

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
 Data File : VN078912.D
 Acq On : 16 Aug 2023 18:55
 Operator : JC\MD
 Sample : 03945-02 20X
 Misc : 6.30g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB01-Z78-80

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: VN078912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.606	1117	1131	1141	rBV2	535151	1492190	2.27%	1.064%
2	9.106	1205	1216	1229	rBV	365832	748973	1.14%	0.534%
3	10.571	1456	1465	1472	rBV	561558	1047003	1.60%	0.747%
4	11.871	1678	1686	1695	rBV	529613	932385	1.42%	0.665%
5	11.971	1695	1703	1712	rVV	5199177	8673949	13.22%	6.185%
6	12.071	1712	1720	1732	rVB	2767344	5302275	8.08%	3.781%
7	12.400	1765	1776	1787	rBV	1563546	2672770	4.07%	1.906%
8	12.700	1817	1827	1833	rBV	476748	789787	1.20%	0.563%
9	12.853	1847	1853	1863	rVB	432916	748485	1.14%	0.534%
10	13.100	1889	1895	1899	rBV	2604940	4604920	7.02%	3.284%
11	13.135	1899	1901	1905	rVV	1592966	2103976	3.21%	1.500%
12	13.176	1905	1908	1916	rVB	653211	1005767	1.53%	0.717%
13	13.341	1928	1936	1943	rBV	476670	786947	1.20%	0.561%
14	13.488	1950	1961	1966	rBV	2083218	3614976	5.51%	2.578%
15	13.535	1966	1969	1976	rVB	474731	720157	1.10%	0.514%
16	13.800	2008	2014	2016	rBV	563846	1053195	1.61%	0.751%
17	13.823	2016	2018	2022	rVV	678283	985238	1.50%	0.703%
18	13.953	2033	2040	2042	rBV	520095	785697	1.20%	0.560%
19	14.000	2042	2048	2062	rVB	11847336	20495333	31.25%	14.614%
20	14.335	2099	2105	2113	rVB	736052	1143264	1.74%	0.815%
21	14.453	2114	2125	2133	rBV3	388084	1021107	1.56%	0.728%
22	14.929	2200	2206	2218	rVB	1069771	1925312	2.94%	1.373%
23	15.047	2218	2226	2233	rBV2	443494	1146542	1.75%	0.818%
24	15.123	2233	2239	2246	rVB	1586656	2744505	4.18%	1.957%
25	15.212	2246	2254	2261	rVB	2754107	5037213	7.68%	3.592%
26	15.317	2264	2272	2279	rBV3	508831	1087135	1.66%	0.775%
27	15.647	2319	2328	2339	rVV2	35521509	65590905	100.00%	46.769%
28	15.753	2339	2346	2358	rVB	483452	1021768	1.56%	0.729%
29	15.988	2381	2386	2403	rVB2	281542	961819	1.47%	0.686%

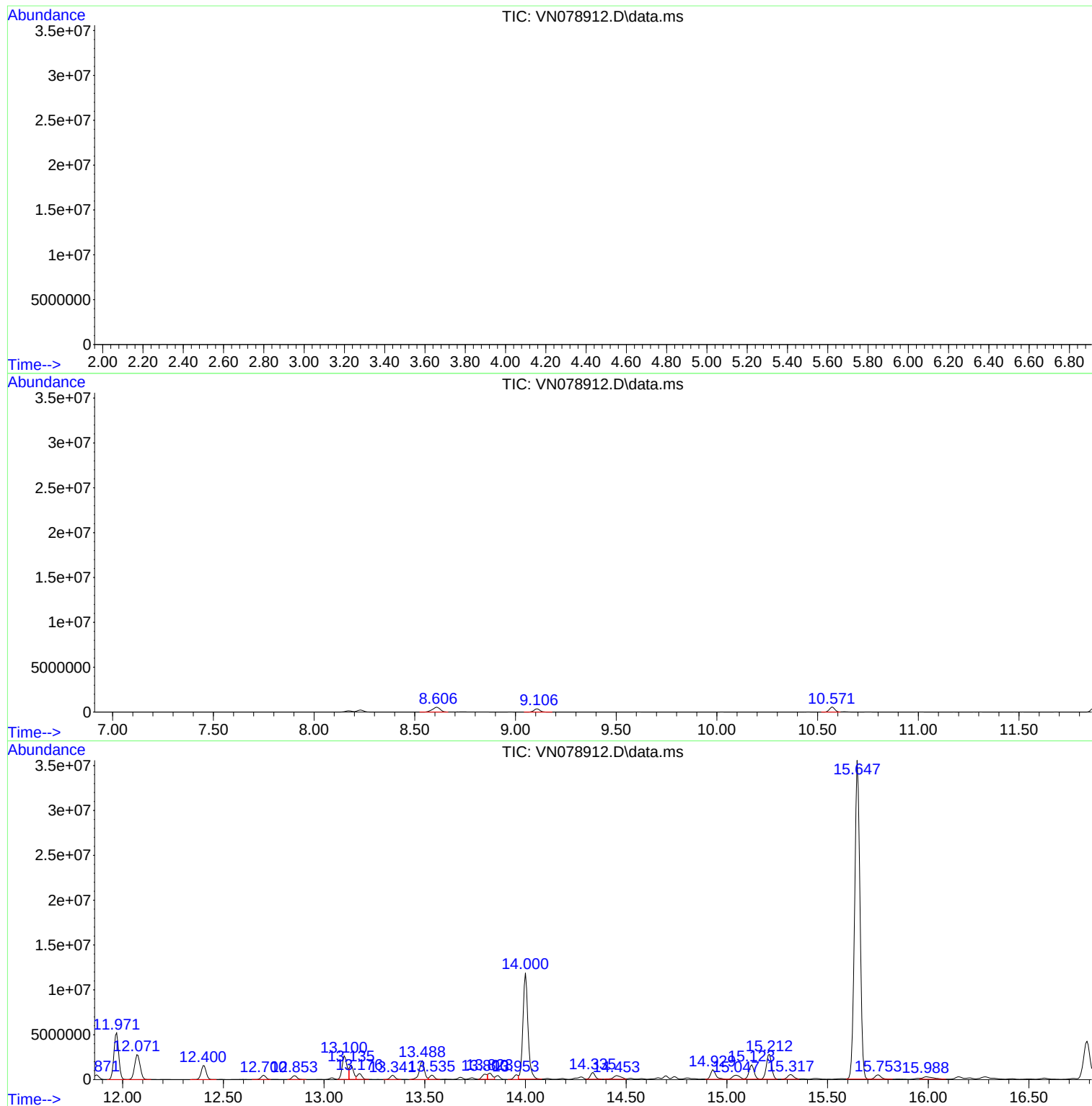
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Instrument :
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ClientSampleId :
NEVINS-SB01-Z78-80

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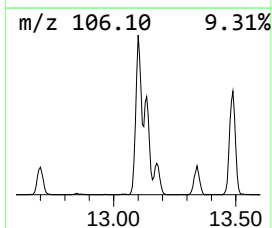
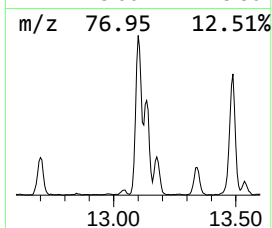
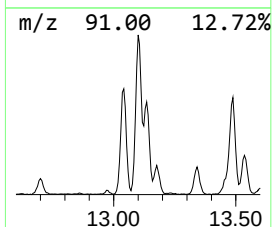
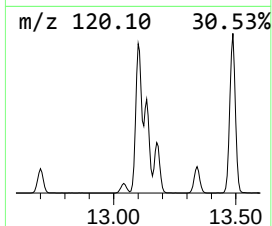
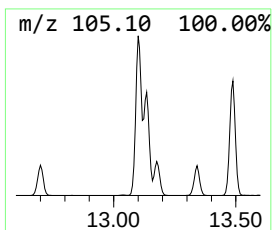
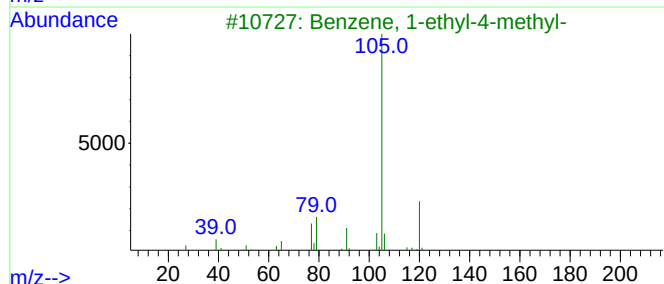
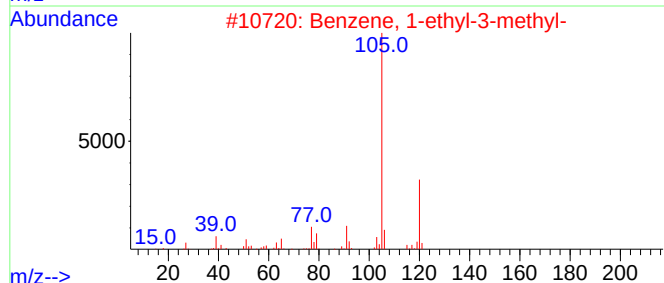
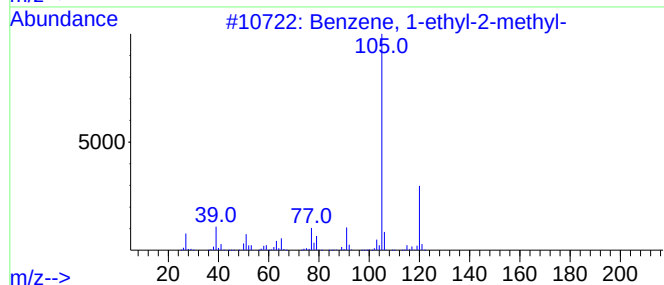
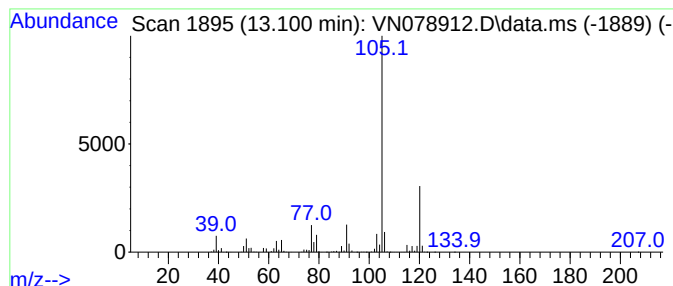
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	218.62 ug/l	4604920	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	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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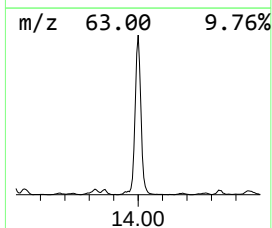
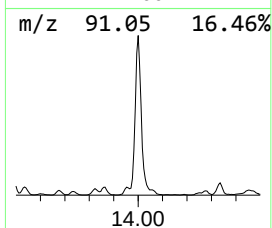
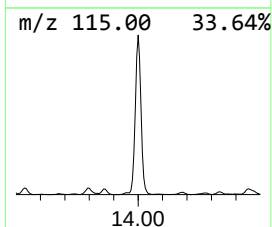
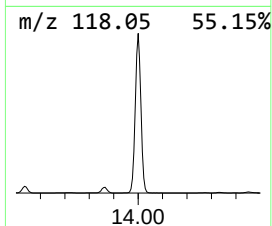
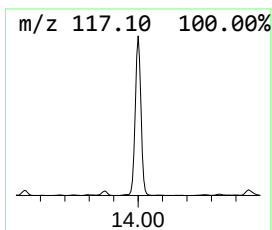
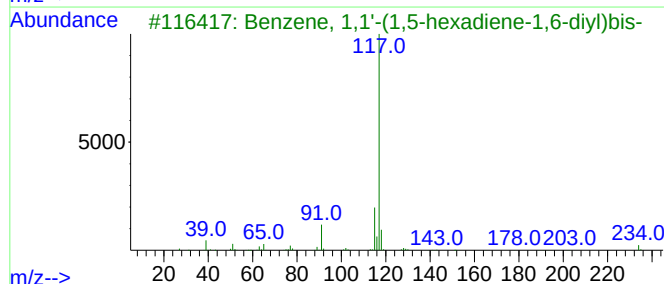
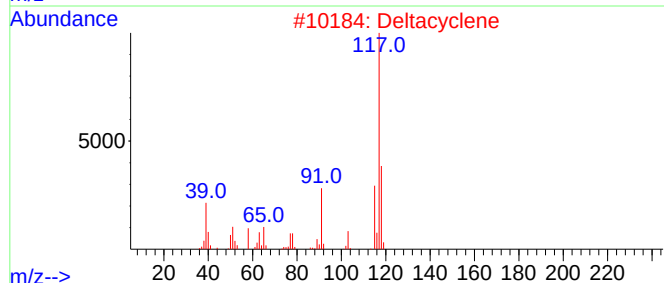
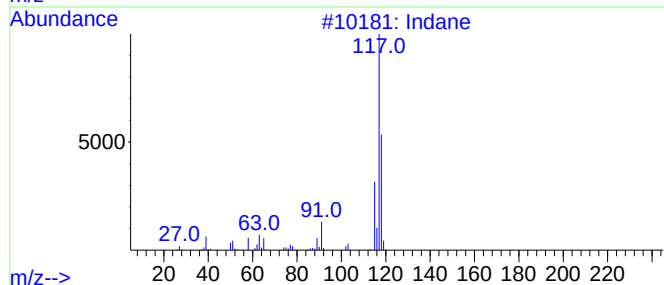
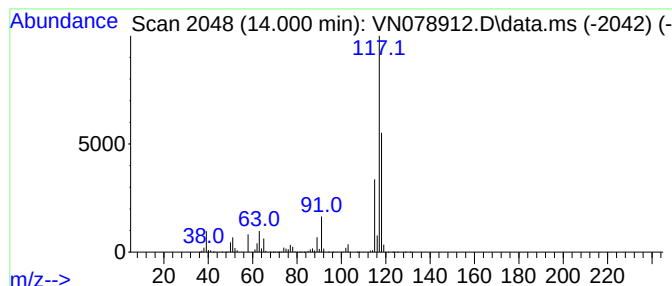
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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	973.01 ug/l	20495300	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Deltacyclene	118	C9H10	007785-10-6	59
3			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
4			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50
5			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	50



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB01-Z78-80

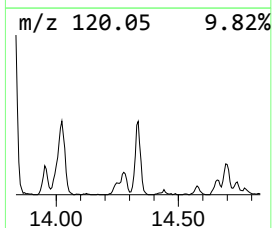
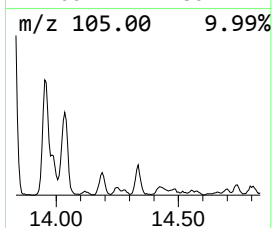
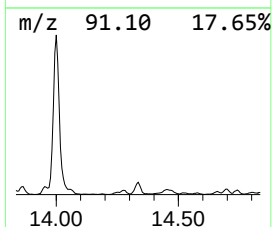
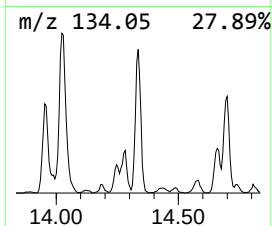
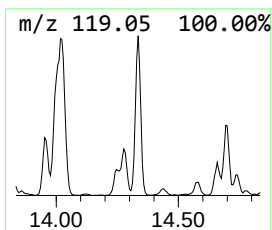
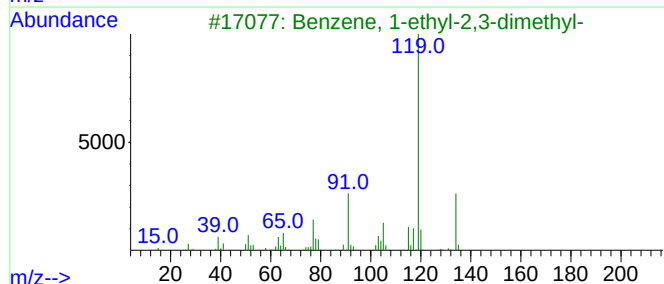
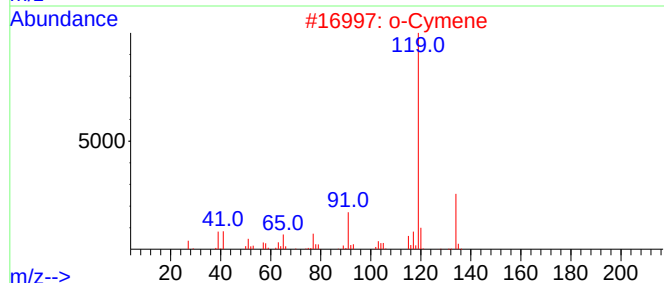
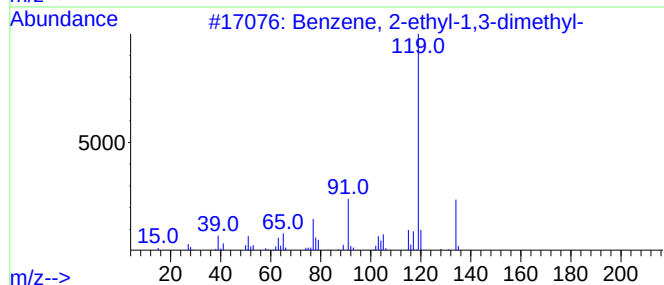
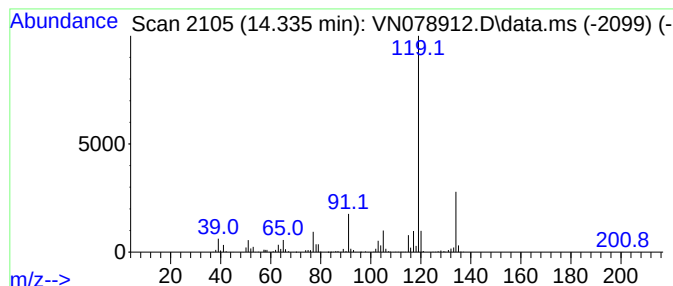
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	54.28 ug/l	1143260	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2			o-Cymene	134	C10H14	000527-84-4	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			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93



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Instrument :
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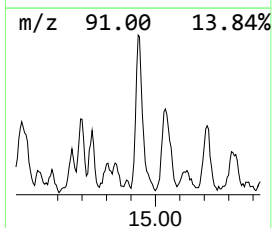
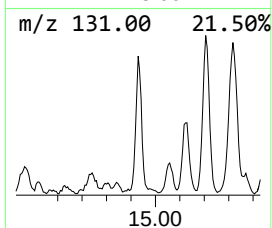
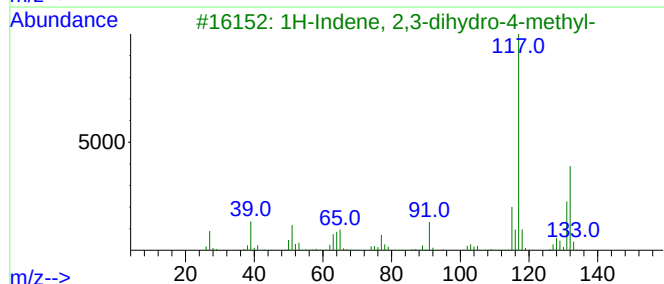
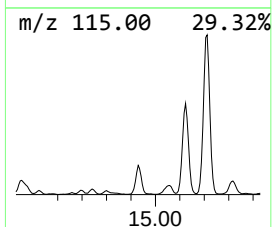
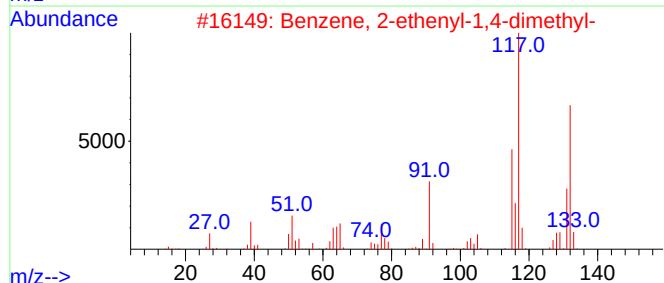
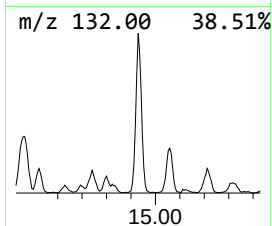
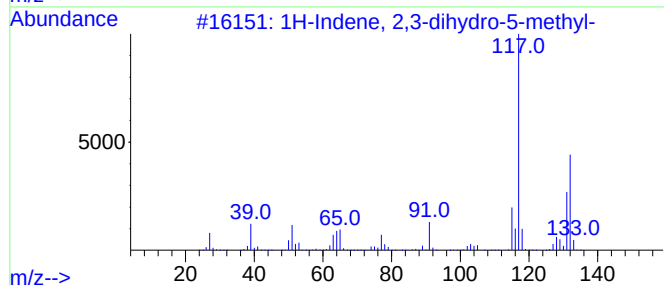
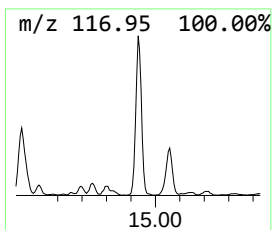
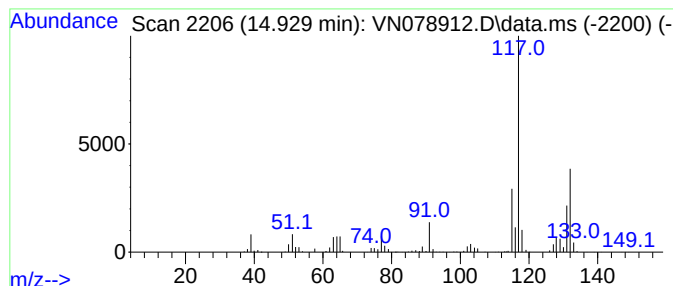
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	91.40 ug/l	1925310	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	96		
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96		
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	96		
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91		
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	90		



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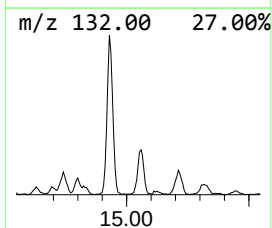
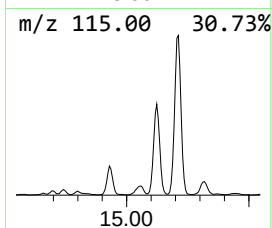
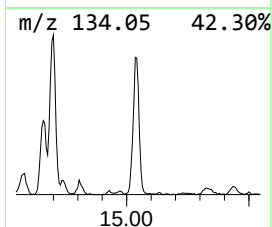
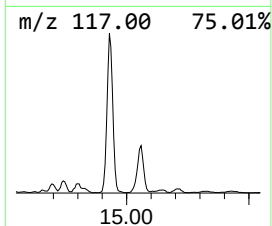
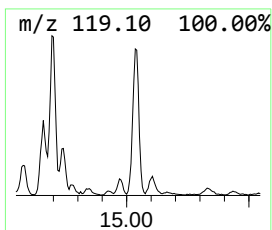
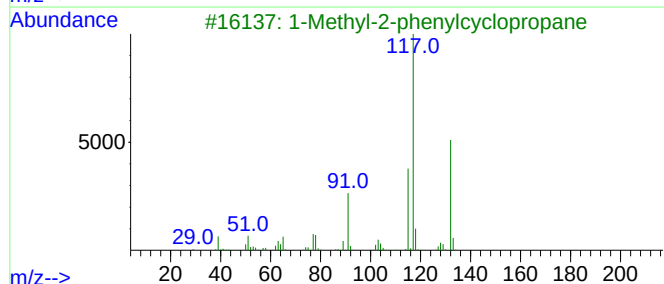
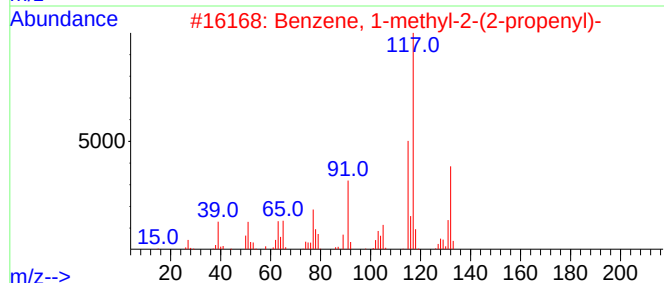
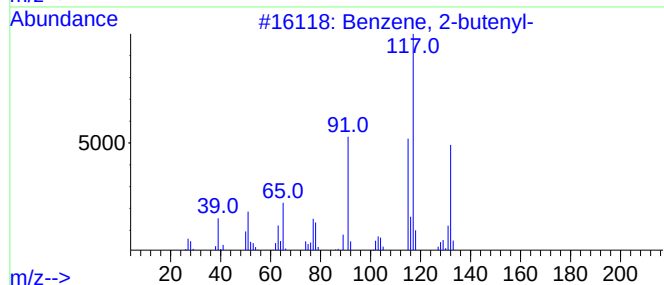
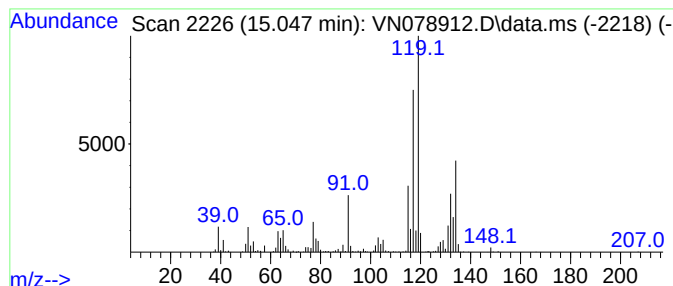
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-butenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	54.43 ug/l	1146540	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
2			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	64
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	50



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NEVINS-SB01-Z78-80

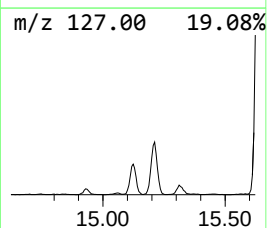
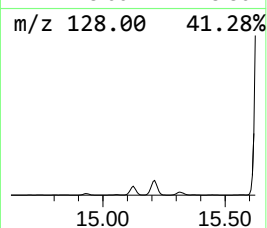
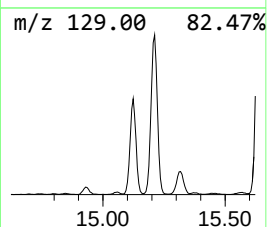
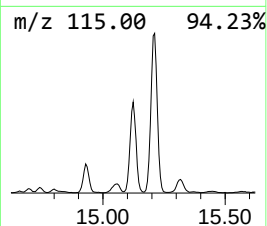
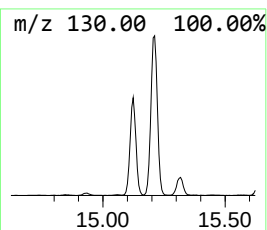
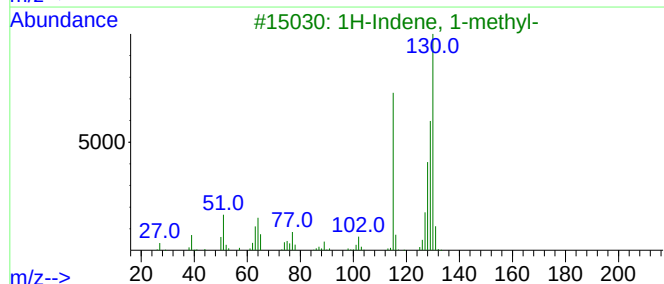
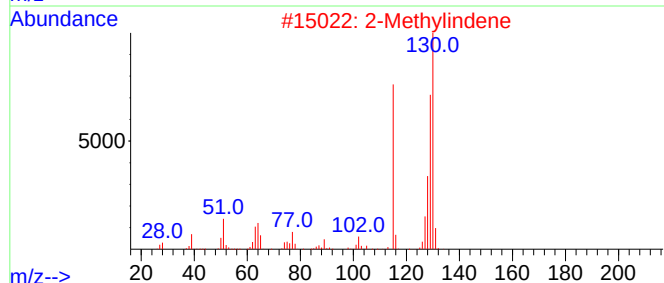
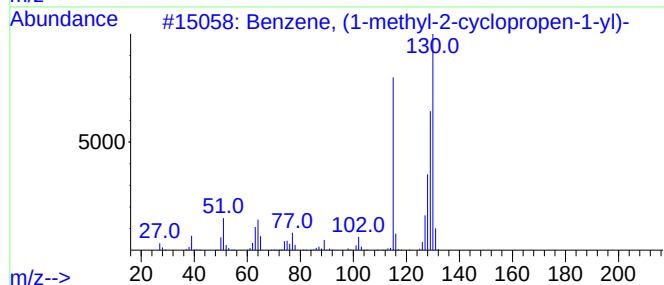
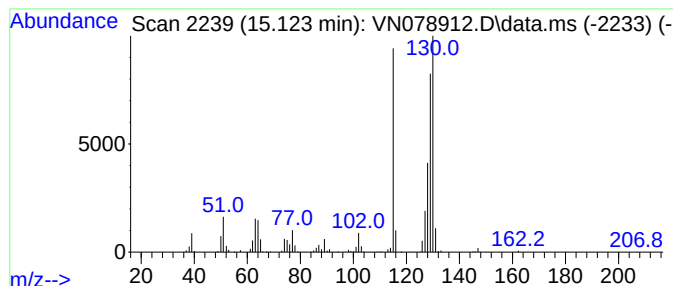
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, (1-methyl-2-cyclop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	130.29 ug/l	2744510	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	97
2			2-Methylindene	130	C10H10	002177-47-1	97
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
5			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078912.D
Acq On : 16 Aug 2023 18:55
Operator : JC\MD
Sample : 03945-02 20X
Misc : 6.30g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB01-Z78-80

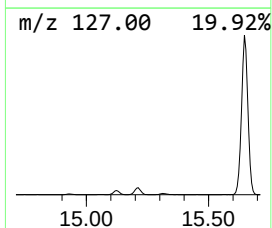
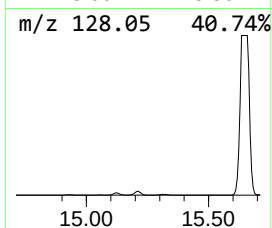
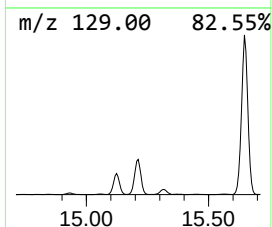
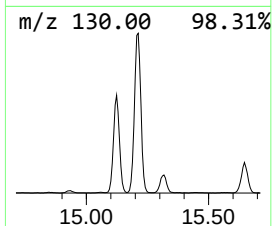
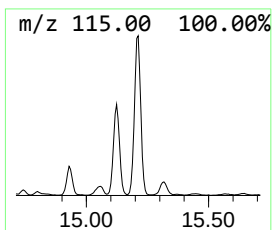
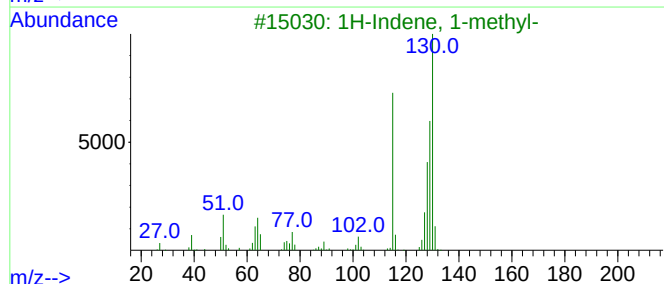
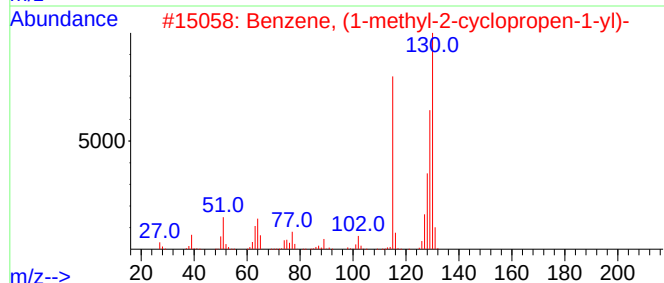
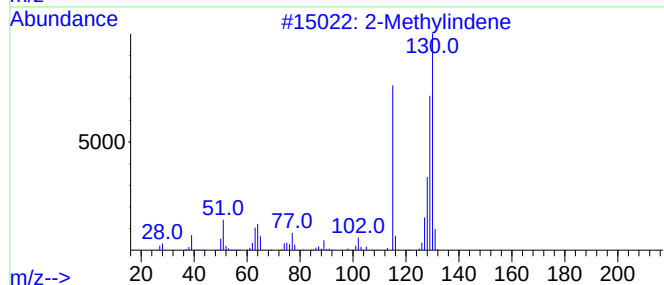
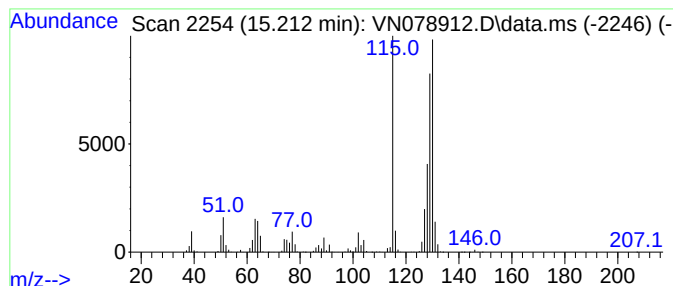
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Quant Title : SW846 8260

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

Peak Number 7 2-Methylindene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	239.14 ug/l	5037210	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...	130	C10H10	065051-83-4	96
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078912.D
Acq On : 16 Aug 2023 18:55
Operator : JC\MD
Sample : 03945-02 20X
Misc : 6.30g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB01-Z78-80

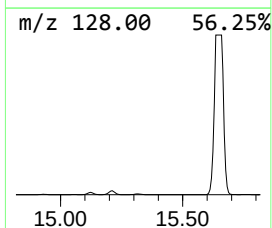
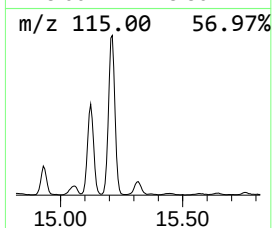
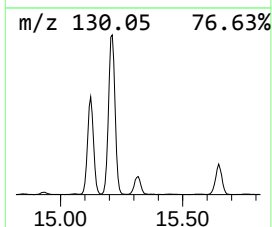
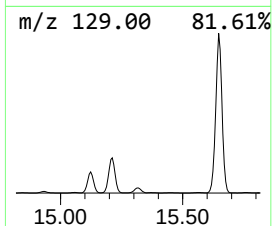
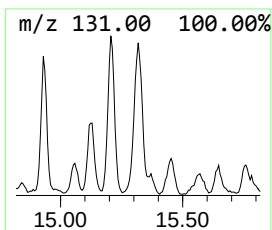
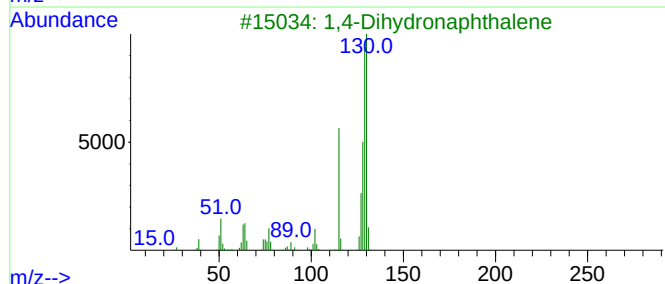
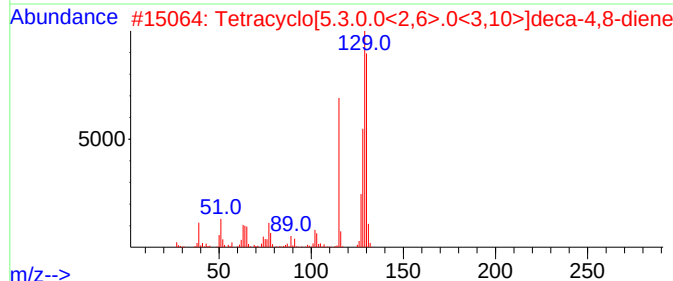
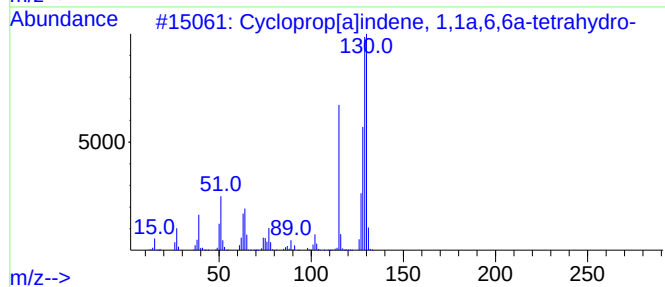
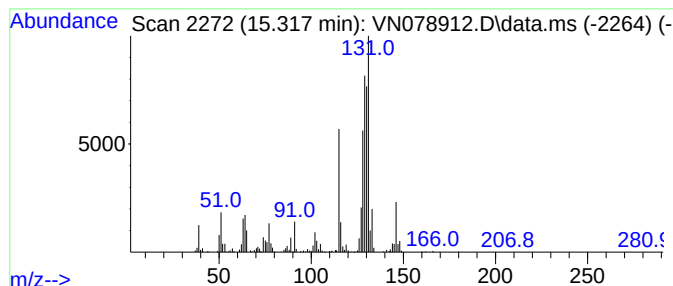
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Quant Title : SW846 8260

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

Peak Number 8 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	51.61 ug/l	1087140	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	90
2			Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	89
3			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	89
4			Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	55
5			Benzene, 1,3-butadienyl-	130	C10H10	001515-78-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078912.D
Acq On : 16 Aug 2023 18:55
Operator : JC\MD
Sample : 03945-02 20X
Misc : 6.30g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB01-Z78-80

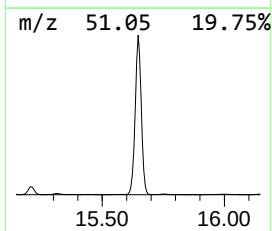
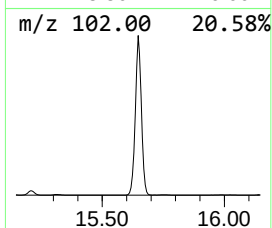
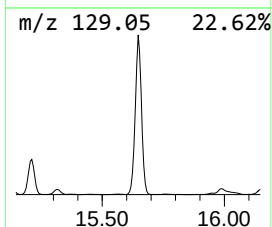
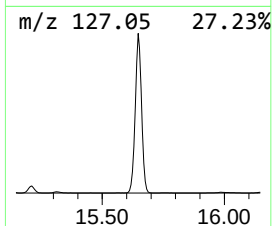
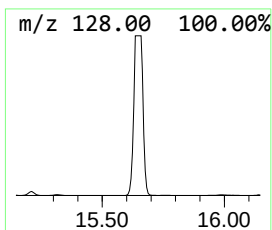
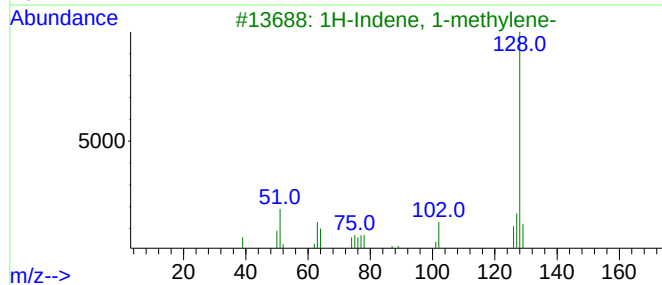
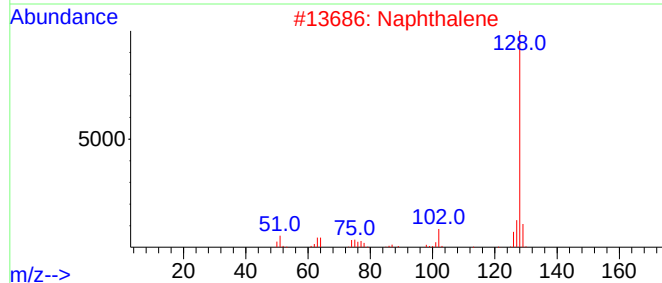
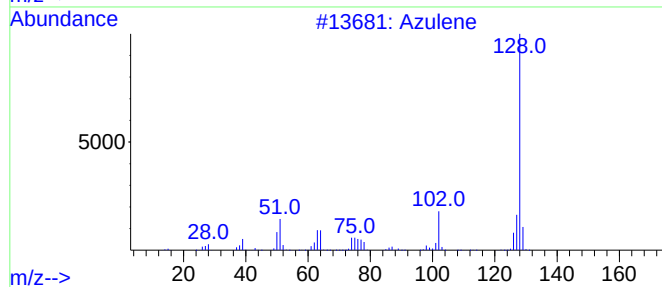
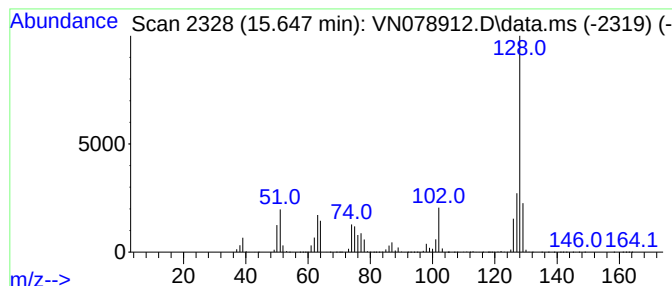
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Quant Title : SW846 8260

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	3113.90 ug/l	65590900	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	90
2			Naphthalene	128	C10H8	000091-20-3	87
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	81
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	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078912.D
Acq On : 16 Aug 2023 18:55
Operator : JC\MD
Sample : 03945-02 20X
Misc : 6.30g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB01-Z78-80

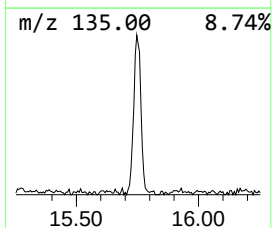
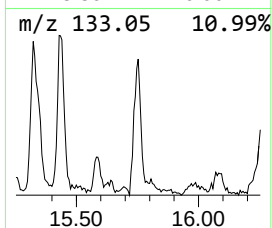
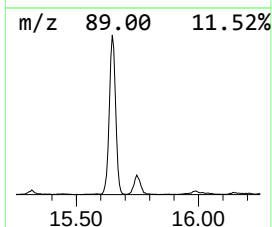
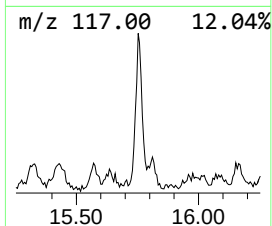
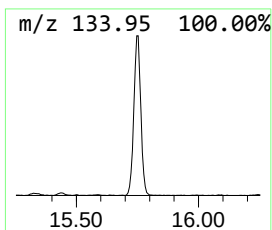
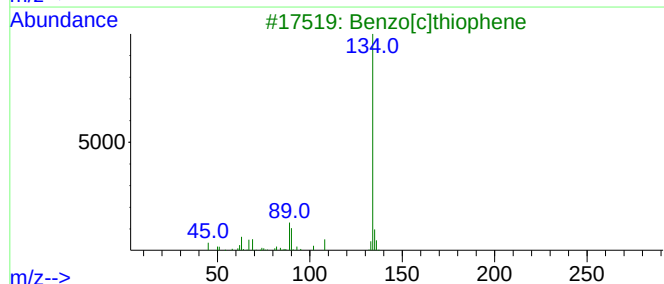
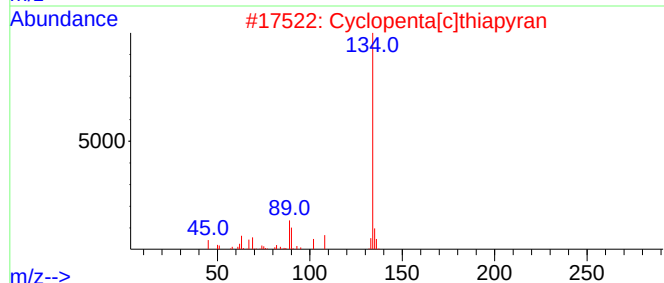
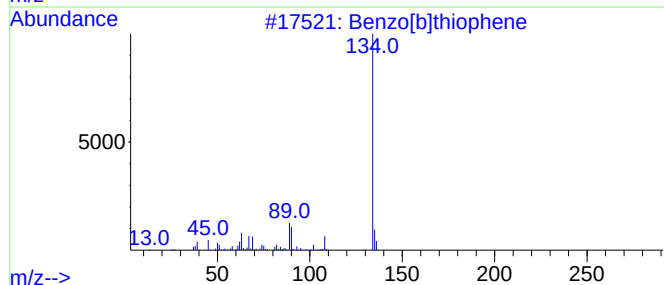
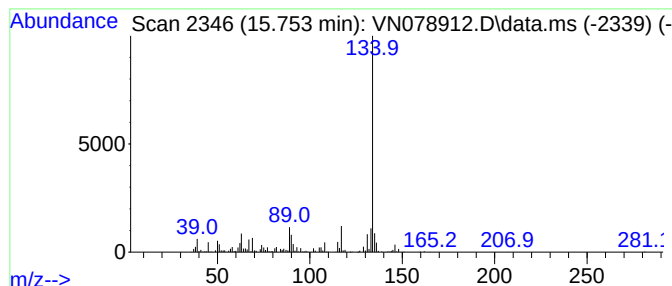
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Quant Title : SW846 8260

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

Peak Number 10 Benzo[b]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.753	48.51 ug/l	1021770	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	93
2			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	81
3			Benzo[c]thiophene	134	C8H6S	000270-82-6	81
4			3-Deazaadenine	134	C6H6N4	006811-77-4	53
5			2-Benzoxazoline	134	C7H6N2O	004570-41-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081623\
Data File : VN078912.D
Acq On : 16 Aug 2023 18:55
Operator : JC\MD
Sample : 03945-02 20X
Misc : 6.30g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB01-Z78-80

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
Benzene, 1-ethy...	13.100	218.6	ug/l	4604920	4	13.794	1053200	50.0
Indane	14.000	973.0	ug/l	20495300	4	13.794	1053200	50.0
Benzene, 2-ethy...	14.335	54.3	ug/l	1143260	4	13.794	1053200	50.0
1H-Indene, 2,3-...	14.929	91.4	ug/l	1925310	4	13.794	1053200	50.0
Benzene, 2-bute...	15.047	54.4	ug/l	1146540	4	13.794	1053200	50.0
Benzene, (1-met...	15.123	130.3	ug/l	2744510	4	13.794	1053200	50.0
2-Methylindene	15.212	239.1	ug/l	5037210	4	13.794	1053200	50.0
Cycloprop[a]ind...	15.318	51.6	ug/l	1087140	4	13.794	1053200	50.0
Azulene	15.647	3113.9	ug/l	65590900	4	13.794	1053200	50.0
Benzo[b]thiophene	15.753	48.5	ug/l	1021770	4	13.794	1053200	50.0