

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
 Data File : VN080503.D
 Acq On : 15 Dec 2023 15:12
 Operator : JC\MD
 Sample : 05862-12
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-LIQUIDS-20231213-01

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\82N121223W.M
 Title : SW846 8260

Signal : TIC: VN080503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.106	1207	1216	1224	rBV	466506	969812	1.33%	0.540%
2	10.571	1457	1465	1470	rBV	688026	1248032	1.72%	0.695%
3	10.629	1470	1475	1488	rVB	459309	848643	1.17%	0.473%
4	11.865	1677	1685	1693	rBV	739423	1321307	1.82%	0.736%
5	11.965	1693	1702	1711	rVV	8152952	13749601	18.92%	7.660%
6	12.070	1711	1720	1736	rVB	6082556	11459284	15.77%	6.384%
7	12.400	1769	1776	1791	rVB	3989988	6732220	9.26%	3.750%
8	12.853	1844	1853	1862	rBV	592210	1003519	1.38%	0.559%
9	13.100	1888	1895	1898	rBV	2247637	3730816	5.13%	2.078%
10	13.129	1898	1900	1905	rVV	1194082	1818261	2.50%	1.013%
11	13.176	1905	1908	1915	rVB	560647	813458	1.12%	0.453%
12	13.335	1928	1935	1945	rVB	473457	862145	1.19%	0.480%
13	13.482	1948	1960	1965	rBV	2298029	3893712	5.36%	2.169%
14	13.794	2007	2013	2015	rBV	820229	1344457	1.85%	0.749%
15	13.823	2015	2018	2021	rVV	985848	1543503	2.12%	0.860%
16	13.859	2021	2024	2033	rVB	561556	851074	1.17%	0.474%
17	14.000	2041	2048	2060	rVB	15511873	26879298	36.99%	14.974%
18	14.176	2069	2078	2086	rBV	4652319	7791899	10.72%	4.341%
19	14.929	2199	2206	2218	rVB	627028	1015215	1.40%	0.566%
20	15.053	2218	2227	2232	rBV3	397914	984793	1.36%	0.549%
21	15.123	2232	2239	2246	rVV	1672541	2922852	4.02%	1.628%
22	15.205	2246	2253	2264	rVV	3079800	5588801	7.69%	3.113%
23	15.647	2318	2328	2338	rBV2	35443273	72675216	100.00%	40.486%
24	15.747	2338	2345	2357	rVB	958728	1937098	2.67%	1.079%
25	16.782	2513	2521	2522	rBV	4989771	7521522	10.35%	4.190%

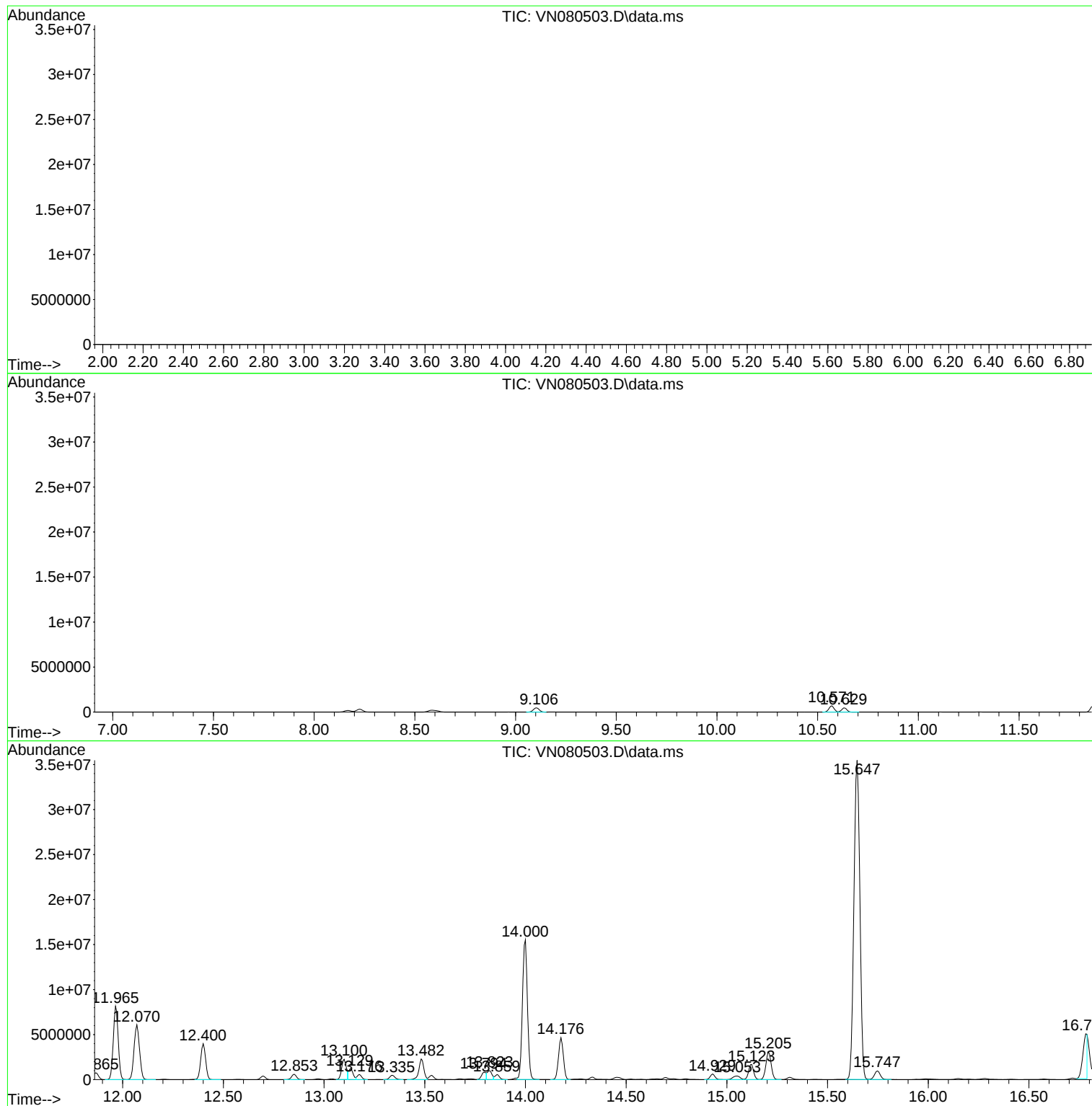
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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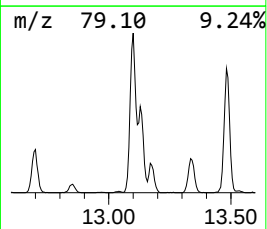
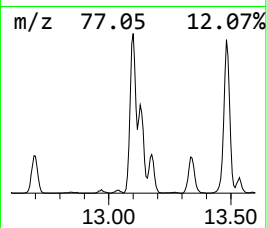
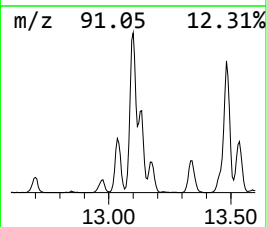
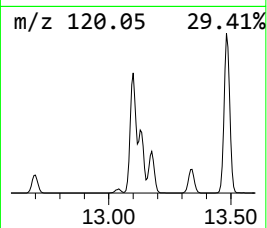
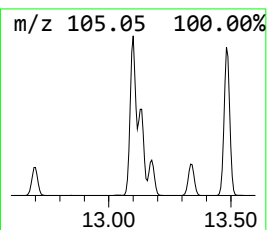
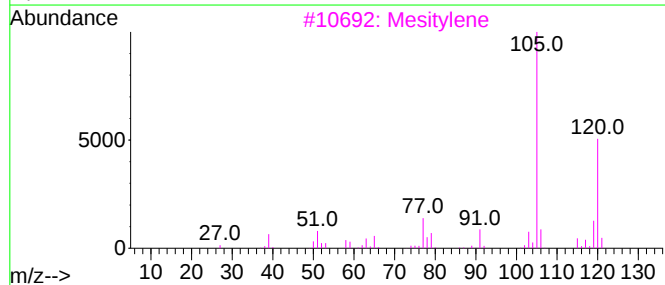
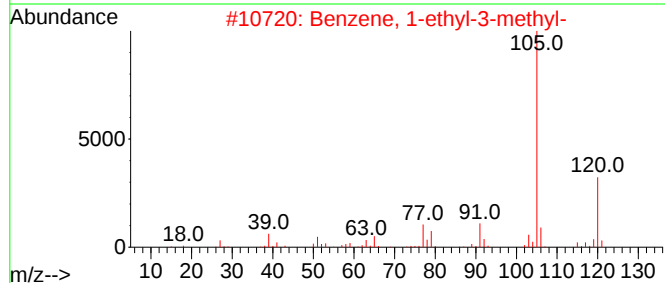
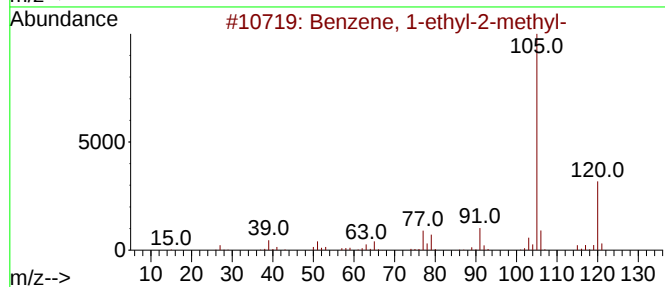
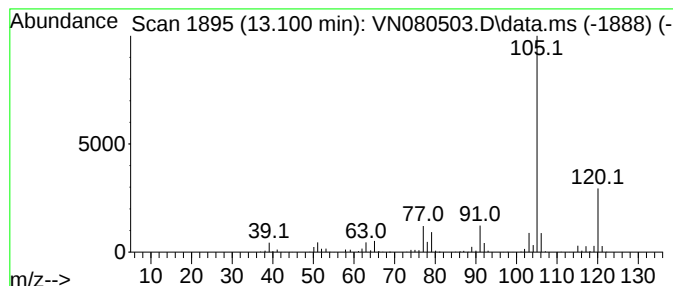
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	138.75 ug/l	3730820	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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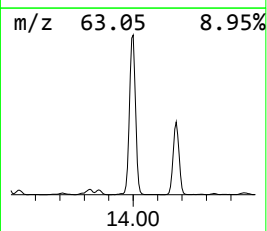
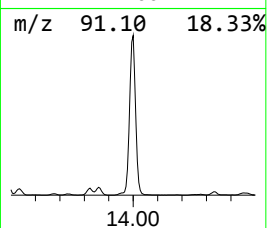
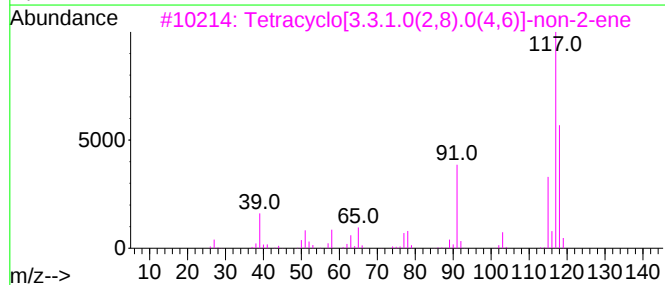
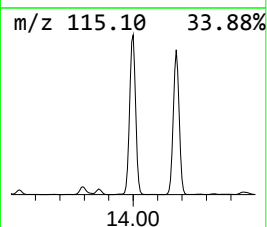
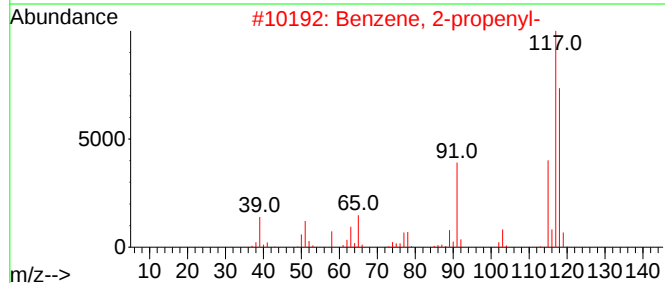
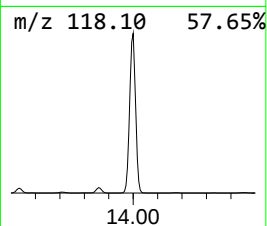
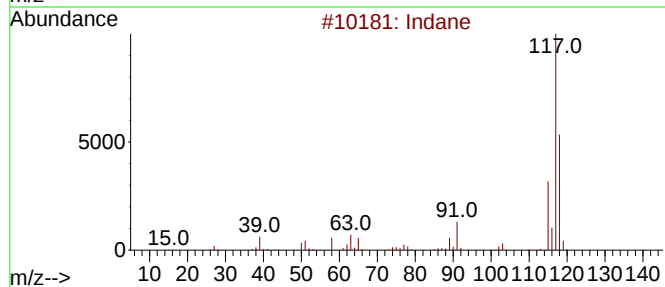
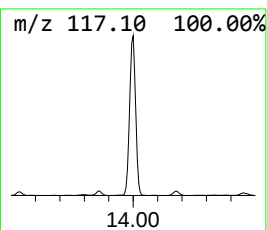
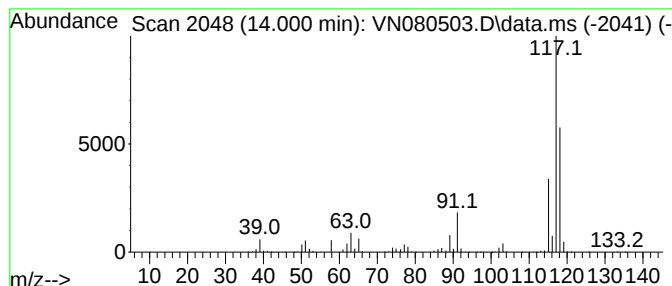
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	999.63 ug/l	26879300	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	68



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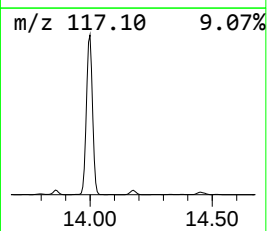
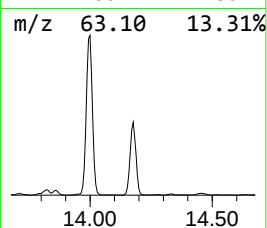
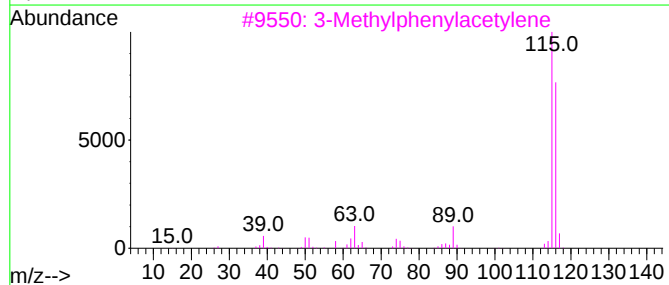
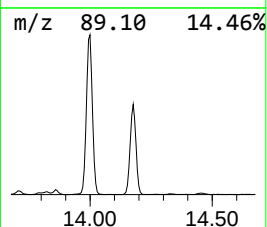
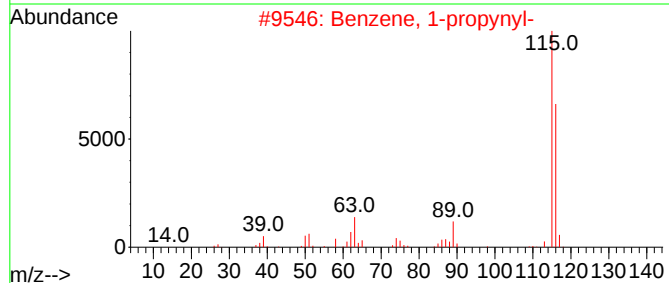
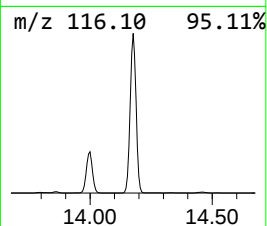
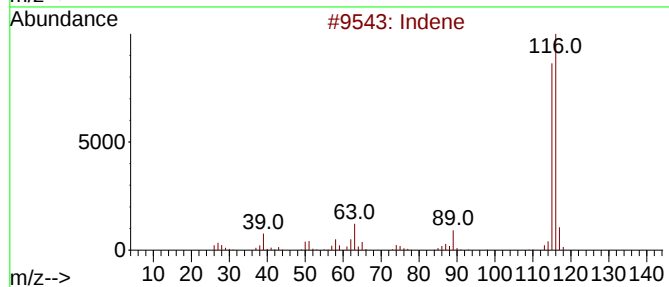
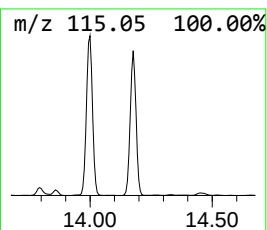
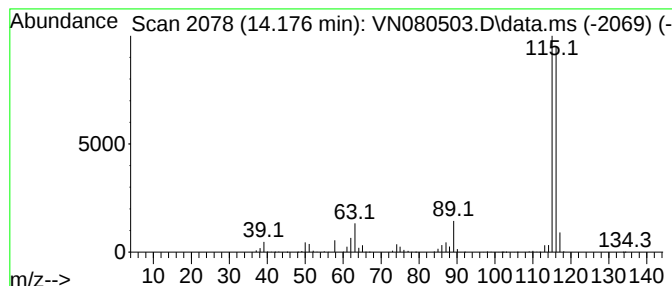
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	289.78 ug/l	7791900	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



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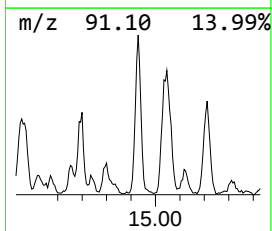
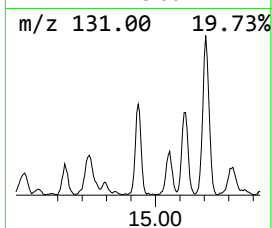
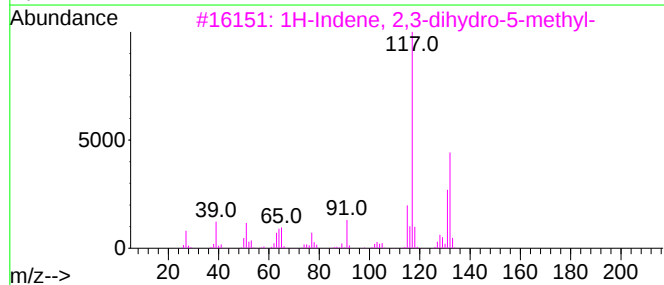
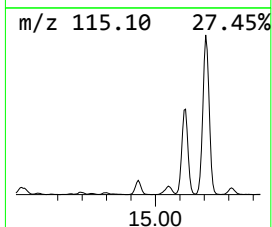
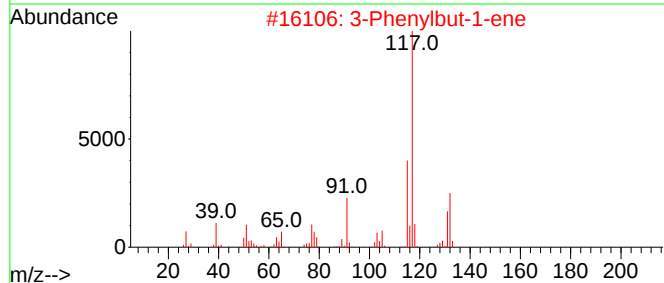
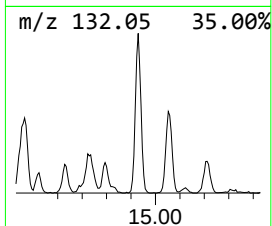
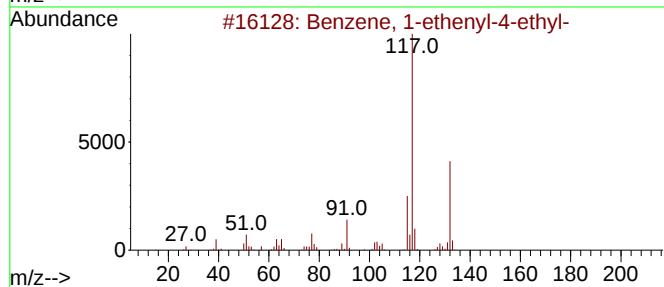
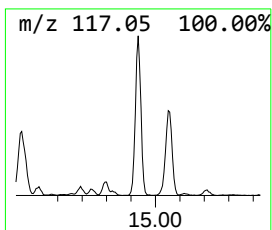
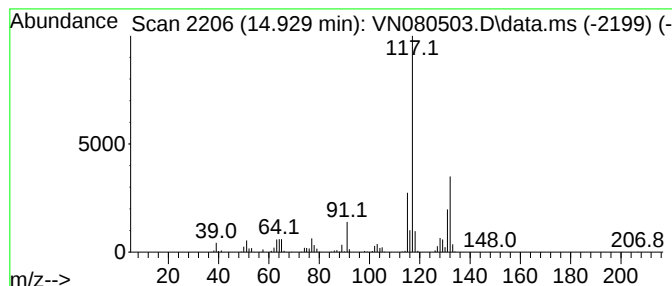
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	37.76 ug/l	1015220	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



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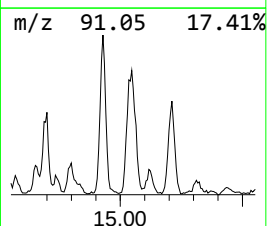
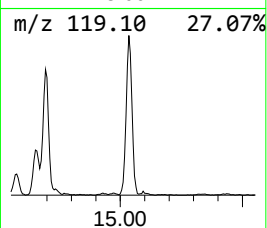
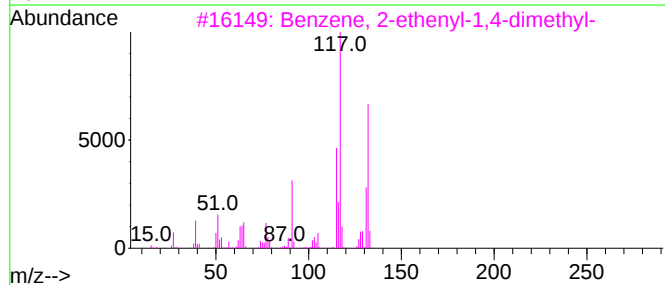
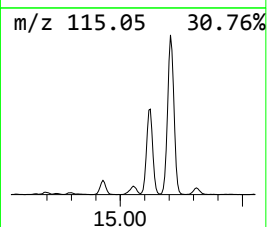
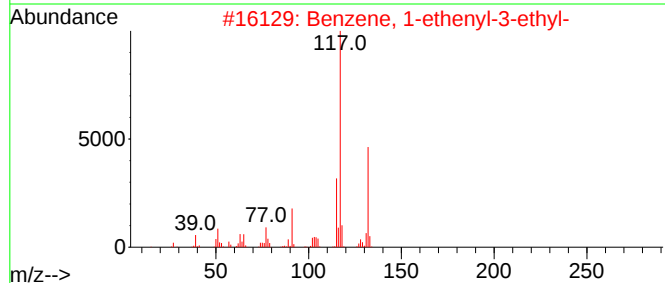
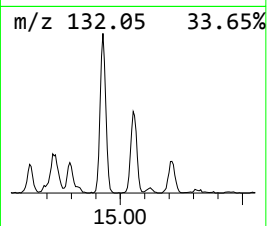
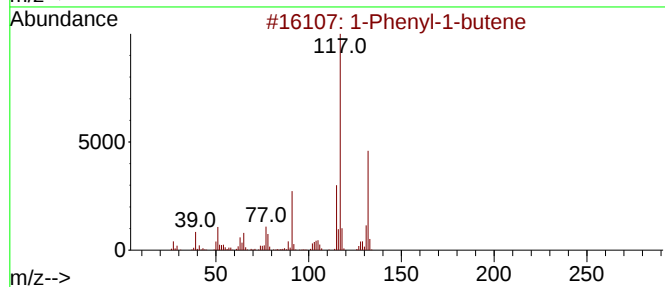
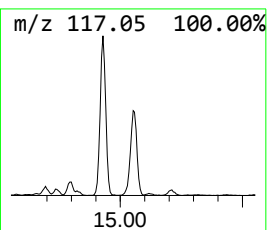
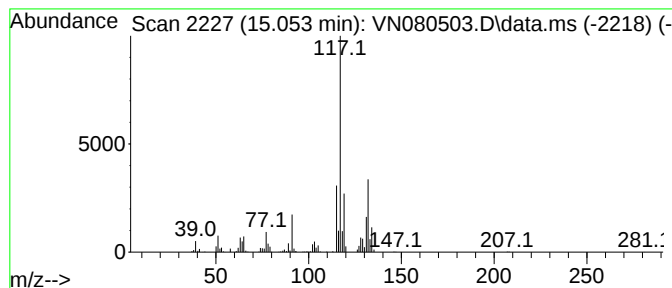
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	36.62 ug/l	984793	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	93
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



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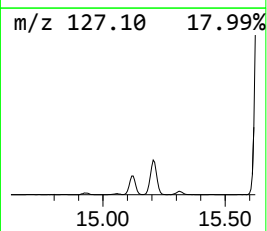
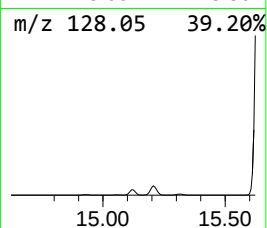
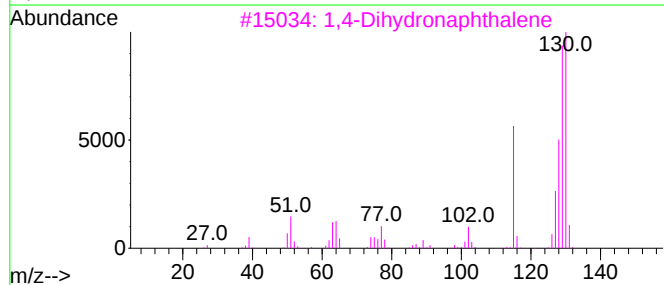
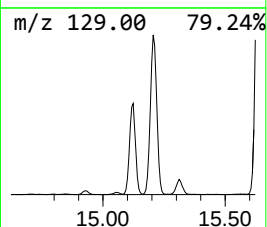
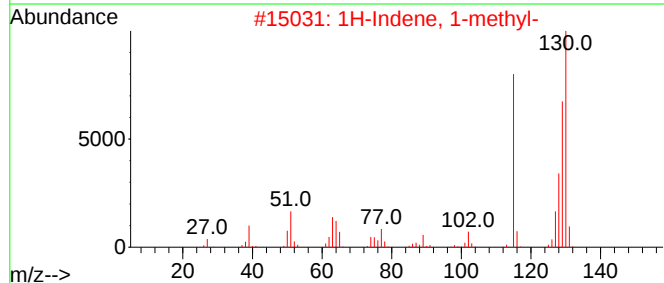
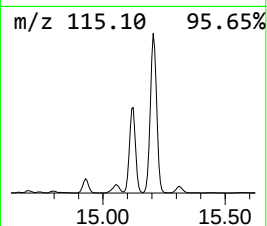
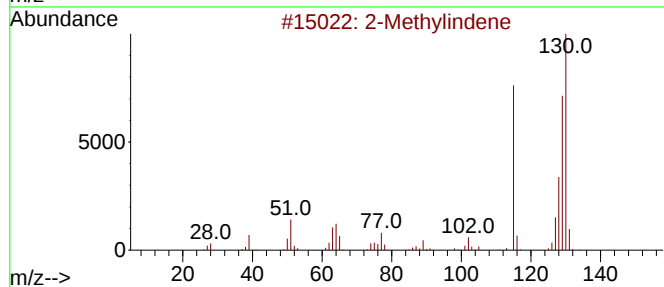
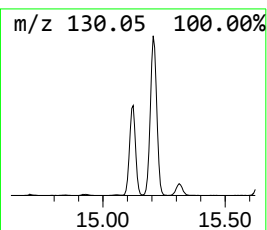
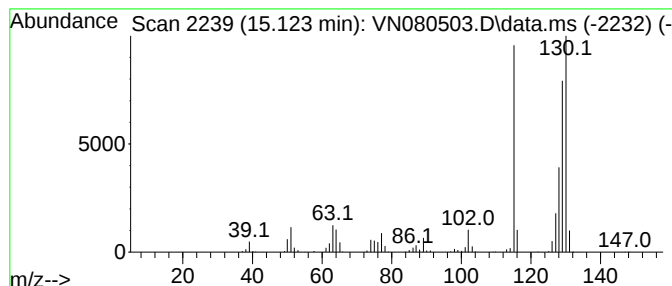
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Quant Title : SW846 8260

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

Peak Number 6 2-Methylindene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	108.70 ug/l	2922850	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	96
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
3			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93
4			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080503.D
Acq On : 15 Dec 2023 15:12
Operator : JC\MD
Sample : 05862-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-LIQUIDS-20231213-01

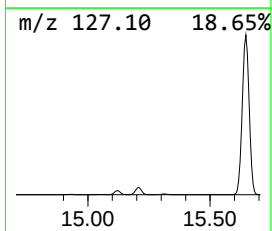
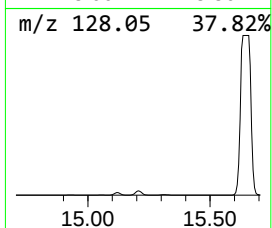
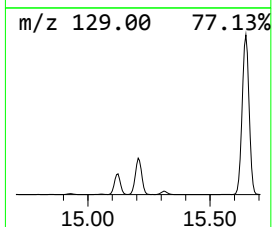
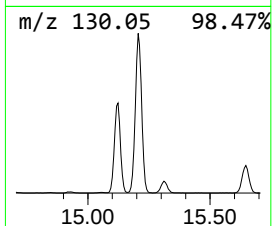
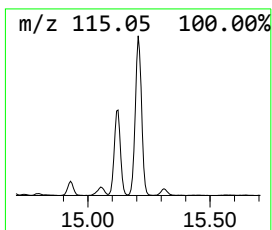
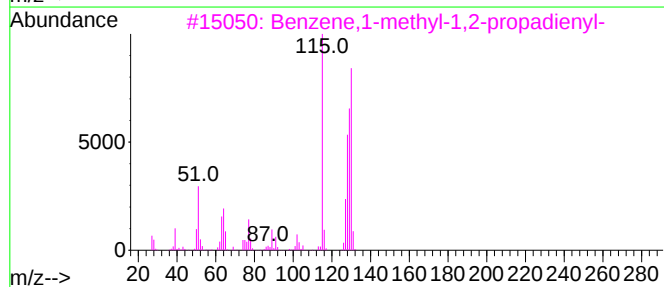
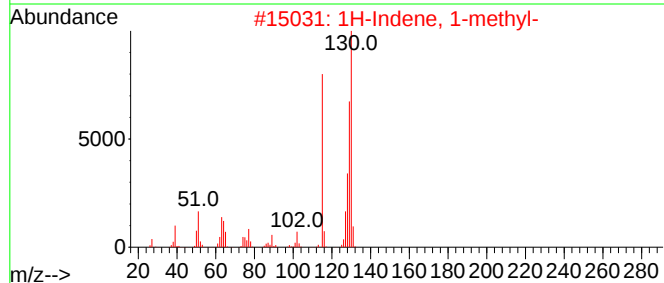
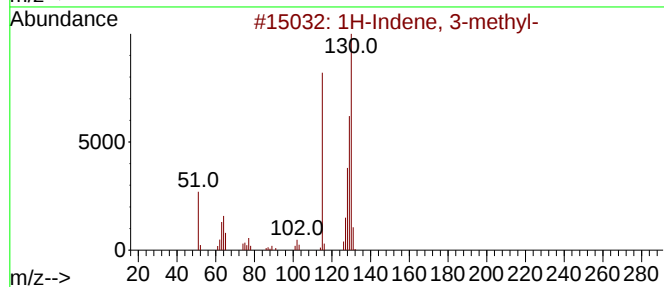
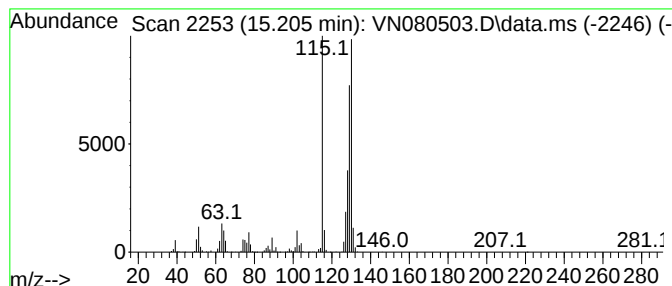
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	207.85 ug/l	5588800	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 3-methyl-	130	C10H10	000767-60-2	95
2		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
3		Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
4		2-Methylindene	130	C10H10	002177-47-1	95
5		Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080503.D
Acq On : 15 Dec 2023 15:12
Operator : JC\MD
Sample : 05862-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-LIQUIDS-20231213-01

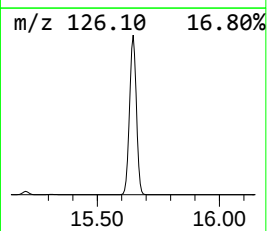
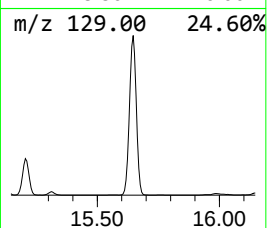
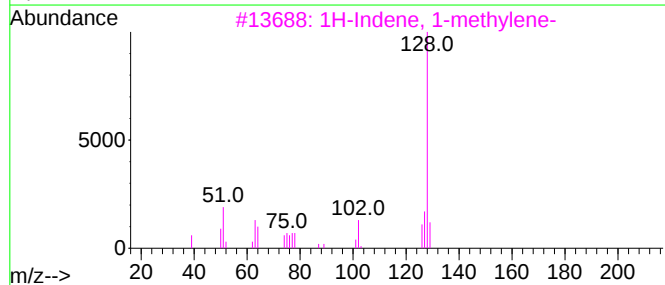
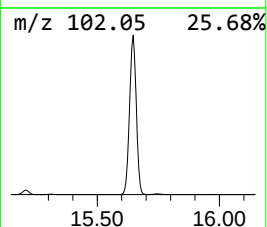
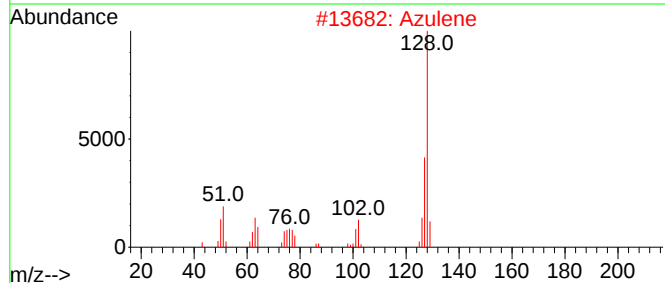
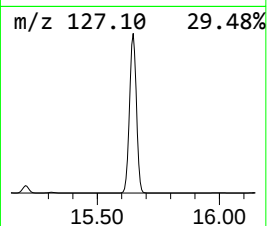
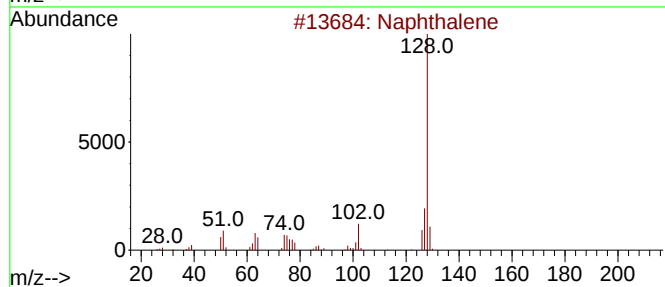
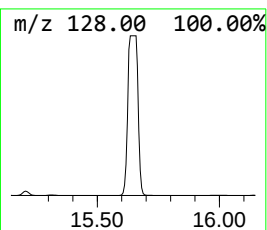
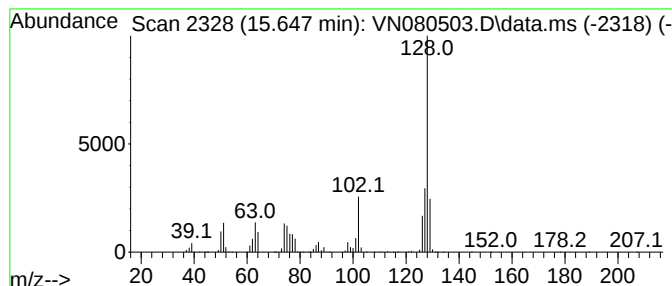
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Quant Title : SW846 8260

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

Peak Number 8 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	2702.77 ug/l	72675200	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	91
2			Azulene	128	C10H8	000275-51-4	81
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	64
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	53
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080503.D
Acq On : 15 Dec 2023 15:12
Operator : JC\MD
Sample : 05862-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-LIQUIDS-20231213-01

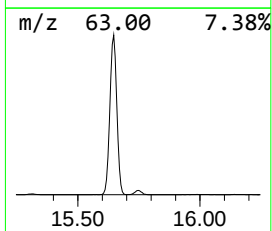
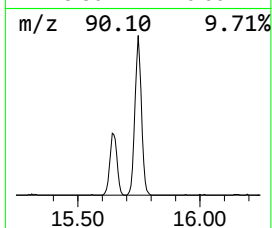
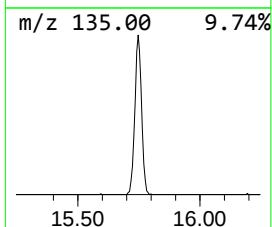
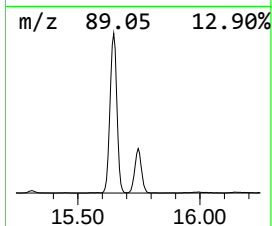
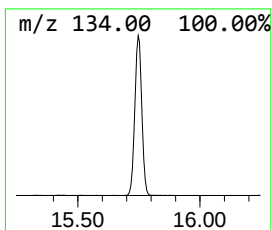
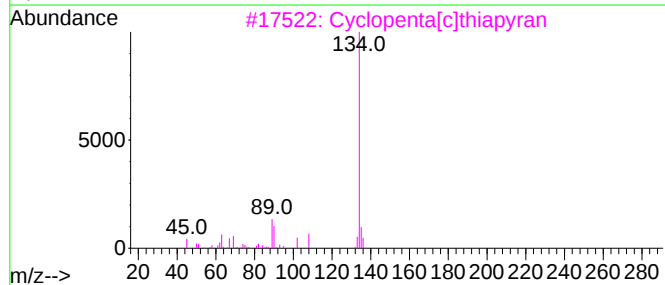
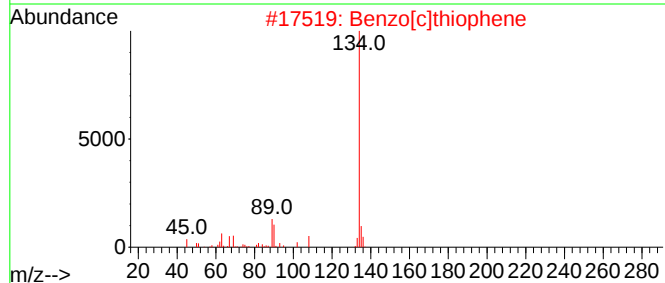
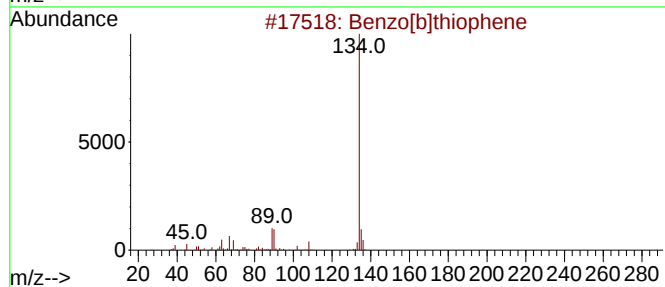
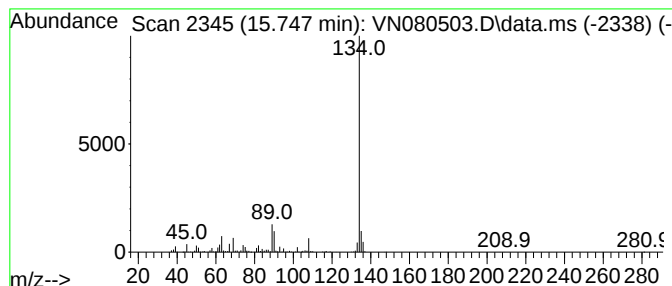
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[b]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.747	72.04 ug/l	1937100	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50
5			3-Deazaadenine	134	C6H6N4	006811-77-4	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080503.D
Acq On : 15 Dec 2023 15:12
Operator : JC\MD
Sample : 05862-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-LIQUIDS-20231213-01

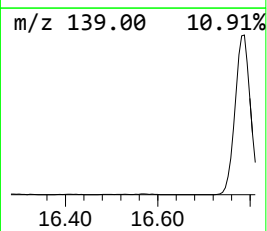
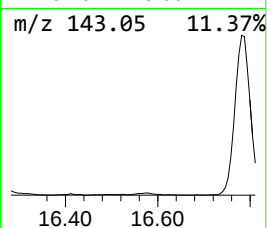
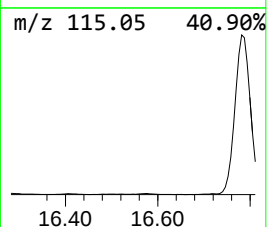
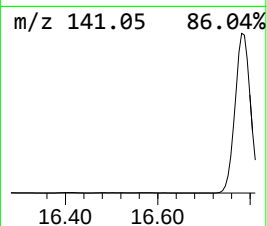
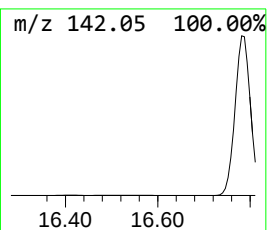
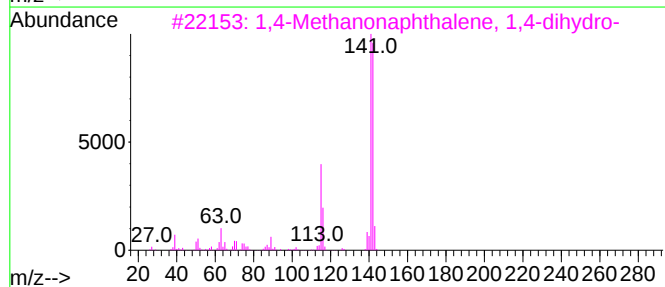
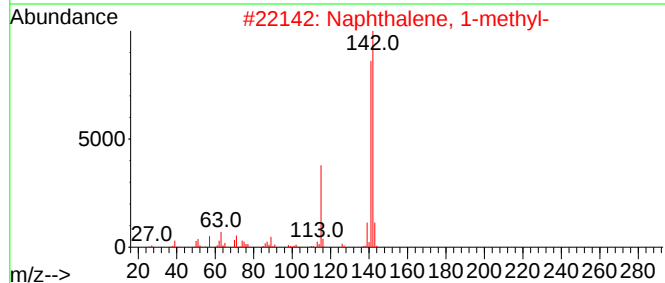
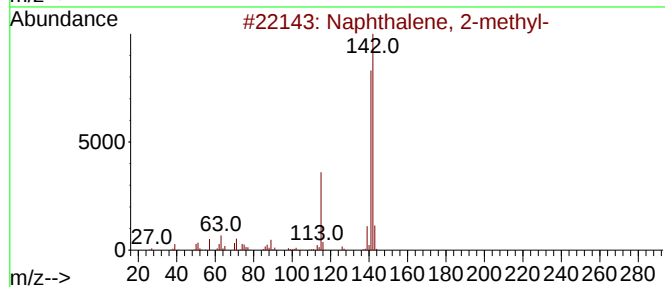
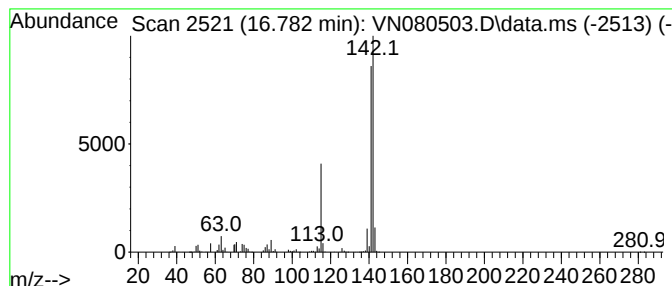
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Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	279.72 ug/l	7521520	1,4-Dichlorobenzene-d4	13.794

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	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080503.D
Acq On : 15 Dec 2023 15:12
Operator : JC\MD
Sample : 05862-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-LIQUIDS-20231213-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.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
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Indane	14.000	999.6	ug/l	26879300	4	13.794	1344460	50.0
Indene	14.176	289.8	ug/l	7791900	4	13.794	1344460	50.0
Benzene, 1-ethe...	14.929	37.8	ug/l	1015220	4	13.794	1344460	50.0
1-Phenyl-1-butene	15.053	36.6	ug/l	984793	4	13.794	1344460	50.0
2-Methylindene	15.123	108.7	ug/l	2922850	4	13.794	1344460	50.0
1H-Indene, 3-me...	15.206	207.8	ug/l	5588800	4	13.794	1344460	50.0
Azulene	15.647	2702.8	ug/l	72675200	4	13.794	1344460	50.0
Benzo[b]thiophene	15.747	72.0	ug/l	1937100	4	13.794	1344460	50.0
1,4-Methanonaph...	16.782	279.7	ug/l	7521520	4	13.794	1344460	50.0