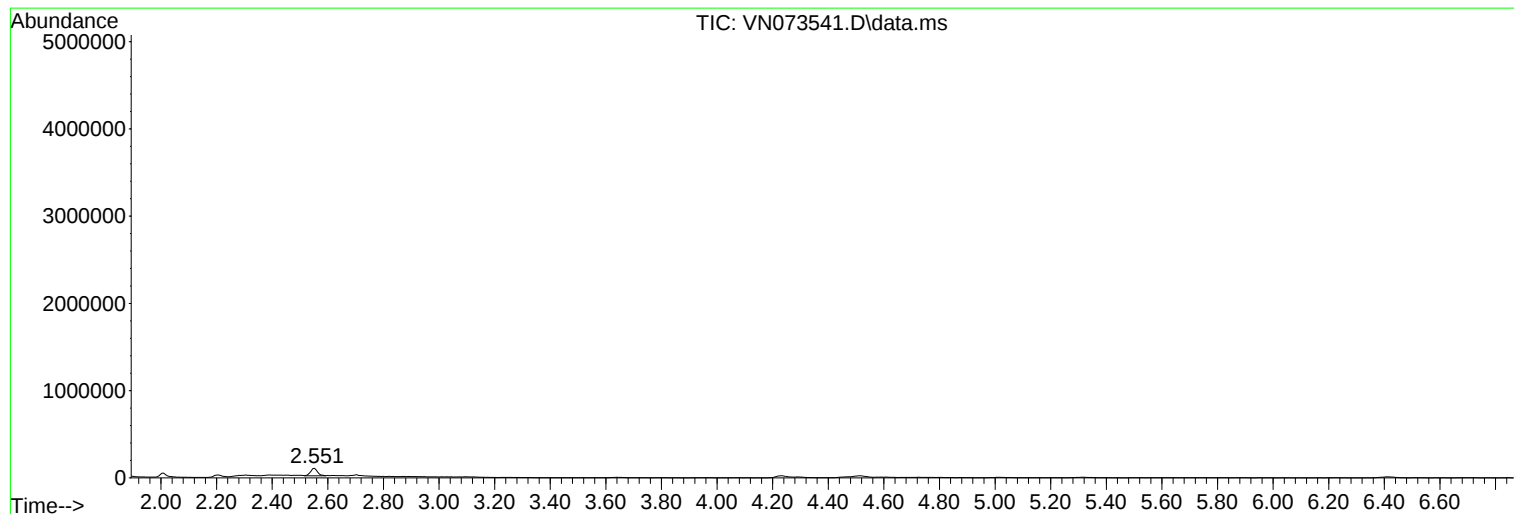
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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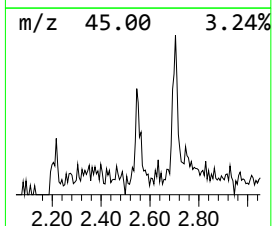
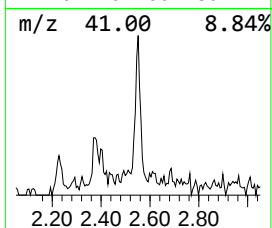
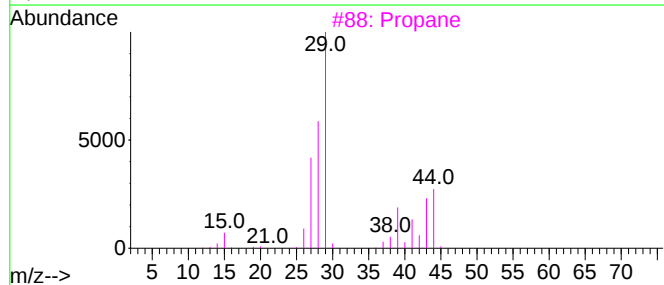
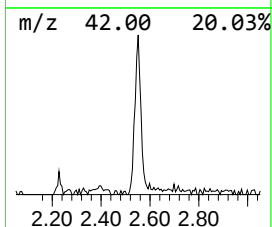
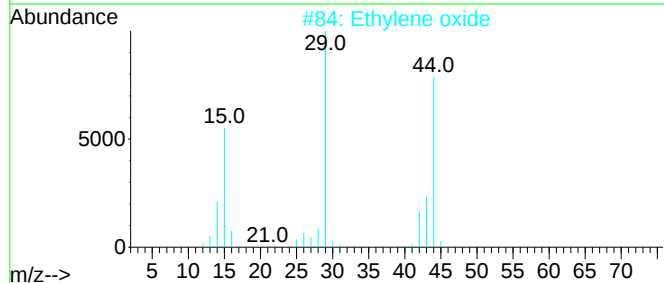
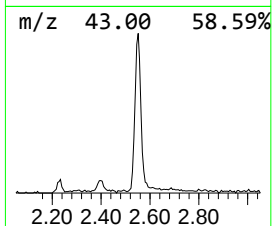
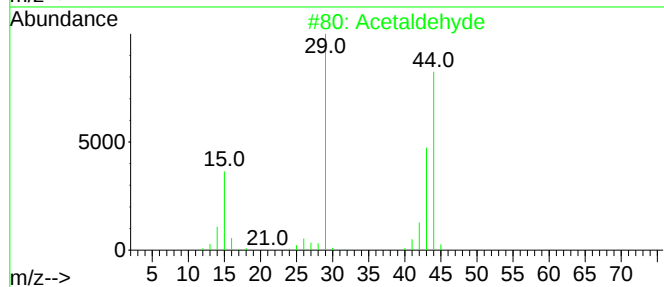
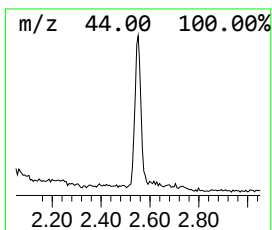
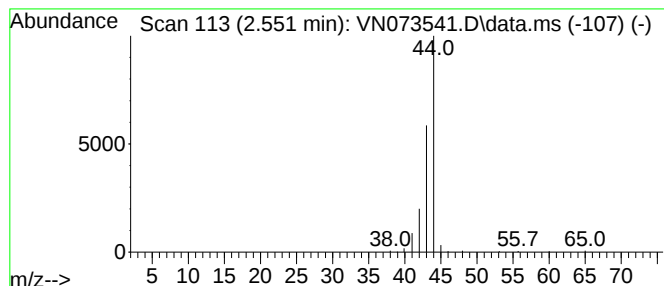
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.551	8.51 ug/l	147767	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			Propane	44	C3H8	000074-98-6	5
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	4
5			Topotecan	421	C23H23N3O5	1000131-70-7	4



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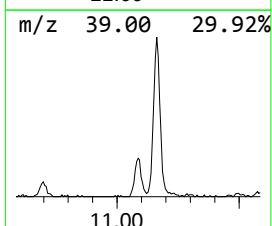
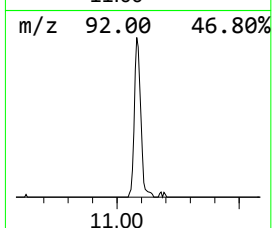
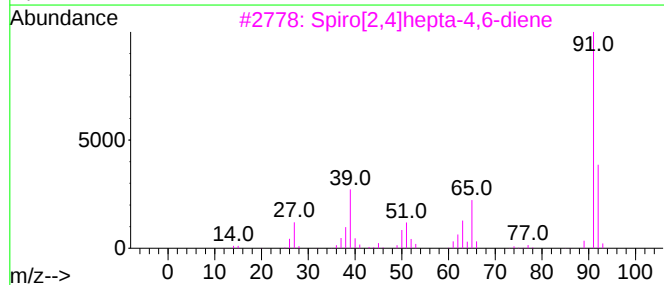
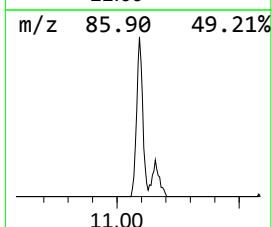
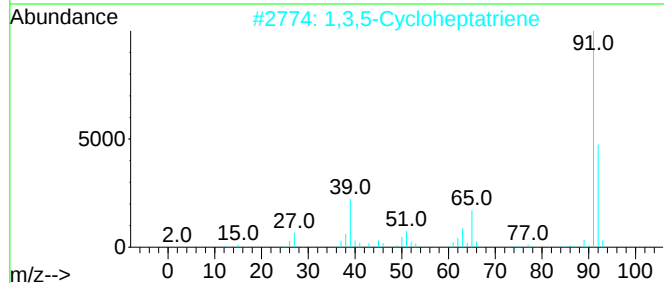
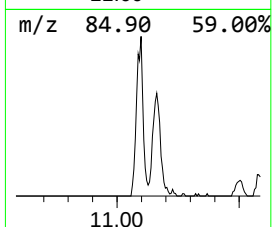
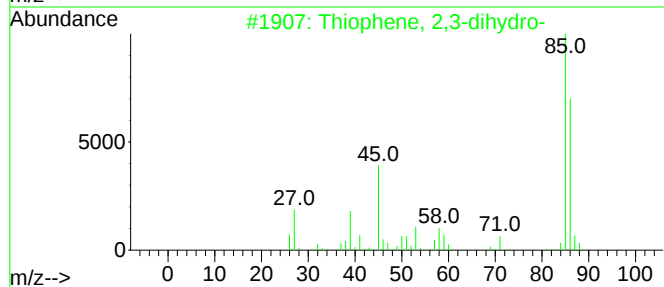
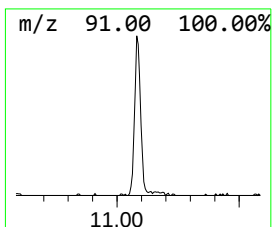
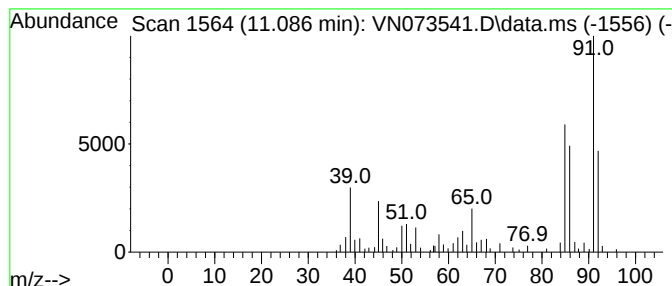
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown11.086 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.086	6.44 ug/l	187948	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2,3-dihydro-	86	C4H6S	001120-59-8	43
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	42
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	42
4			Toluene	92	C7H8	000108-88-3	38
5			Thiophene, 2,5-dihydro-	86	C4H6S	001708-32-3	38



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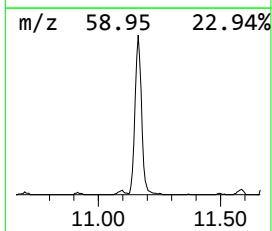
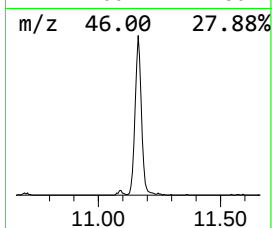
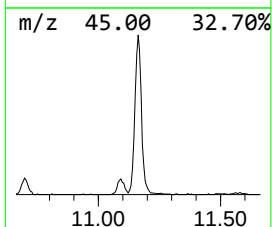
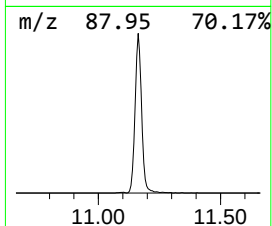
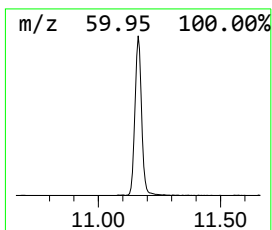
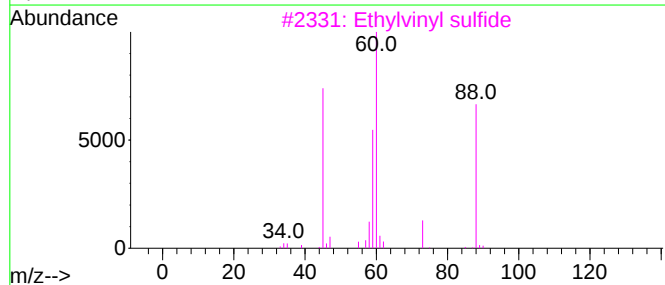
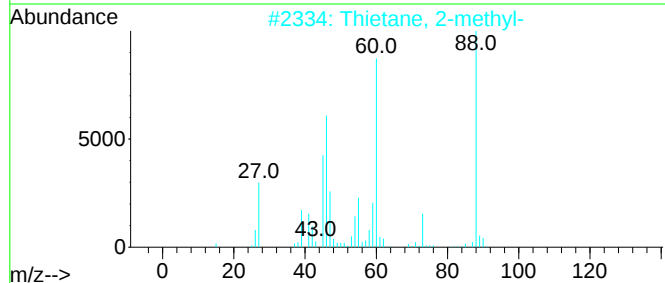
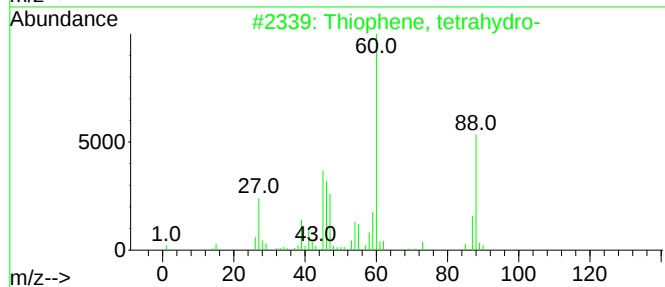
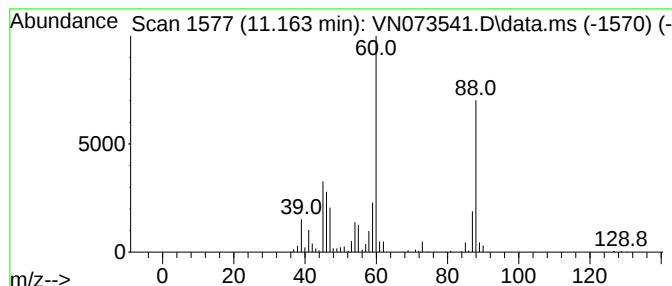
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	40.78 ug/l	1189980	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
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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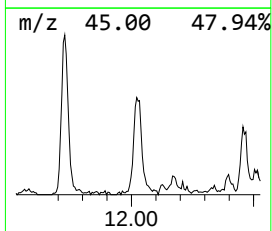
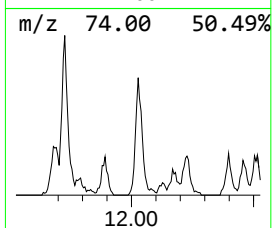
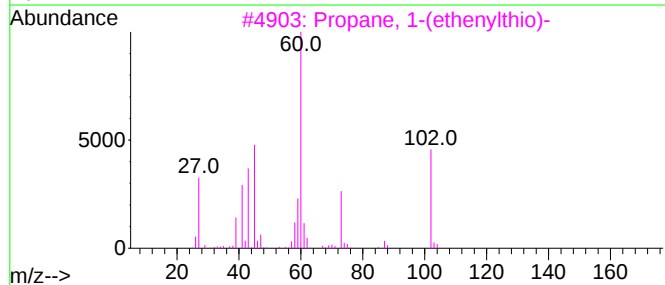
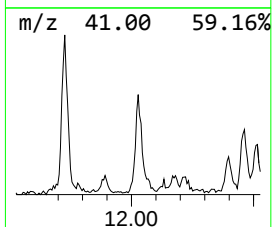
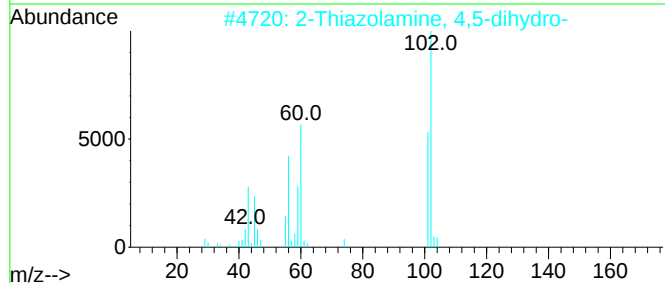
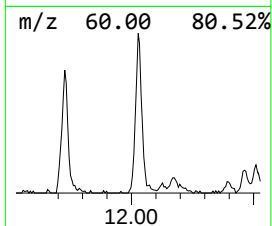
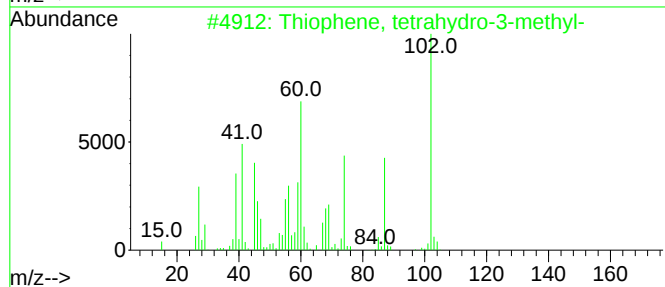
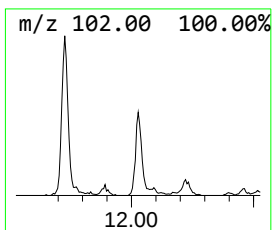
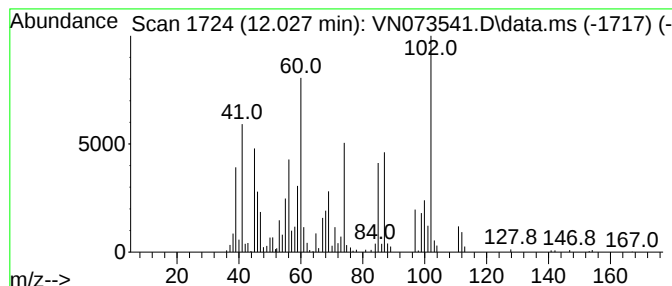
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.027	14.02 ug/l	409210	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	37
3			Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	16
4			Methyl.alpha.d-rhamnopyranoside	178	C7H14O5	001128-40-1	16
5			2,5,6-Trimethyl-1,3-oxathiane	146	C7H14O5	114376-06-6	16



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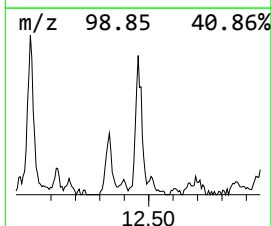
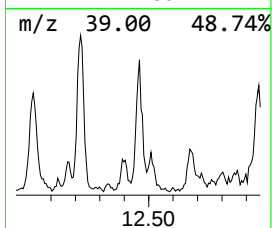
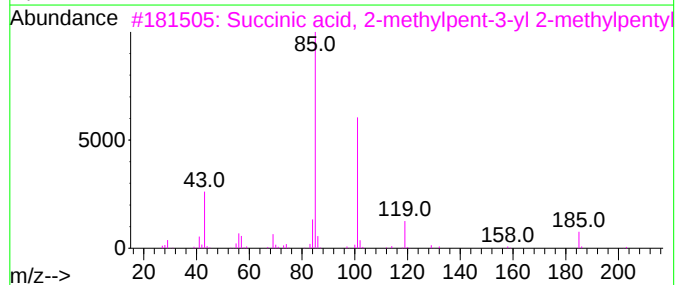
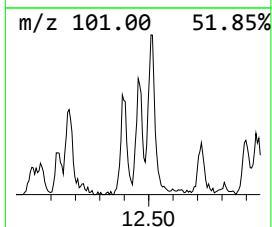
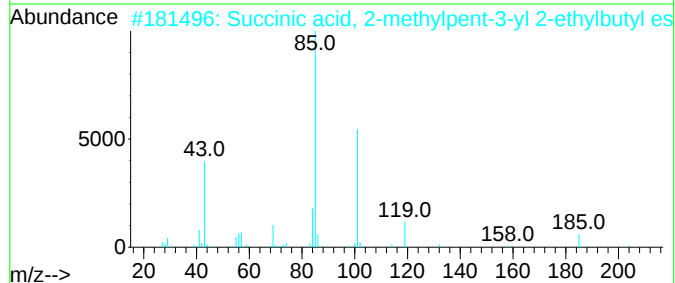
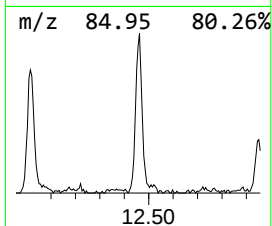
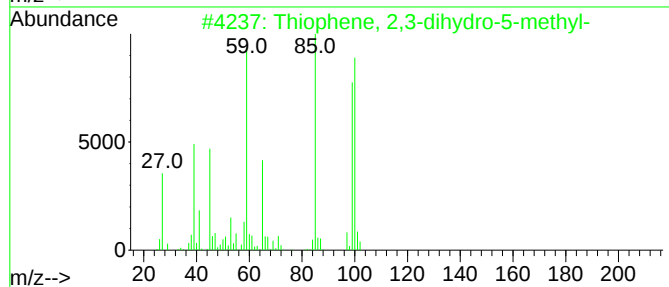
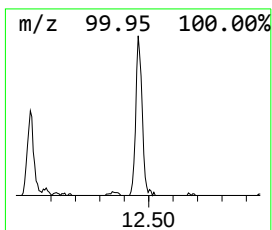
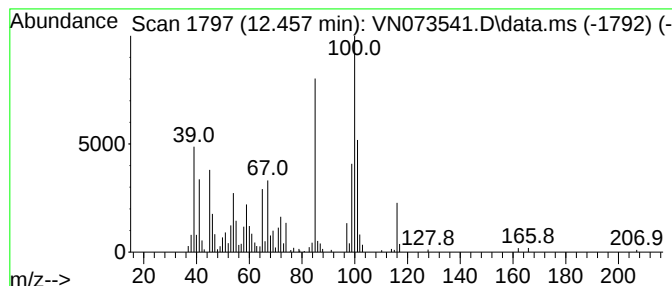
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Quant Title : SW846 8260

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

Peak Number 5 Thiophene, 2,3-dihydro-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	9.49 ug/l	276982	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	53
2			Succinic acid, 2-methylpent-3-yl...	286	C16H30O4	1000389-60-8	22
3			Succinic acid, 2-methylpent-3-yl...	286	C16H30O4	1010389-64-9	22
4			Succinic acid, 2-methylpent-3-yl...	300	C17H32O4	1000390-46-9	22
5			2-Butenoic acid, 2-methyl-, (Z)-	100	C5H8O2	000565-63-9	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073541.D
Acq On : 20 Jul 2022 23:02
Operator : JC\MD
Sample : N3779-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-G

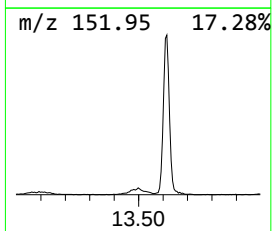
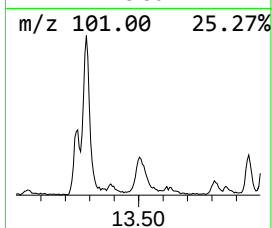
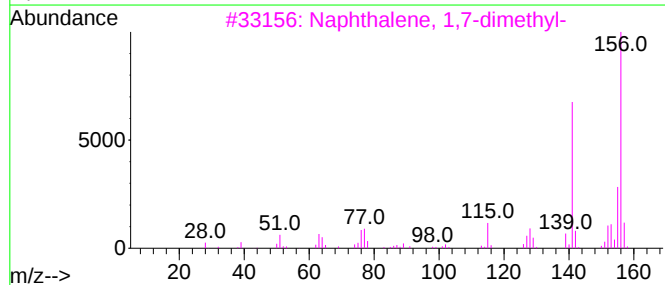
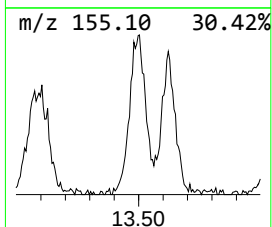
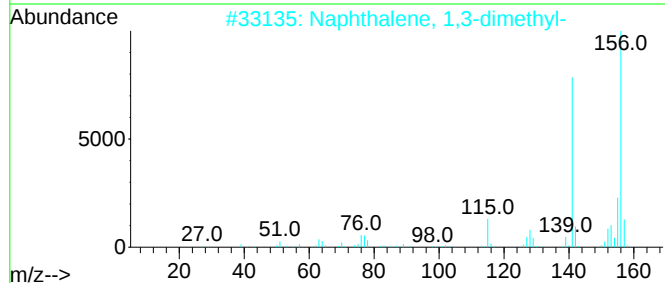
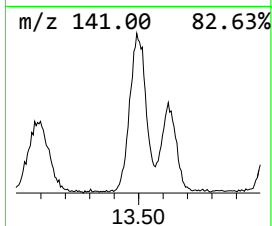
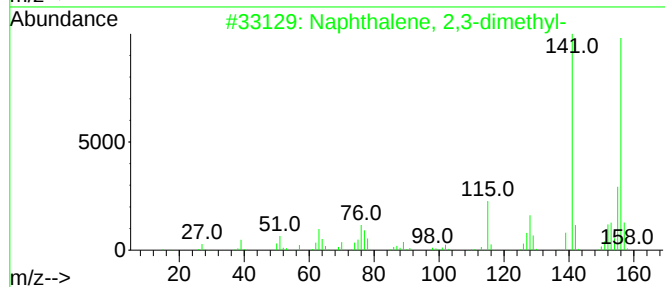
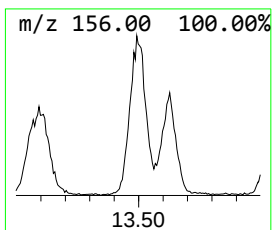
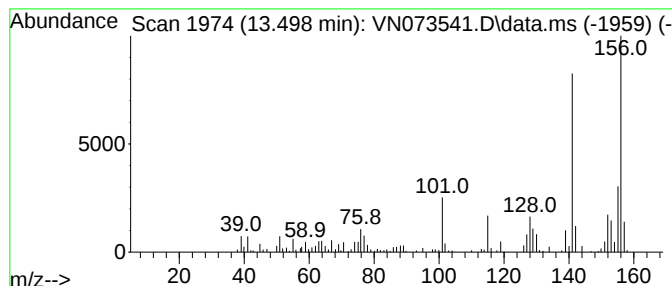
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	22.70 ug/l	968658	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
5			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073541.D
Acq On : 20 Jul 2022 23:02
Operator : JC\MD
Sample : N3779-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-G

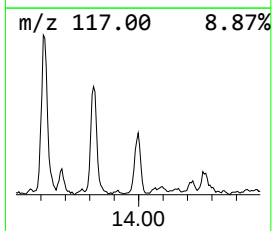
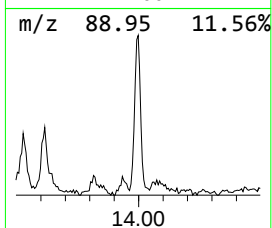
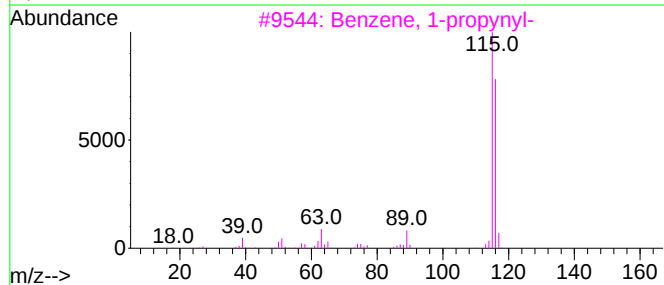
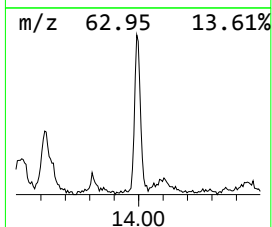
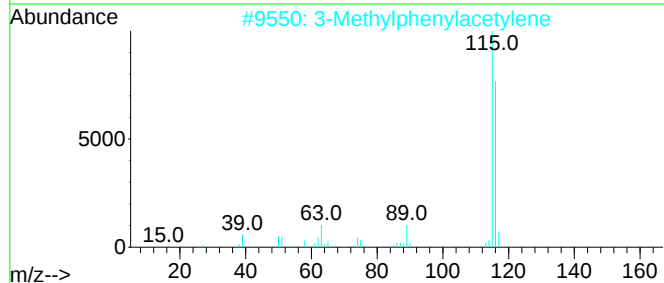
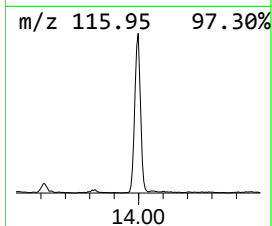
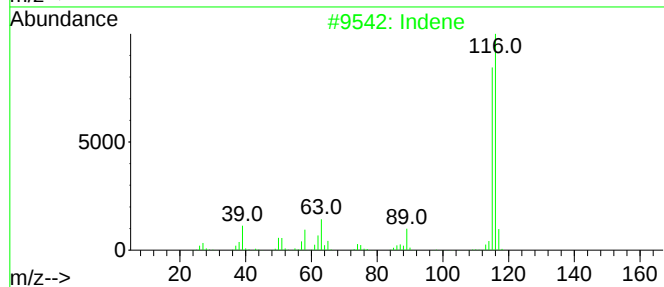
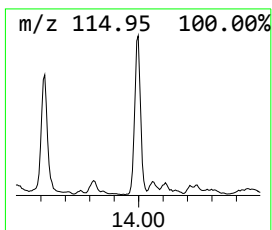
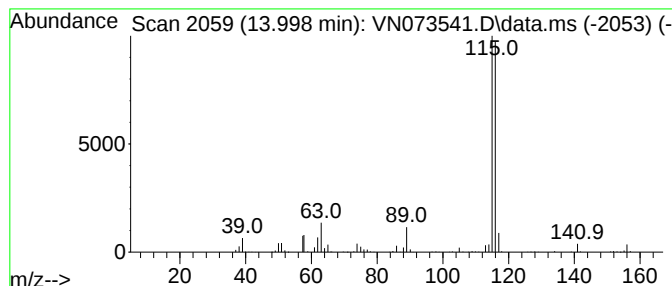
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Quant Title : SW846 8260

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	16.93 ug/l	722254	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073541.D
Acq On : 20 Jul 2022 23:02
Operator : JC\MD
Sample : N3779-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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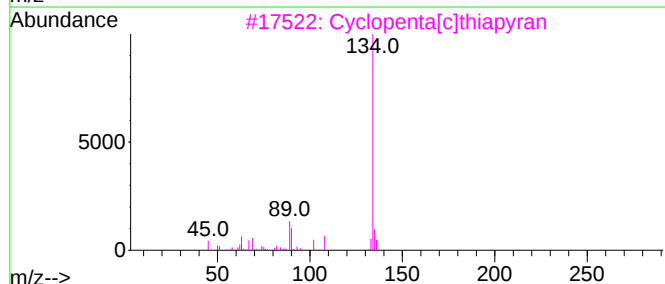
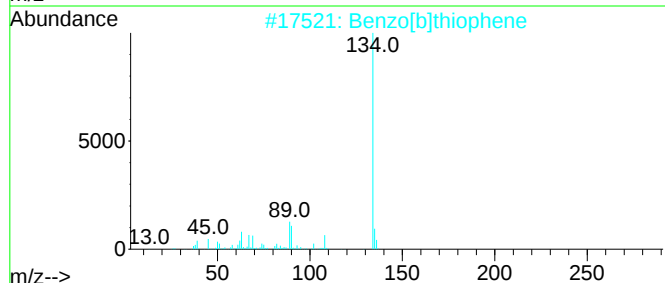
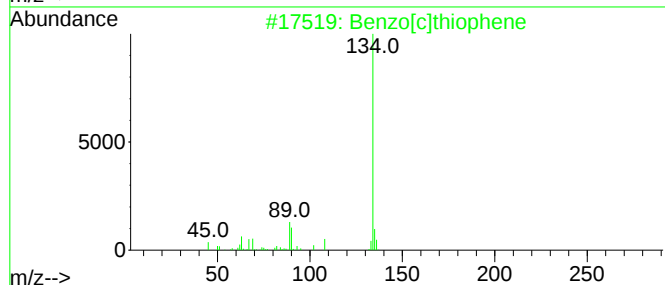
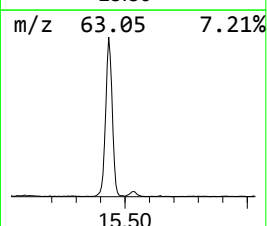
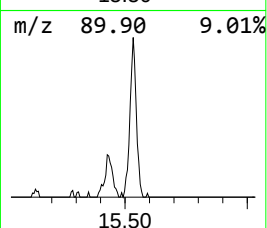
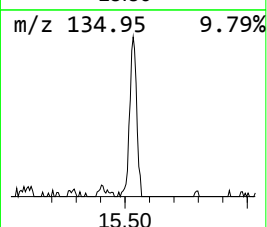
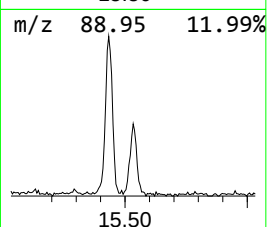
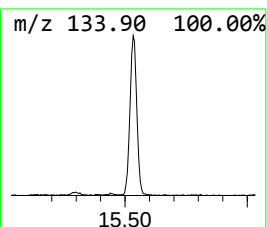
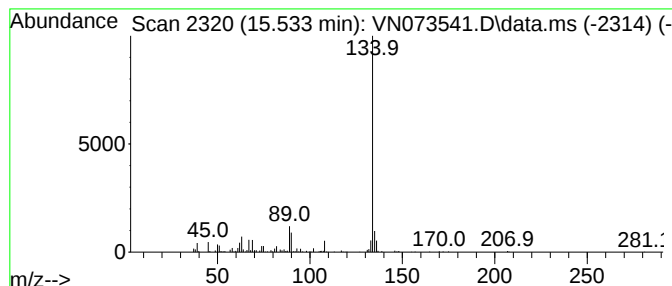
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Quant Title : SW846 8260

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

Peak Number 8 Benzo[c]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	7.77 ug/l	331389	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			5-Benzylidene-3-(2,5-dimethylani...	338	C19H18N2O2S	302955-01-7	64
5			3-Deazaadenine	134	C6H6N4	006811-77-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073541.D
Acq On : 20 Jul 2022 23:02
Operator : JC\MD
Sample : N3779-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-G

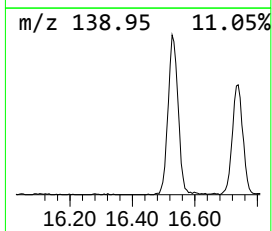
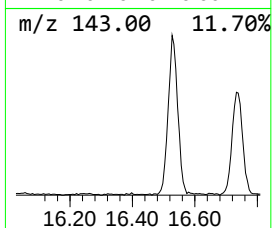
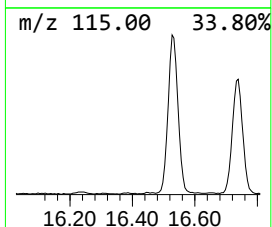
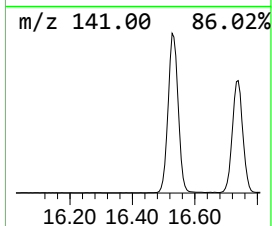
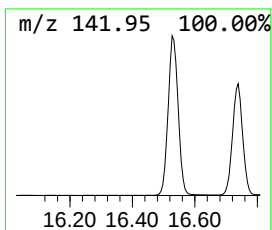
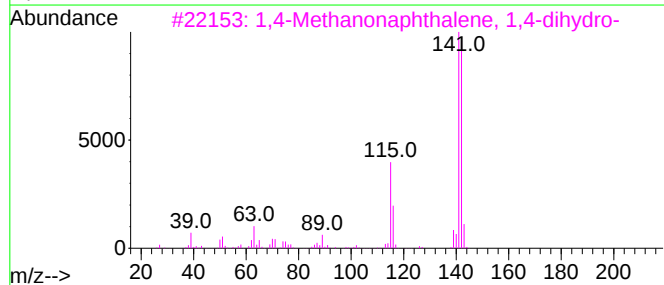
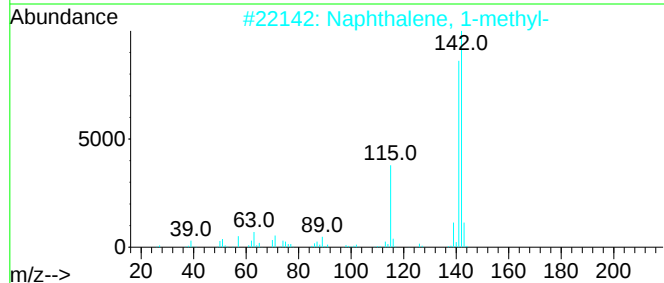
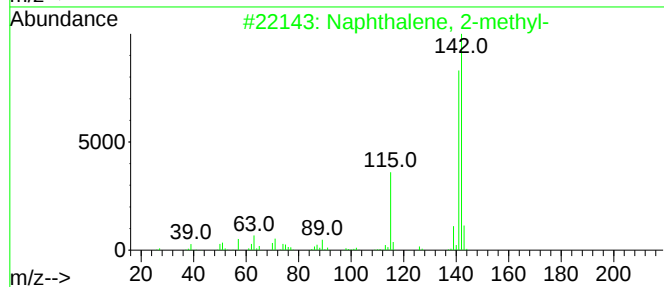
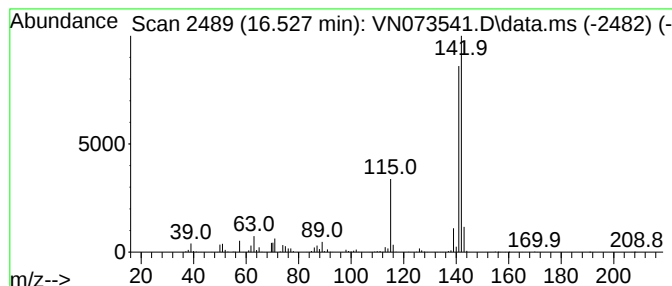
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Quant Title : SW846 8260

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	77.89 ug/l	3323090	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	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	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073541.D
Acq On : 20 Jul 2022 23:02
Operator : JC\MD
Sample : N3779-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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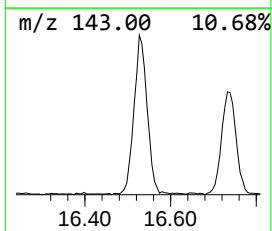
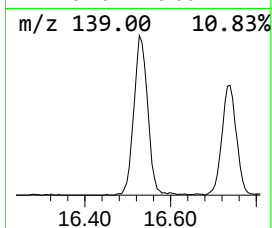
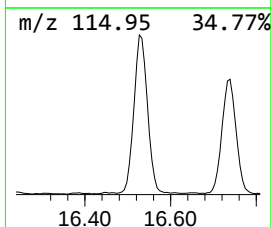
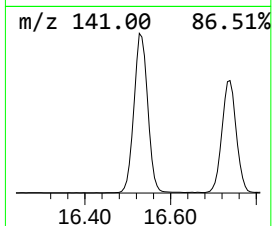
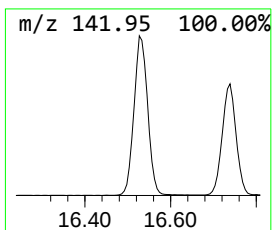
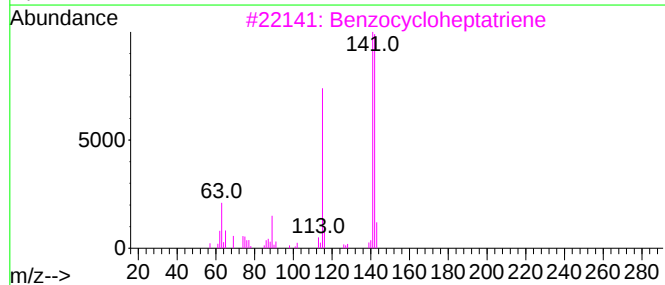
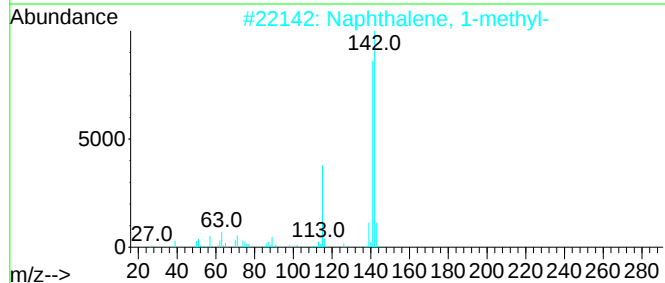
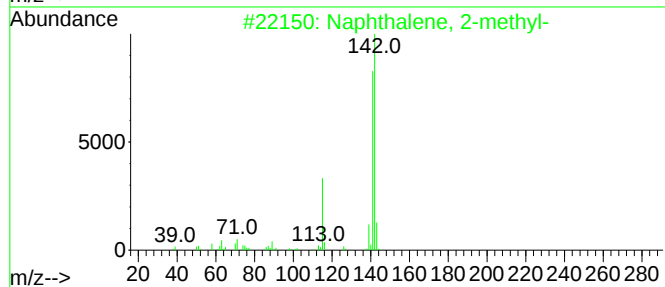
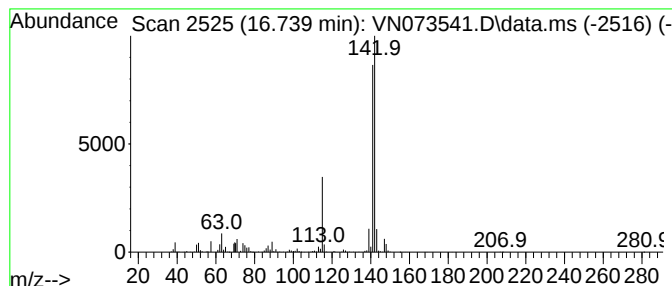
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	57.95 ug/l	2472190	1,4-Dichlorobenzene-d4	13.615

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	90
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072022\
Data File : VN073541.D
Acq On : 20 Jul 2022 23:02
Operator : JC\MD
Sample : N3779-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
070622-G

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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unknown11.086	11.086	6.4	ug/l	187948	3	11.686	1459120	50.0
Thiophene, tetr...	11.163	40.8	ug/l	1189980	3	11.686	1459120	50.0
Thiophene, tetr...	12.027	14.0	ug/l	409210	3	11.686	1459120	50.0
Thiophene, 2,3-...	12.457	9.5	ug/l	276982	3	11.686	1459120	50.0
Naphthalene, 2,...	13.498	22.7	ug/l	968658	4	13.615	2133190	50.0
Indene	13.998	16.9	ug/l	722254	4	13.615	2133190	50.0
Benzo[c]thiophene	15.533	7.8	ug/l	331389	4	13.615	2133190	50.0
Naphthalene, 2-...	16.527	77.9	ug/l	3323090	4	13.615	2133190	50.0
Naphthalene, 1-...	16.739	58.0	ug/l	2472190	4	13.615	2133190	50.0