

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
 Data File : VX027259.D
 Acq On : 01 Mar 2022 19:24
 Operator : JC/MD
 Sample : N1725-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-03

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_X\Method\82X022322W.M
 Title : SW846 8260

Signal : TIC: VX027259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	43	rBV	20803	53429	1.64%	0.775%
2	5.391	696	706	722	rBV	49952	143863	4.40%	2.087%
3	5.556	722	733	749	rVV	86997	243226	7.44%	3.528%
4	5.964	790	800	809	rBV	52015	139727	4.28%	2.027%
5	6.769	922	932	948	rBV	133846	319332	9.77%	4.632%
6	8.653	1234	1241	1250	rBV	283795	437196	13.38%	6.341%
7	10.055	1465	1471	1482	rBV	288635	379485	11.61%	5.504%
8	11.085	1634	1640	1646	rBV	226513	294420	9.01%	4.270%
9	12.024	1789	1794	1801	rBV	316715	381081	11.66%	5.527%
10	12.244	1825	1830	1839	rBV	337082	404632	12.38%	5.869%
11	13.780	2076	2082	2091	rBV	2613634	3267674	100.00%	47.395%
12	13.871	2091	2097	2104	rVB	134253	168483	5.16%	2.444%
13	14.640	2218	2223	2233	rVB	217543	266023	8.14%	3.858%
14	14.780	2241	2246	2260	rVB	167051	204053	6.24%	2.960%
15	16.328	2493	2500	2513	rBV	110026	191960	5.87%	2.784%

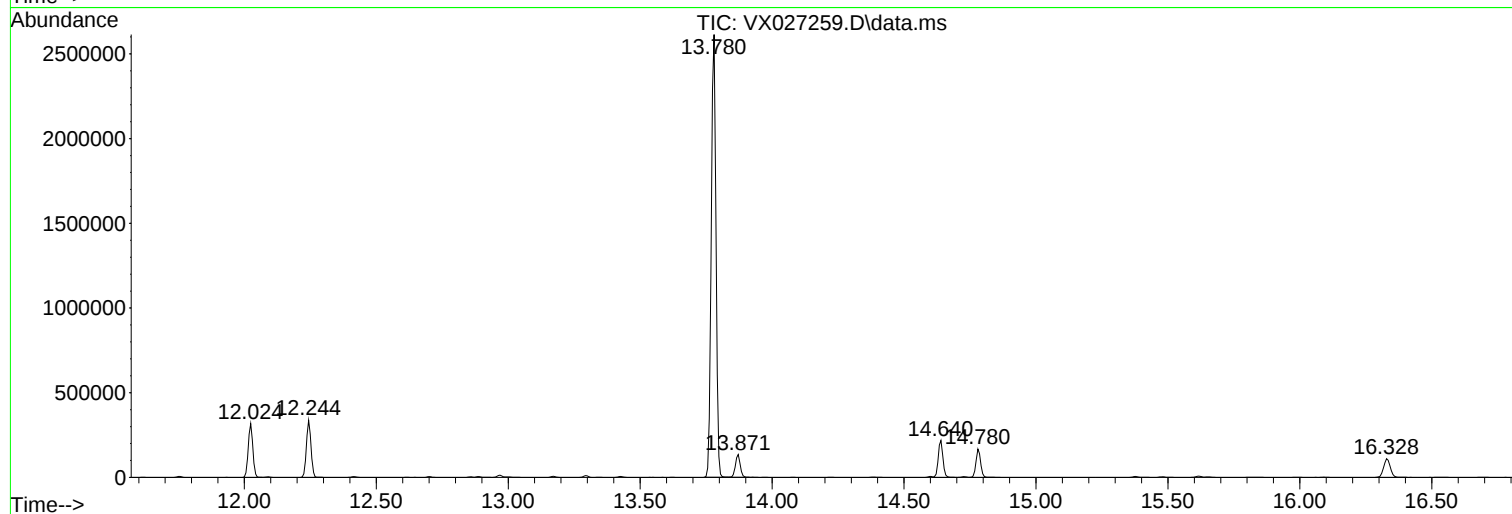
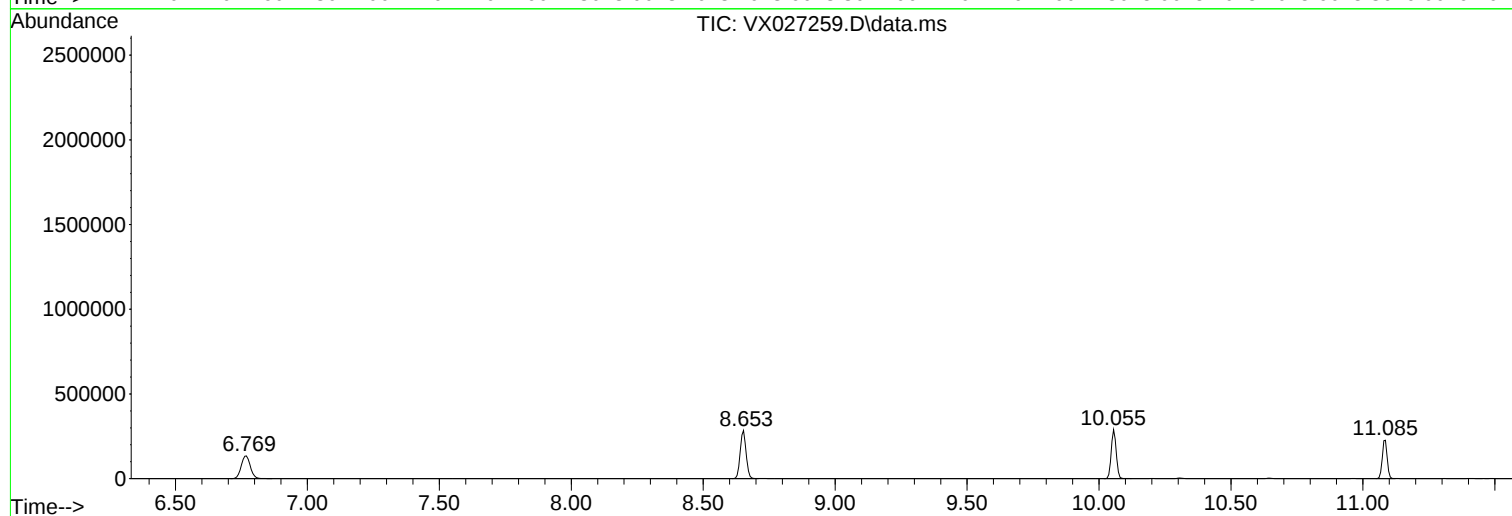
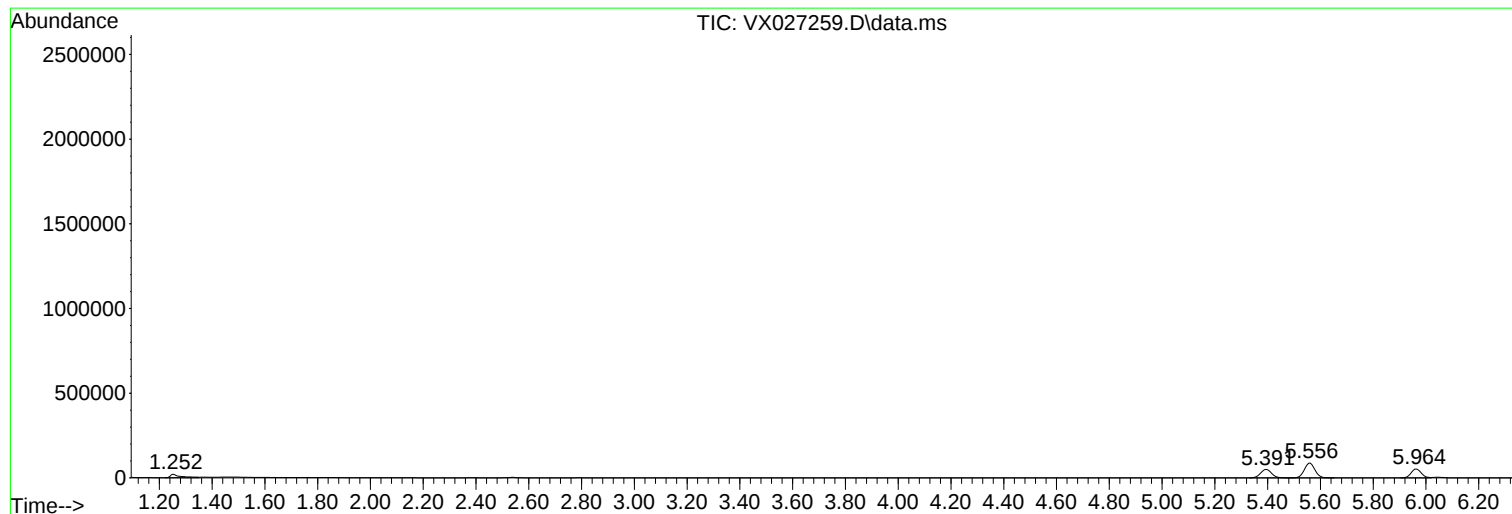
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



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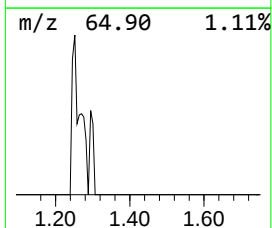
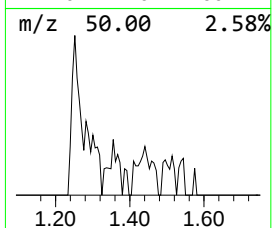
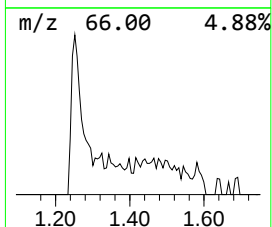
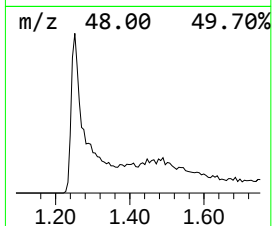
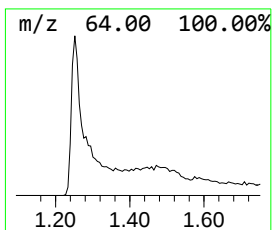
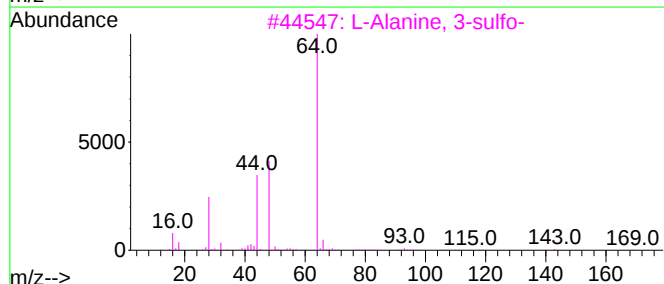
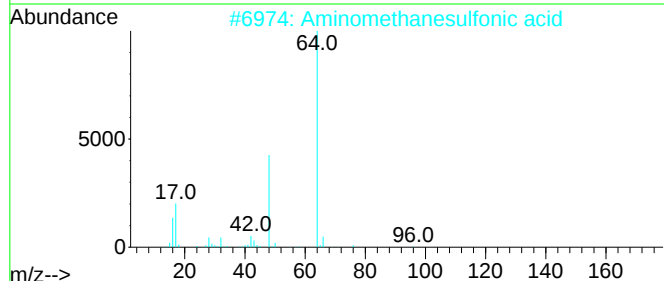
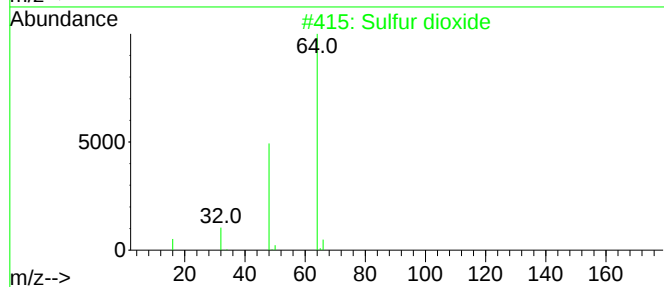
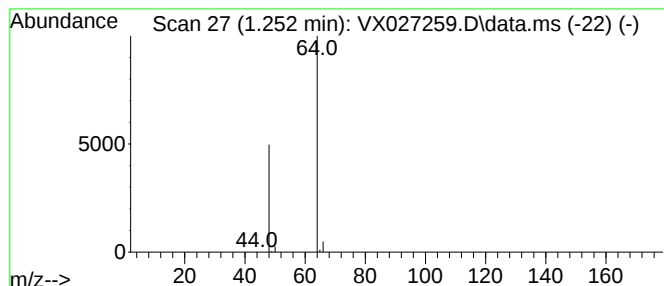
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	10.98 ug/l	53429	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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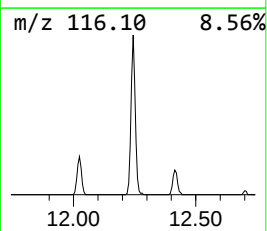
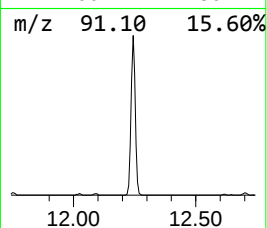
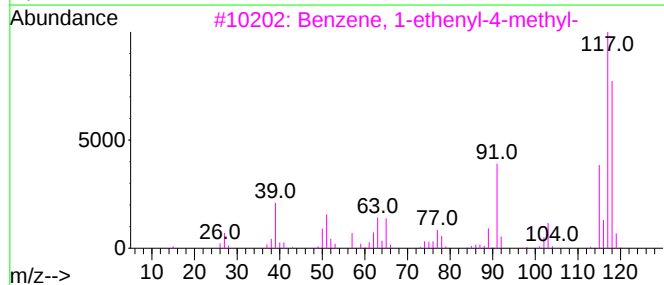
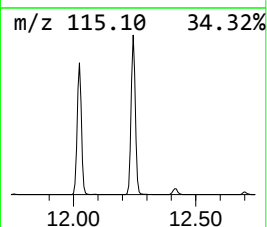
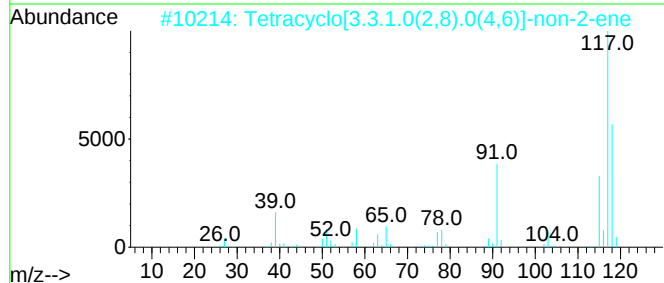
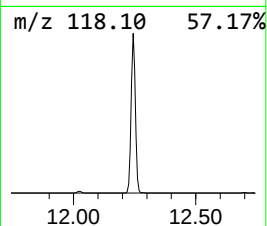
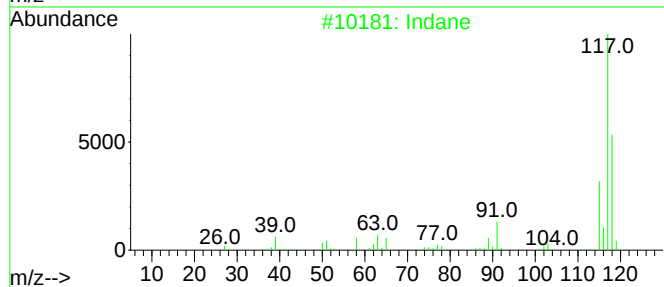
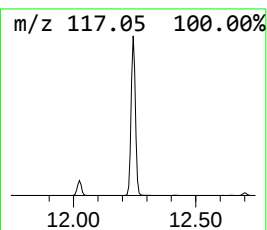
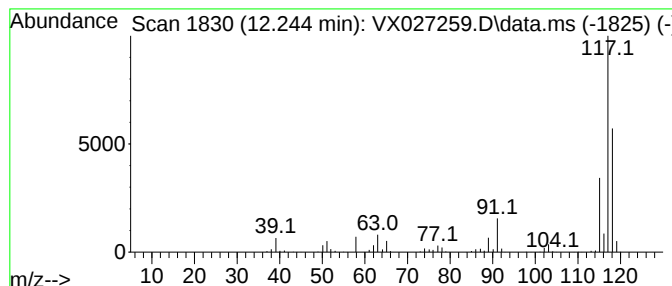
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	53.09 ug/l	404632	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74
4			Deltacyclene	118	C9H10	007785-10-6	72
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64



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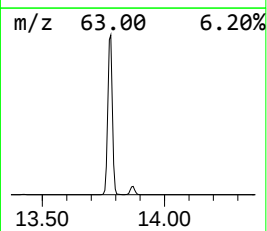
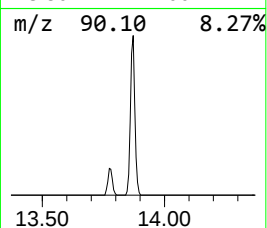
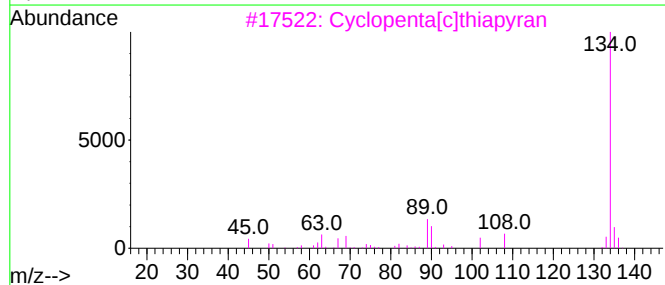
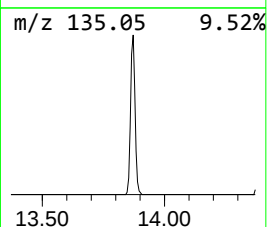
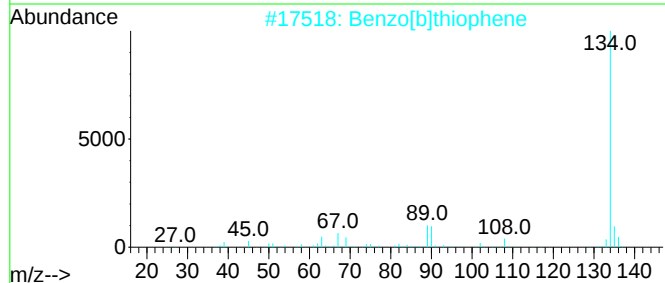
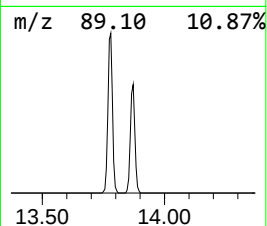
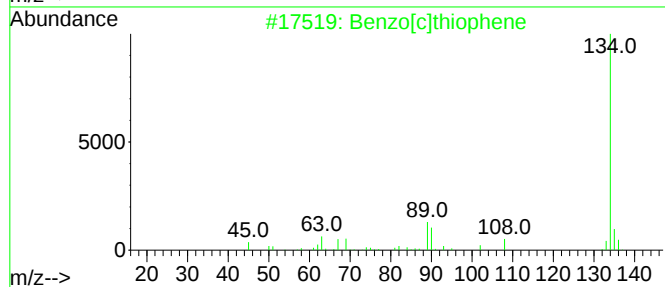
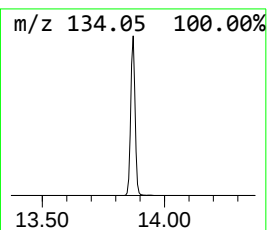
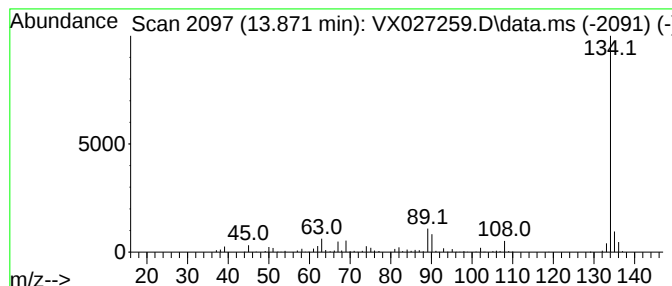
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzo[c]thiophene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	22.11 ug/l	168483	1,4-Dichlorobenzene-d4	12.024

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			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



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Instrument :
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ClientSampleId :
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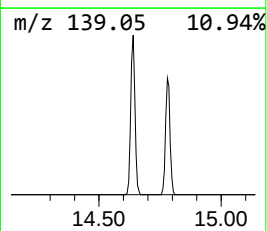
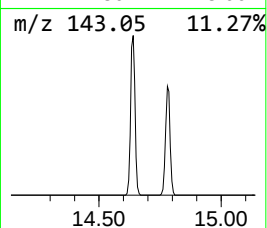
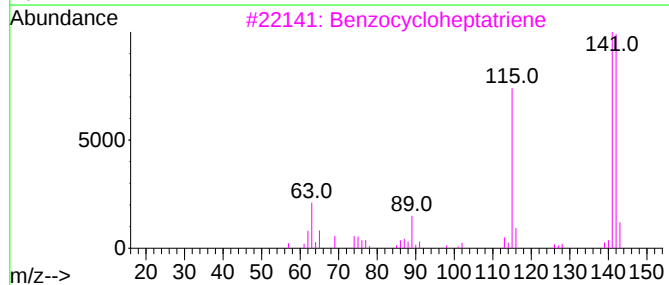
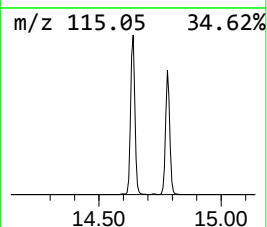
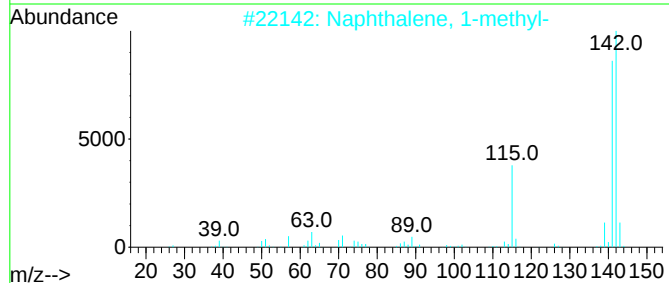
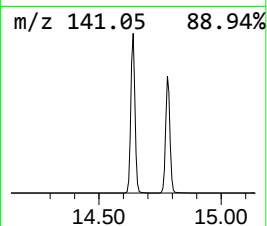
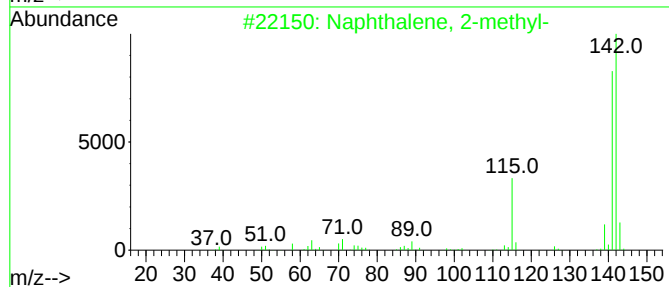
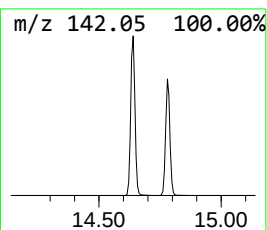
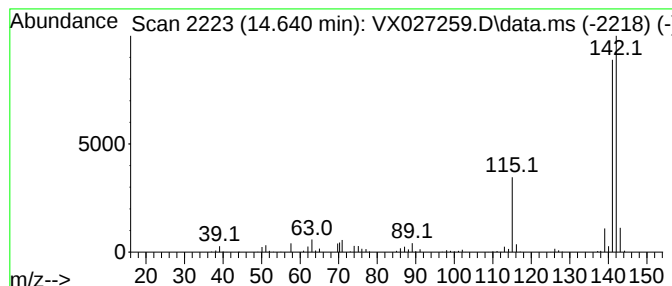
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	34.90 ug/l	266023	1,4-Dichlorobenzene-d4	12.024

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



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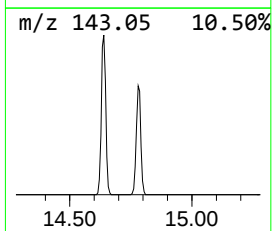
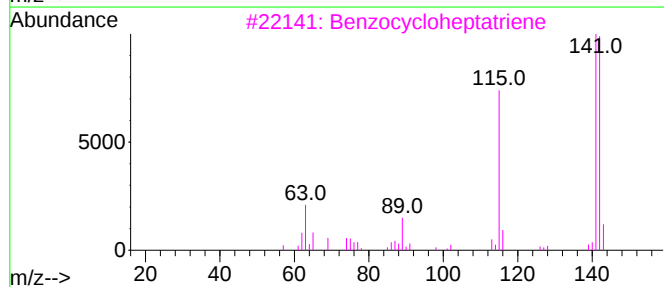
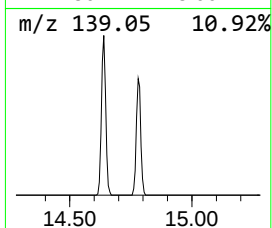
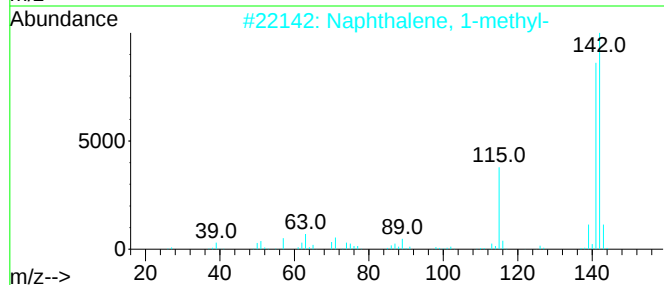
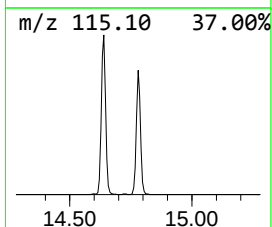
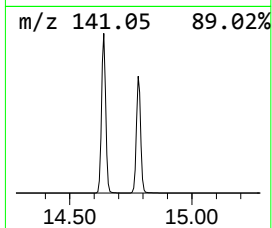
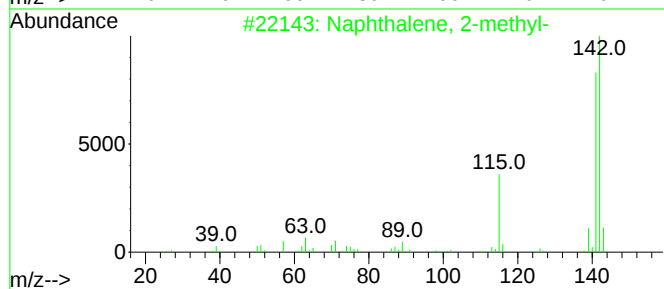
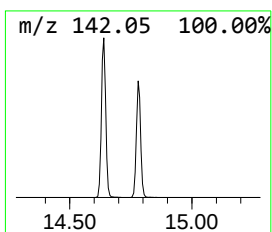
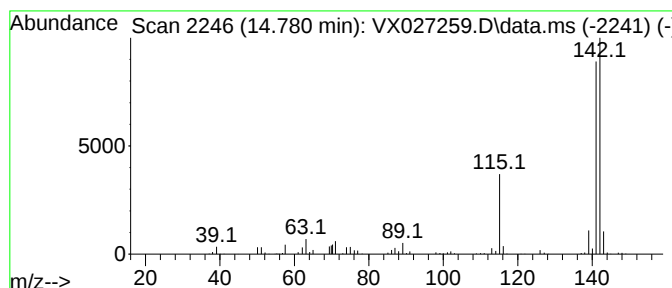
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Methanonaphthalene, 1,4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	26.77 ug/l	204053	1,4-Dichlorobenzene-d4	12.024

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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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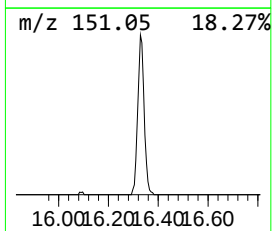
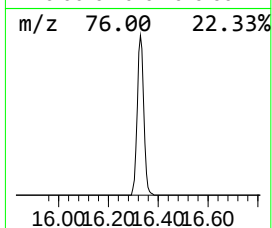
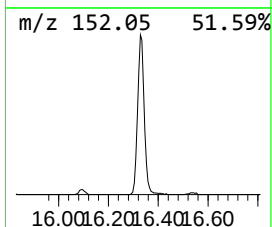
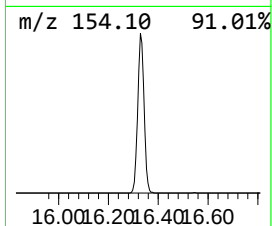
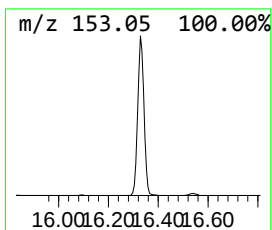
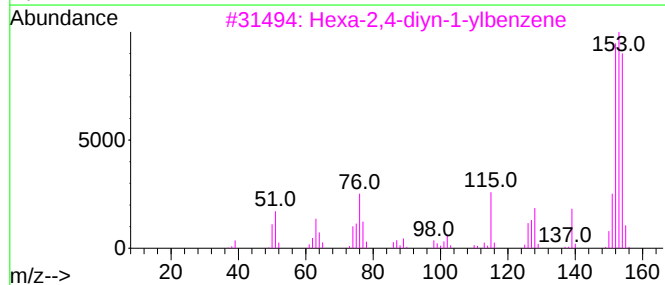
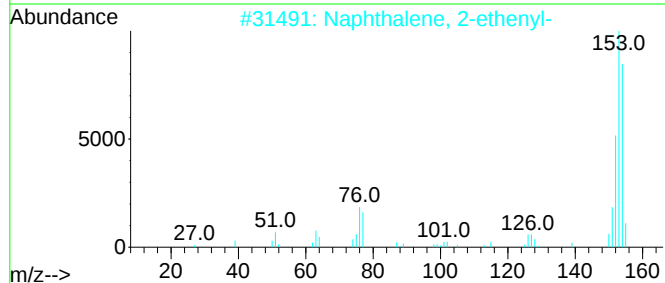
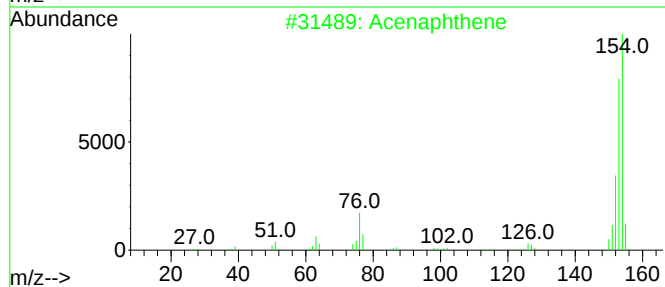
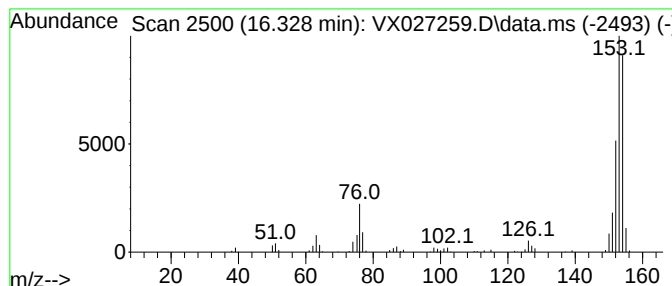
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	25.19 ug/l	191960	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	68
3			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53
5			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027259.D
Acq On : 01 Mar 2022 19:24
Operator : JC/MD
Sample : N1725-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	11.0	ug/l	53429	1	5.556	243226	50.0
Indane	12.244	53.1	ug/l	404632	4	12.024	381081	50.0
Benzo[c]thiophene	13.871	22.1	ug/l	168483	4	12.024	381081	50.0
Benzocyclohepta...	14.640	34.9	ug/l	266023	4	12.024	381081	50.0
1,4-Methanonaph...	14.780	26.8	ug/l	204053	4	12.024	381081	50.0
Hexa-2,4-diyne-1...	16.328	25.2	ug/l	191960	4	12.024	381081	50.0