

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079030.D
 Acq On : 24 Aug 2023 14:41
 Operator : JC\MD
 Sample : 04047-01 20X
 Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB05-Z26-27

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\82N081523W.M
 Title : SW846 8260

Signal : TIC: VN079030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.230	1061	1067	1081	rVB	332869	788396	1.03%	0.520%
2	8.612	1119	1132	1144	rBV	2228248	5425974	7.08%	3.582%
3	9.106	1206	1216	1230	rBV	501465	1018941	1.33%	0.673%
4	10.571	1457	1465	1472	rBV	790509	1487063	1.94%	0.982%
5	11.870	1678	1686	1695	rBV	716040	1276048	1.67%	0.842%
6	11.970	1695	1703	1712	rVV	5598387	9496029	12.40%	6.269%
7	12.070	1712	1720	1731	rVB	2651770	5184194	6.77%	3.422%
8	12.400	1765	1776	1786	rBV	1610344	2794838	3.65%	1.845%
9	12.853	1847	1853	1862	rVB	604547	1067189	1.39%	0.705%
10	13.100	1889	1895	1898	rBV	1242489	2124526	2.77%	1.403%
11	13.135	1898	1901	1905	rVV	1407889	2207175	2.88%	1.457%
12	13.176	1905	1908	1915	rVB	536003	821812	1.07%	0.543%
13	13.341	1928	1936	1943	rBV	593648	1015857	1.33%	0.671%
14	13.488	1951	1961	1966	rBV	1675971	2923788	3.82%	1.930%
15	13.794	2007	2013	2016	rBV	740419	1332718	1.74%	0.880%
16	13.953	2033	2040	2042	rBV	552672	831088	1.09%	0.549%
17	14.000	2042	2048	2063	rVB	11186096	19122678	24.97%	12.624%
18	14.335	2099	2105	2114	rBV	744164	1181632	1.54%	0.780%
19	14.470	2118	2128	2134	rVB3	675625	1554226	2.03%	1.026%
20	14.929	2200	2206	2218	rVB	1066447	1853021	2.42%	1.223%
21	15.041	2218	2225	2233	rBV3	463644	1132343	1.48%	0.748%
22	15.123	2233	2239	2246	rVB	1310239	2252905	2.94%	1.487%
23	15.211	2246	2254	2261	rVB	2501647	4674626	6.10%	3.086%
24	15.317	2263	2272	2279	rBV3	493835	1101687	1.44%	0.727%
25	15.647	2319	2328	2338	rVB2	41340304	76584194	100.00%	50.558%
26	15.747	2338	2345	2353	rBV	728593	1422729	1.86%	0.939%
27	15.988	2381	2386	2401	rVB	235527	801923	1.05%	0.529%

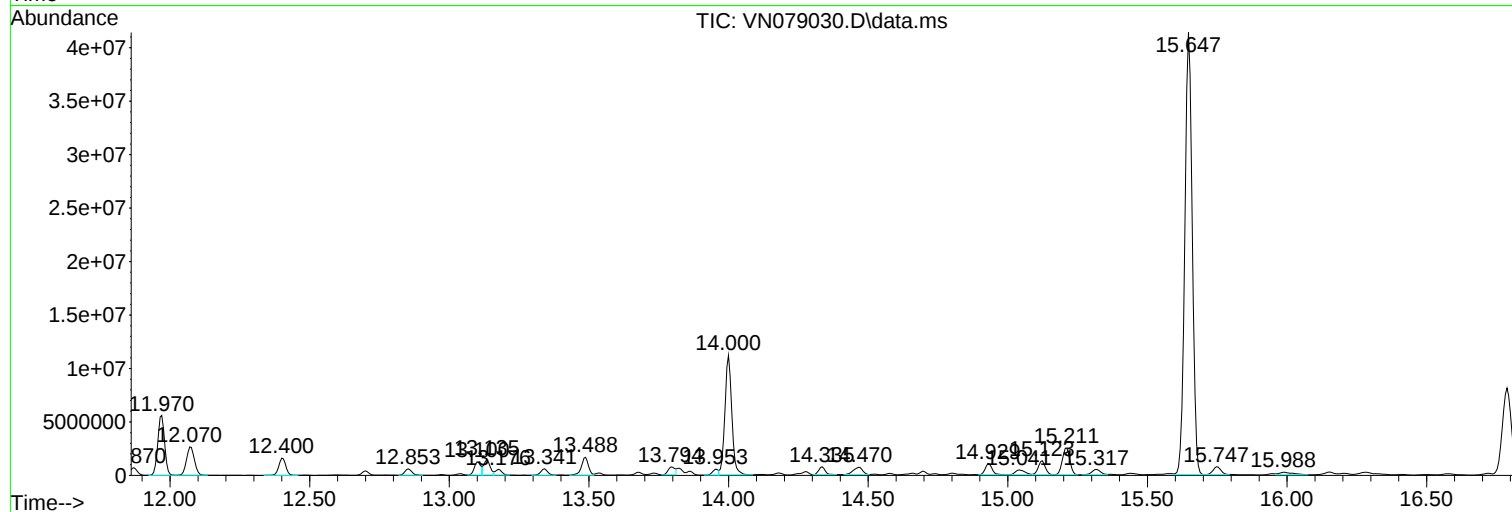
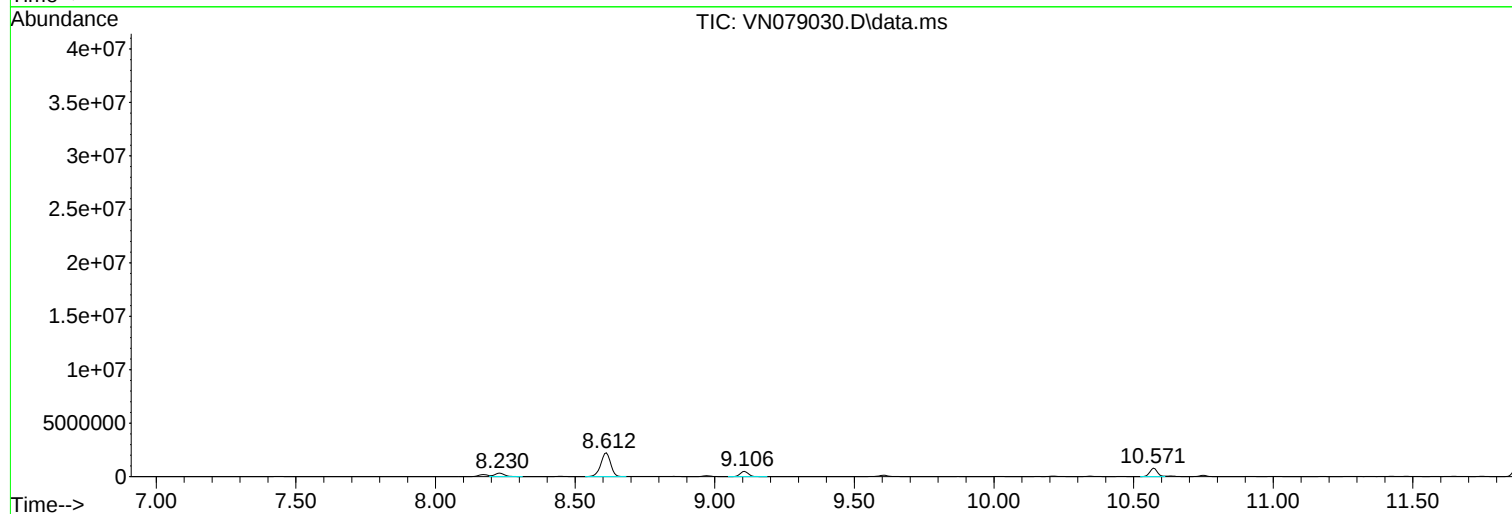
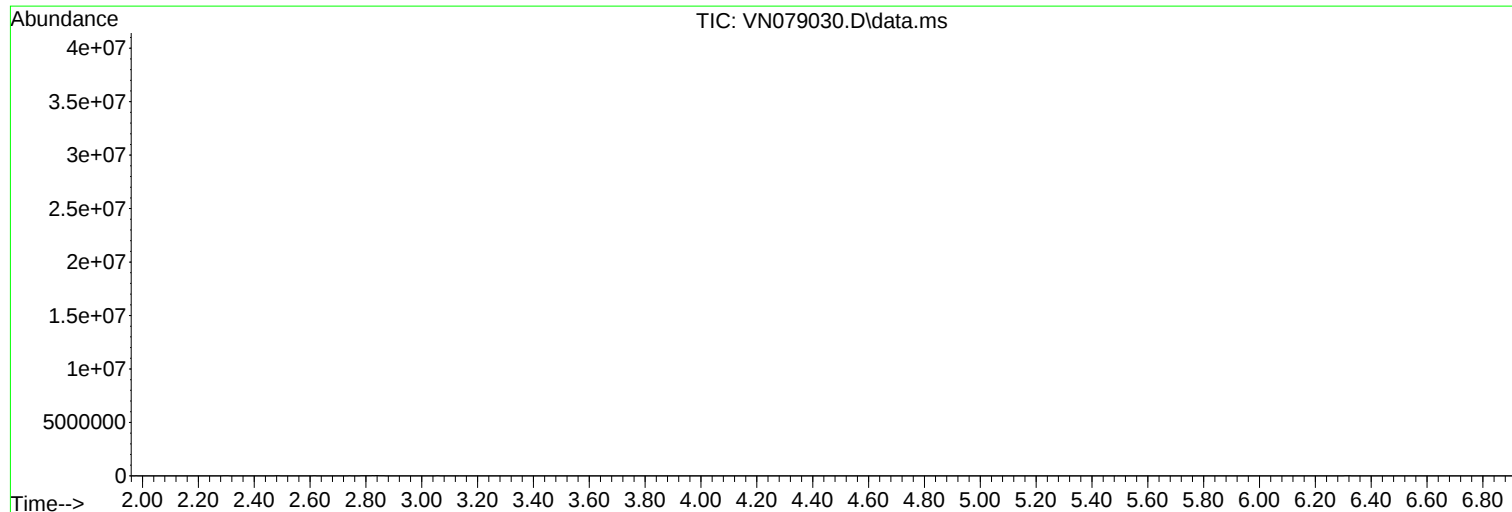
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

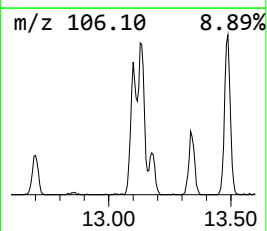
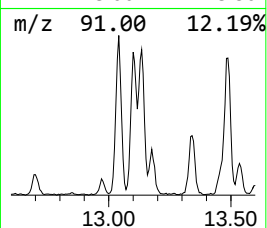
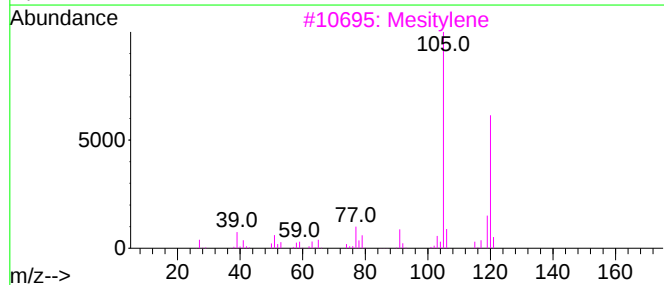
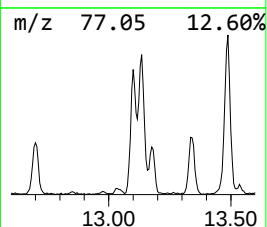
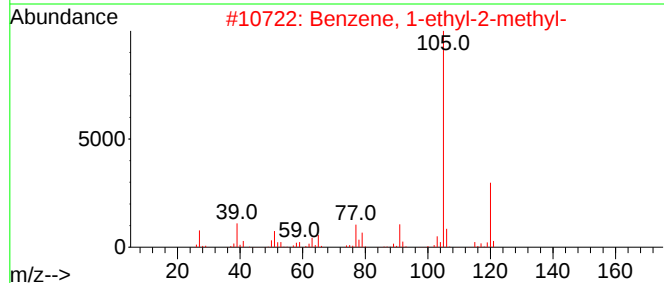
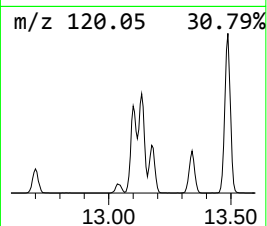
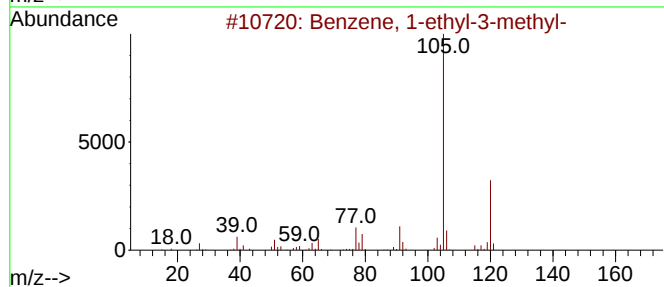
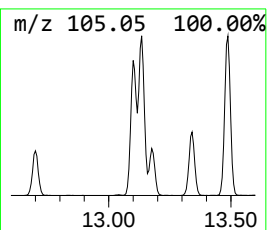
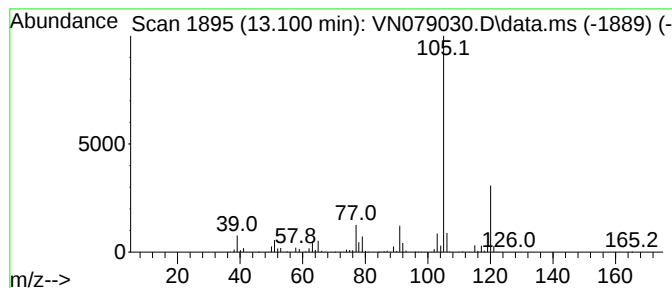
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Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	79.71 ug/l	2124530	1,4-Dichlorobenzene-d4	13.794

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

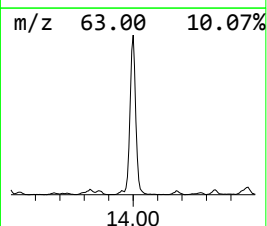
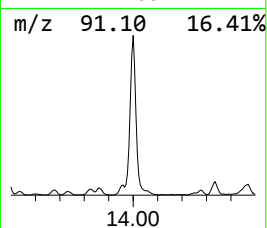
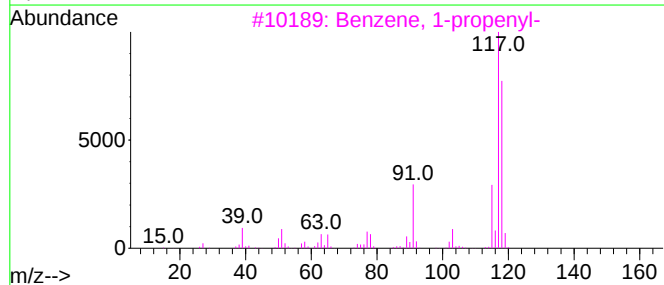
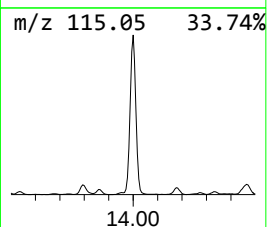
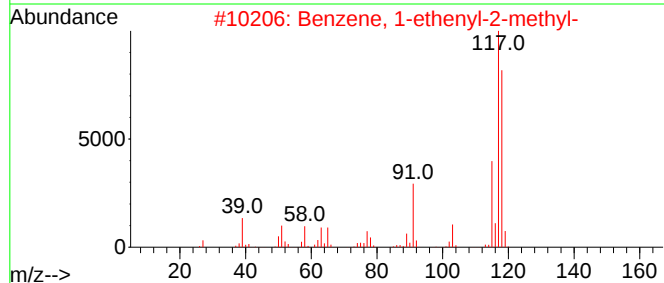
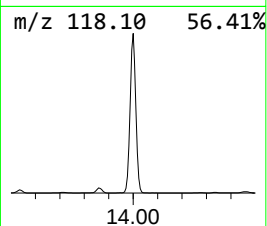
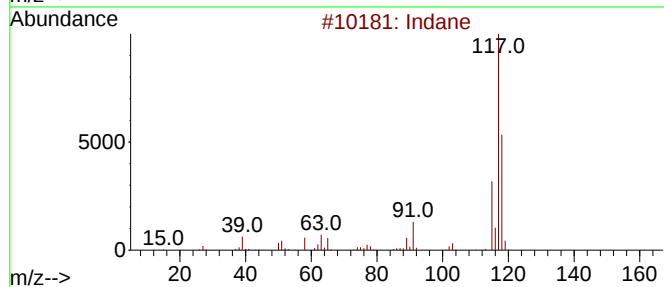
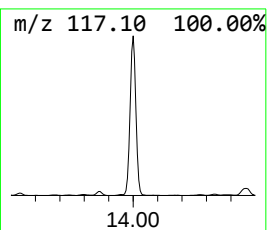
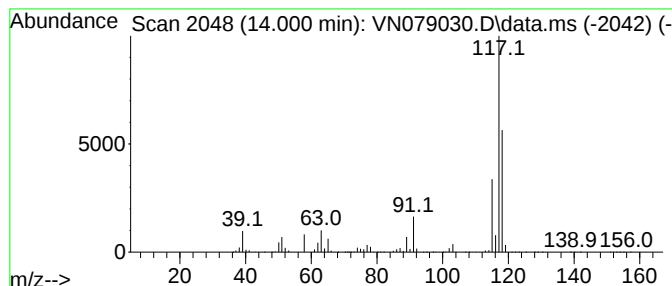
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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	717.43 ug/l	19122700	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, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	59
4			Delta-cyclene	118	C9H10	007785-10-6	59
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

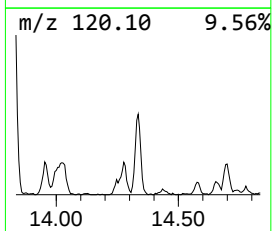
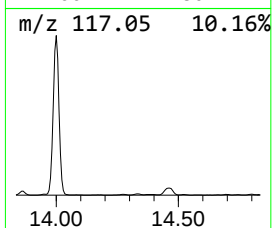
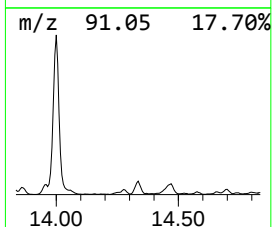
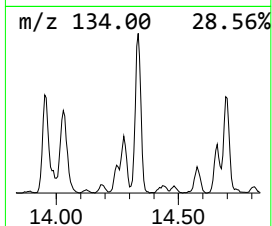
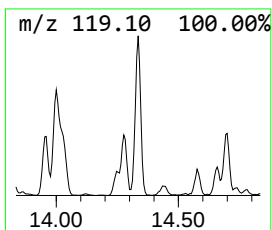
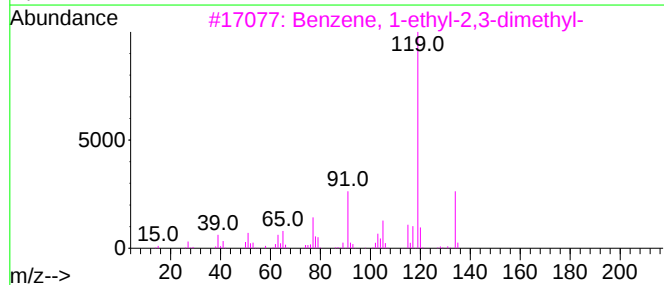
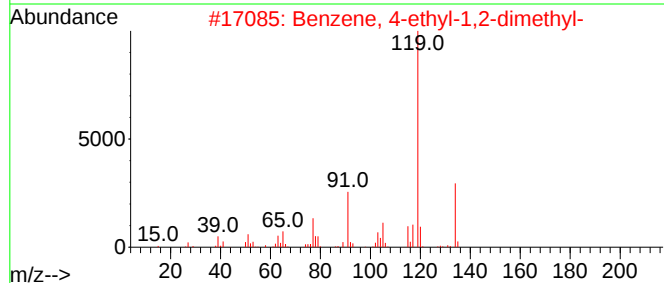
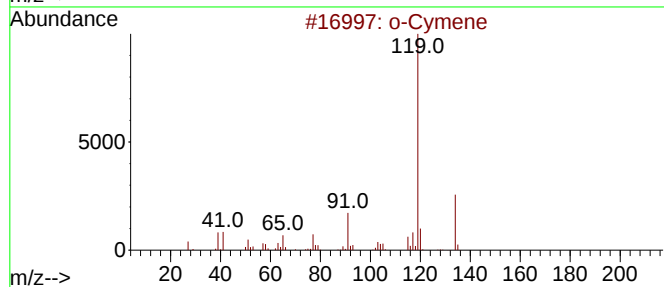
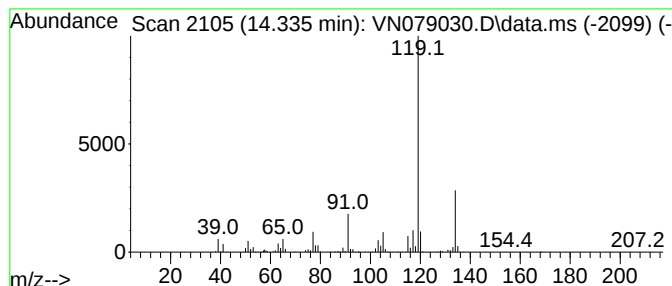
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Quant Title : SW846 8260

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

Peak Number 3 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	44.33 ug/l	1181630	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5			p-Cymene	134	C10H14	000099-87-6	94



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Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

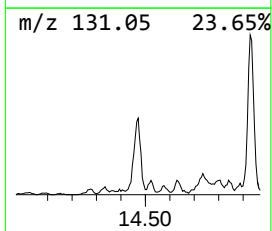
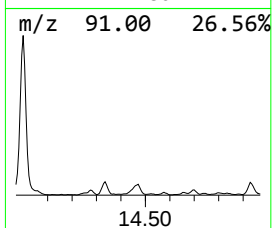
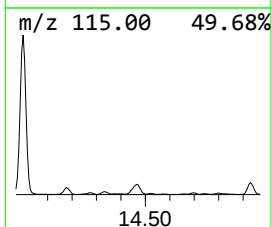
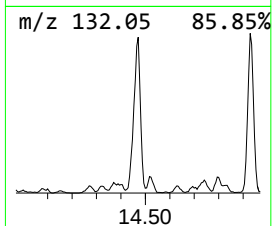
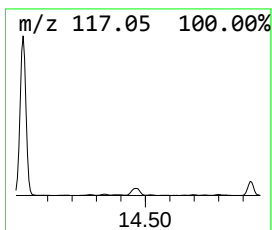
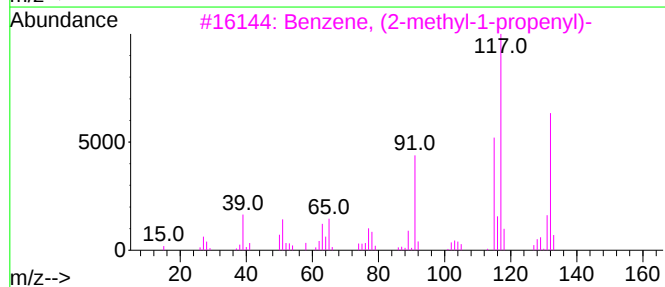
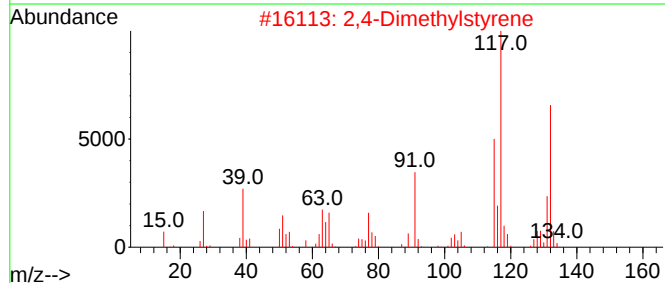
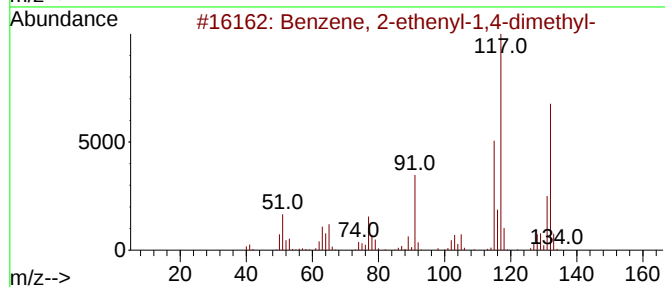
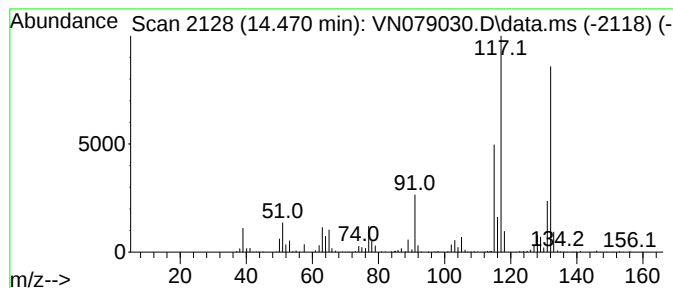
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.470	58.31 ug/l	1554230	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	97
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	96
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	95
4			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	95
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	94



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

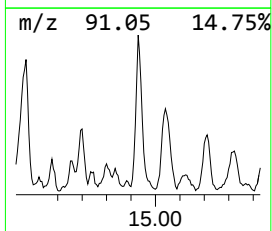
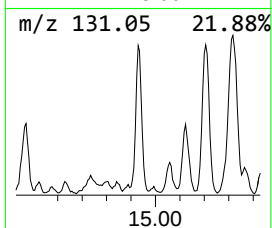
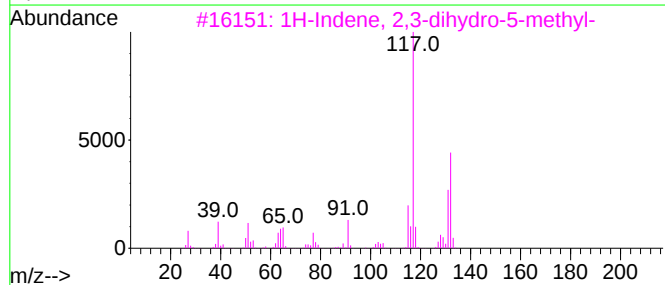
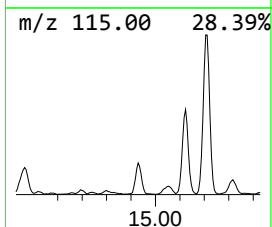
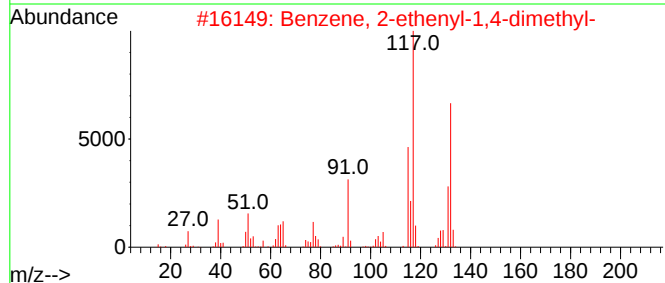
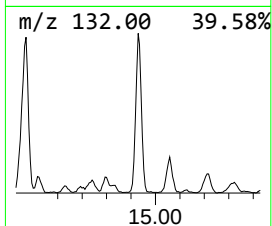
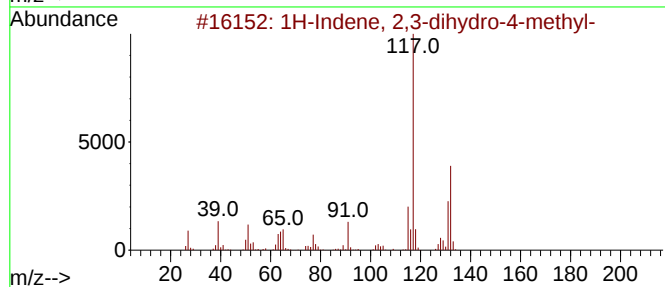
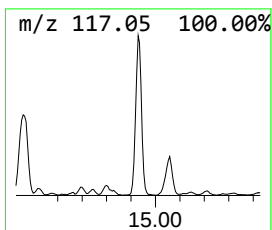
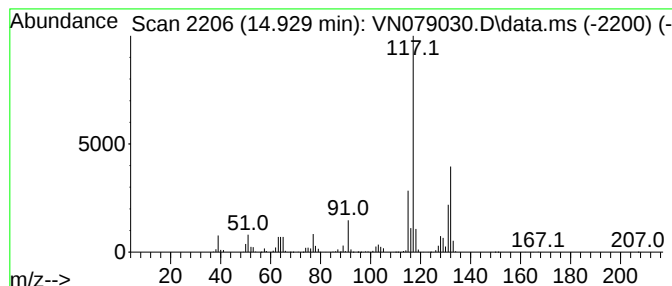
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 5 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	69.52 ug/l	1853020	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91



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Sample : 04047-01 20X
Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

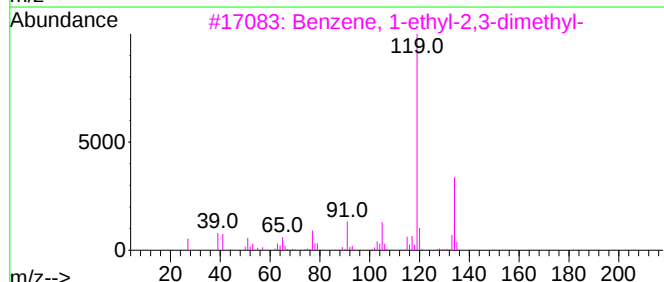
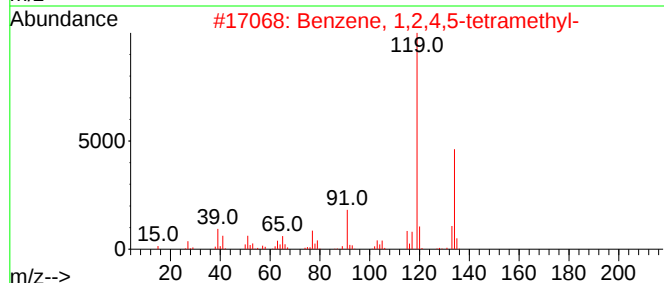
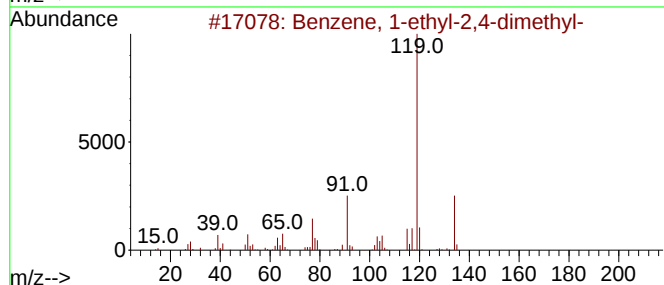
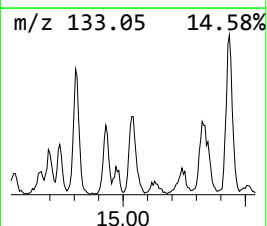
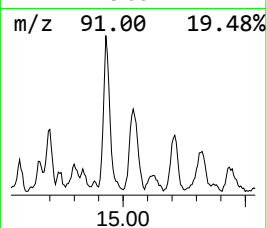
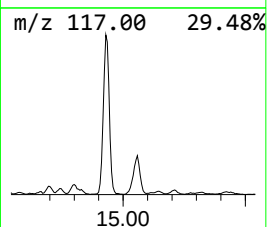
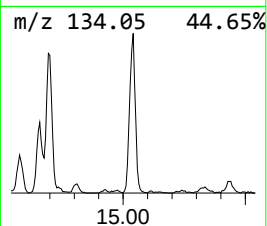
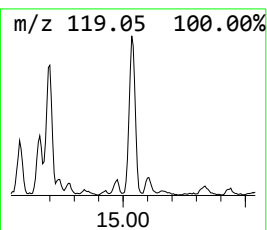
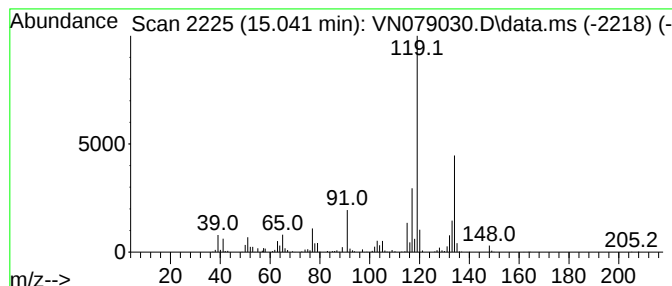
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	42.48 ug/l	1132340	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
4			o-Cymene	134	C10H14	000527-84-4	87
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079030.D
Acq On : 24 Aug 2023 14:41
Operator : JC\MD
Sample : 04047-01 20X
Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

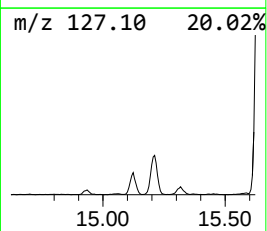
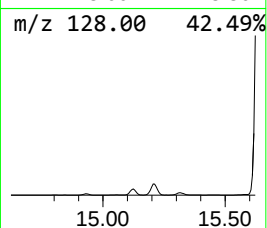
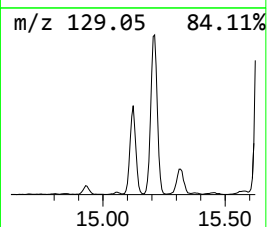
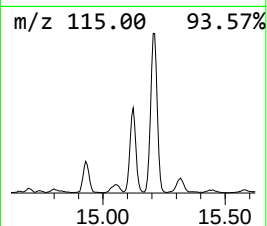
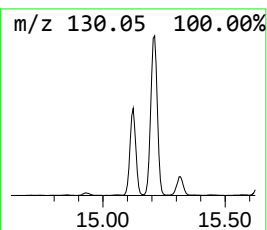
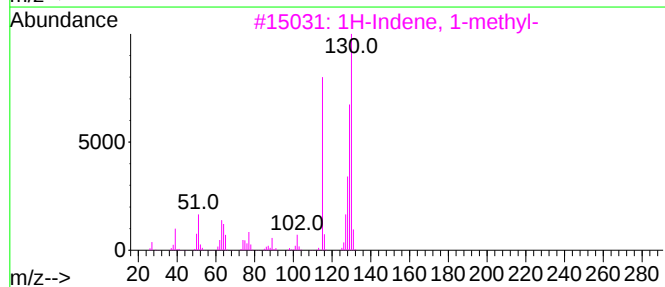
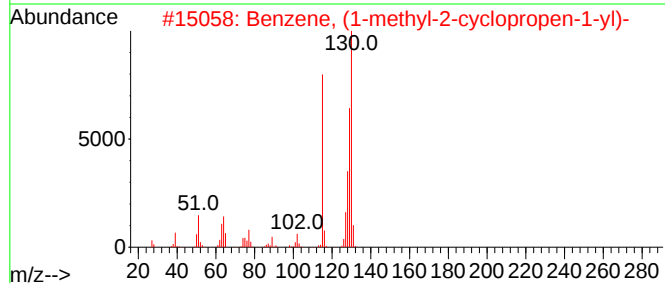
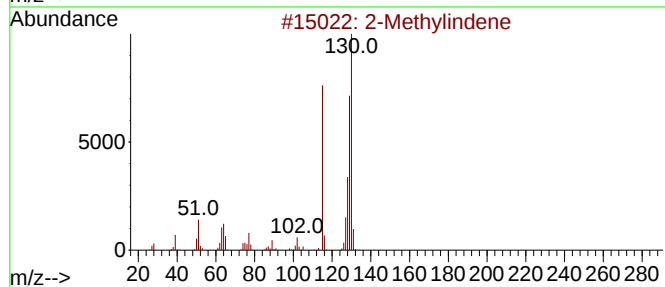
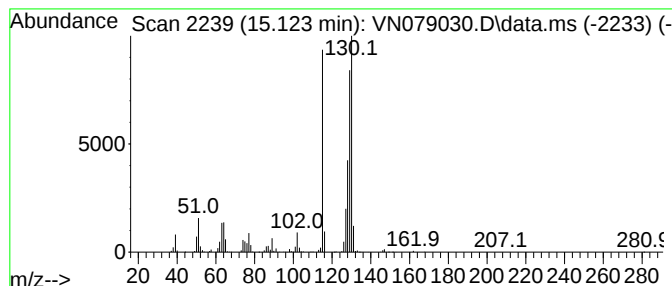
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Quant Title : SW846 8260

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

Peak Number 7 2-Methylindene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	84.52 ug/l	2252910	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	97
2			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	97
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
5			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079030.D
Acq On : 24 Aug 2023 14:41
Operator : JC\MD
Sample : 04047-01 20X
Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

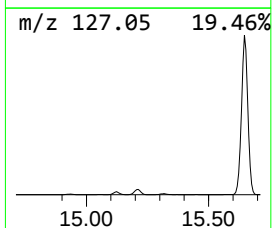
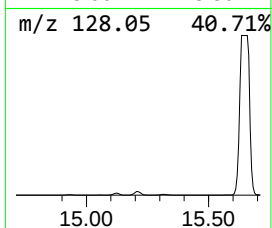
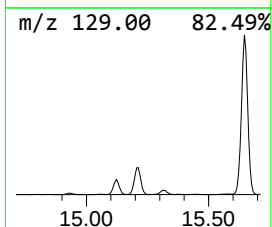
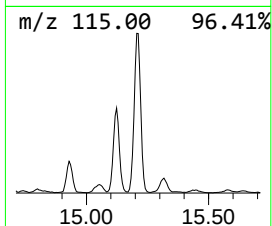
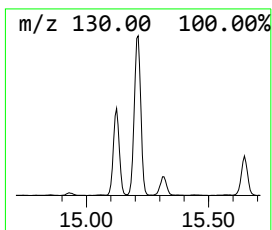
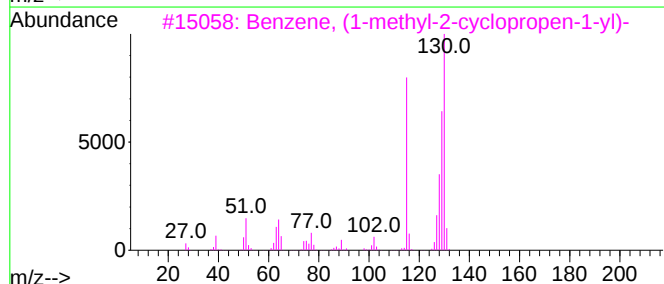
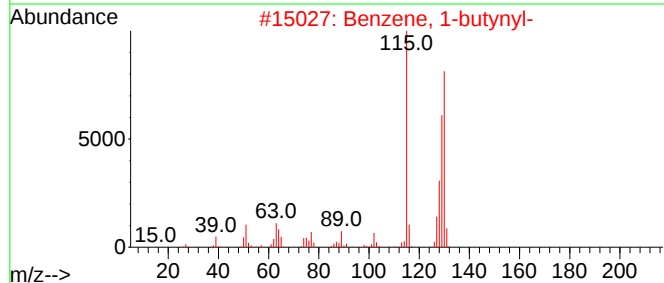
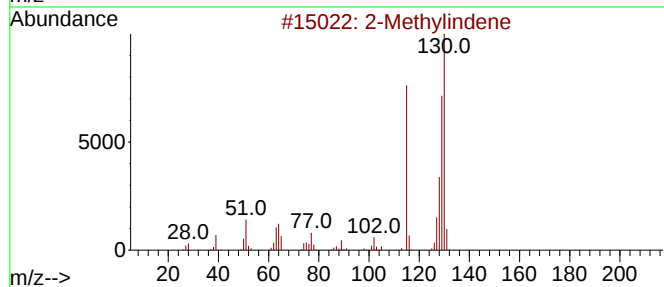
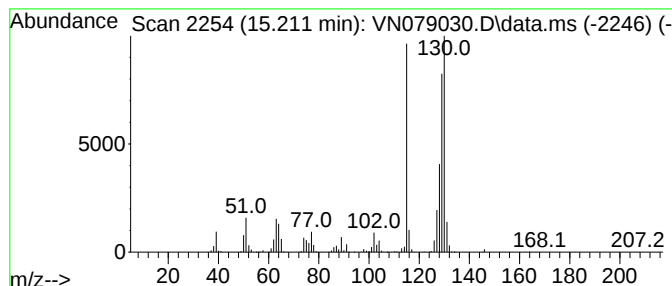
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-butynyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	175.38 ug/l	4674630	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene			130	C10H10	002177-47-1	97
2	Benzene, 1-butynyl-			130	C10H10	000622-76-4	97
3	Benzene, (1-methyl-2-cyclopropen-1-yl)-			130	C10H10	065051-83-4	96
4	1H-Indene, 1-methyl-			130	C10H10	000767-59-9	96
5	Benzene,1-methyl-1,2-propadienyl-			130	C10H10	022433-39-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079030.D
Acq On : 24 Aug 2023 14:41
Operator : JC\MD
Sample : 04047-01 20X
Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

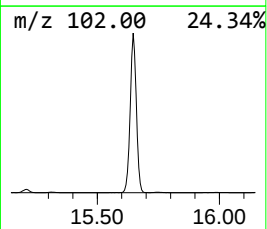
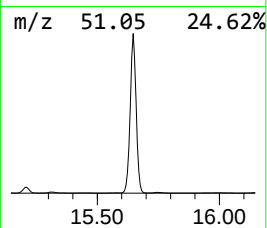
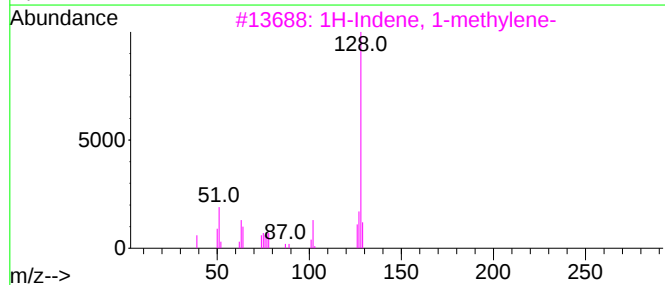
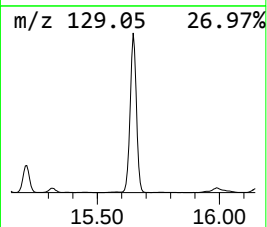
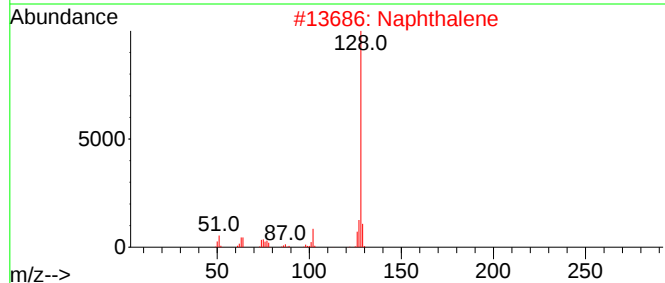
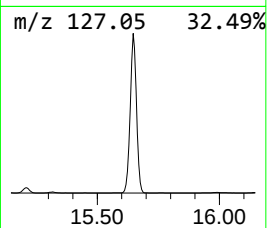
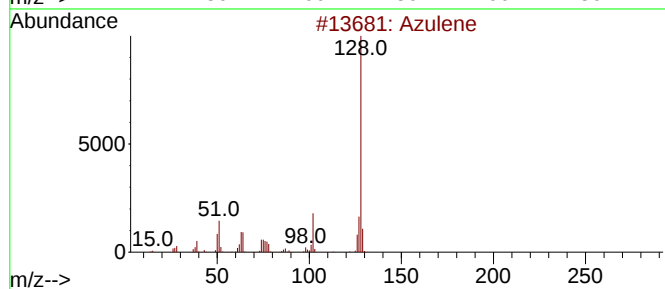
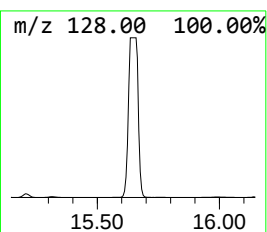
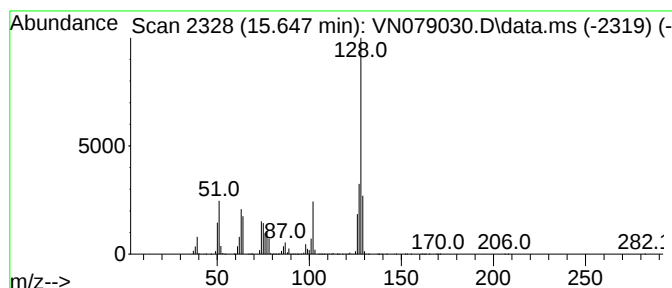
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Quant Title : SW846 8260

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

Peak Number 9 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	2873.23 ug/l	76584200	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	87
2			Naphthalene	128	C10H8	000091-20-3	87
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	86
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	64
5			4-Phenylbut-3-ene-1-yne	128	C10H8	100022-12-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079030.D
Acq On : 24 Aug 2023 14:41
Operator : JC\MD
Sample : 04047-01 20X
Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

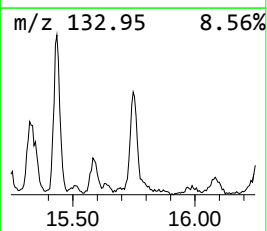
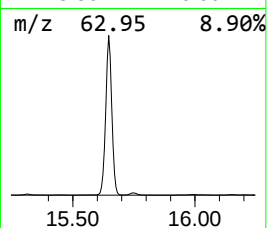
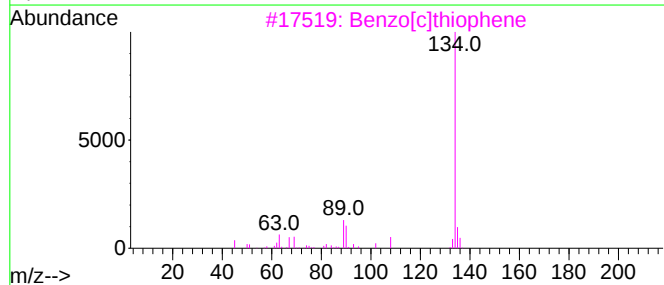
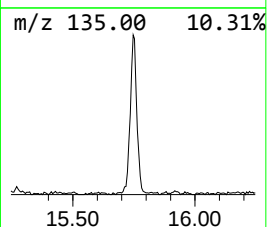
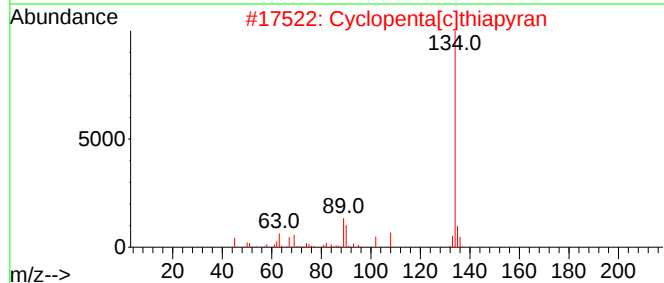
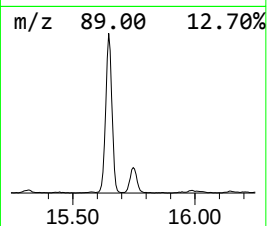
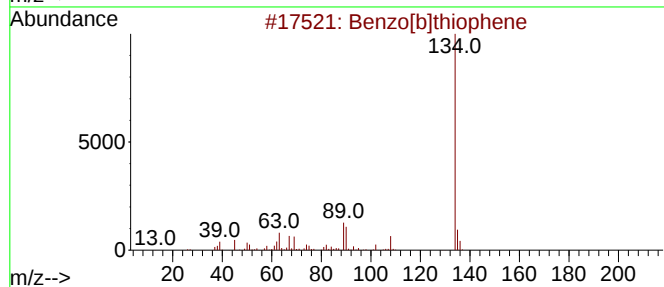
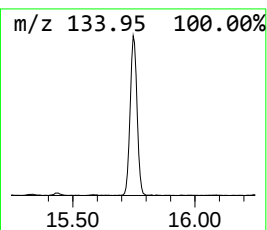
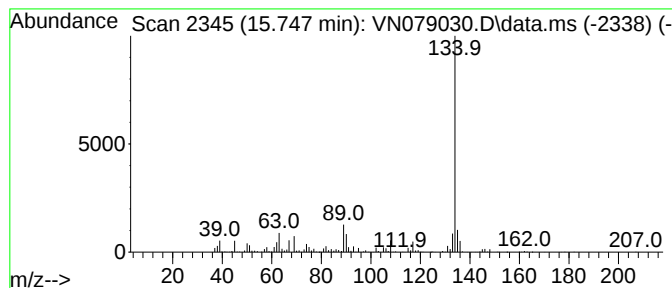
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Quant Title : SW846 8260

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

Peak Number 10 Benzo[b]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.747	53.38 ug/l	1422730	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			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
3			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
4			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	72
5			[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079030.D
Acq On : 24 Aug 2023 14:41
Operator : JC\MD
Sample : 04047-01 20X
Misc : 7.07g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z26-27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.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	717.4	ug/l	19122700	4	13.794	1332720	50.0
o-Cymene	14.335	44.3	ug/l	1181630	4	13.794	1332720	50.0
Benzene, 2-ethe...	14.470	58.3	ug/l	1554230	4	13.794	1332720	50.0
1H-Indene, 2,3-...	14.929	69.5	ug/l	1853020	4	13.794	1332720	50.0
Benzene, 1-ethy...	15.041	42.5	ug/l	1132340	4	13.794	1332720	50.0
2-Methylindene	15.123	84.5	ug/l	2252910	4	13.794	1332720	50.0
Benzene, 1-buty...	15.211	175.4	ug/l	4674630	4	13.794	1332720	50.0
Azulene	15.647	2873.2	ug/l	76584200	4	13.794	1332720	50.0
Benzo[b]thiophene	15.747	53.4	ug/l	1422730	4	13.794	1332720	50.0