

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079033.D
 Acq On : 24 Aug 2023 15:54
 Operator : JC\MD
 Sample : 04075-02 20X
 Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB04-Z23-24

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: VN079033.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.612	1117	1132	1145	rBV2	1499504	3778971	4.44%	2.394%
2	9.106	1206	1216	1231	rBV	536820	1115393	1.31%	0.707%
3	10.571	1456	1465	1472	rBV	829939	1529943	1.80%	0.969%
4	11.871	1677	1686	1695	rBV	788122	1419664	1.67%	0.900%
5	11.971	1695	1703	1712	rVV	5442453	9331538	10.97%	5.913%
6	12.076	1712	1721	1733	rVB	2030292	4015486	4.72%	2.544%
7	12.400	1762	1776	1785	rBV	1570625	2700423	3.17%	1.711%
8	12.853	1846	1853	1861	rVB	651424	1128752	1.33%	0.715%
9	13.135	1897	1901	1905	rVV	1286669	2095915	2.46%	1.328%
10	13.488	1950	1961	1966	rBV	1574824	2770025	3.26%	1.755%
11	13.794	2007	2013	2016	rBV	825112	1446678	1.70%	0.917%
12	14.000	2042	2048	2061	rVB	13319794	23214981	27.28%	14.710%
13	14.335	2099	2105	2110	rBV	825735	1295820	1.52%	0.821%
14	14.459	2117	2126	2133	rBV4	483207	1341441	1.58%	0.850%
15	14.929	2200	2206	2219	rVB	1054584	1960129	2.30%	1.242%
16	15.041	2219	2225	2233	rBV3	519456	1342757	1.58%	0.851%
17	15.123	2233	2239	2246	rVB	1518375	2746090	3.23%	1.740%
18	15.212	2246	2254	2262	rVB	2802936	5182112	6.09%	3.284%
19	15.317	2262	2272	2279	rBV2	588897	1363634	1.60%	0.864%
20	15.647	2319	2328	2338	rVB2	45075664	85093005	100.00%	53.918%
21	15.747	2338	2345	2357	rVB	747564	1556605	1.83%	0.986%
22	15.988	2373	2386	2401	rBV3	364024	1390039	1.63%	0.881%

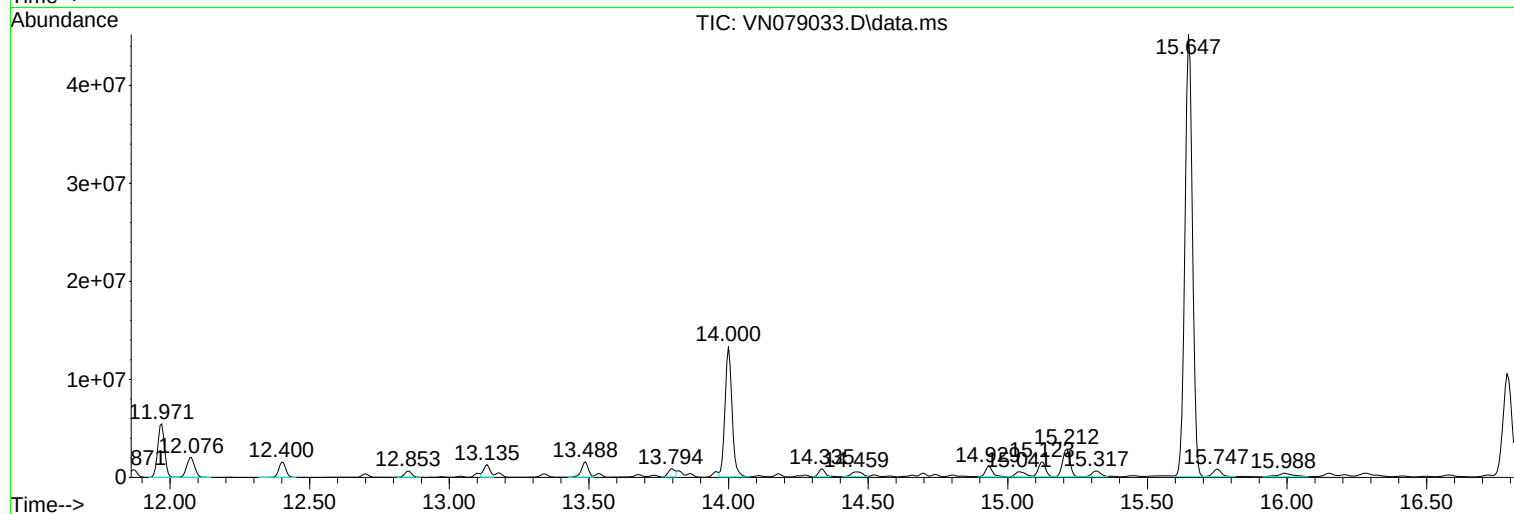
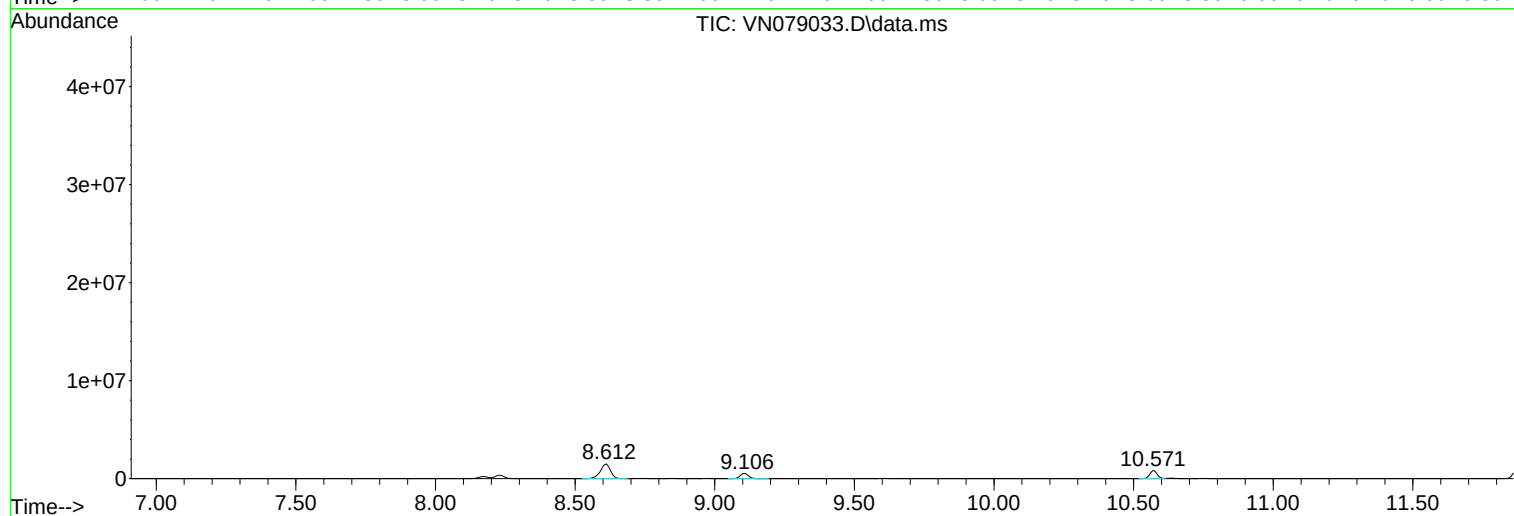
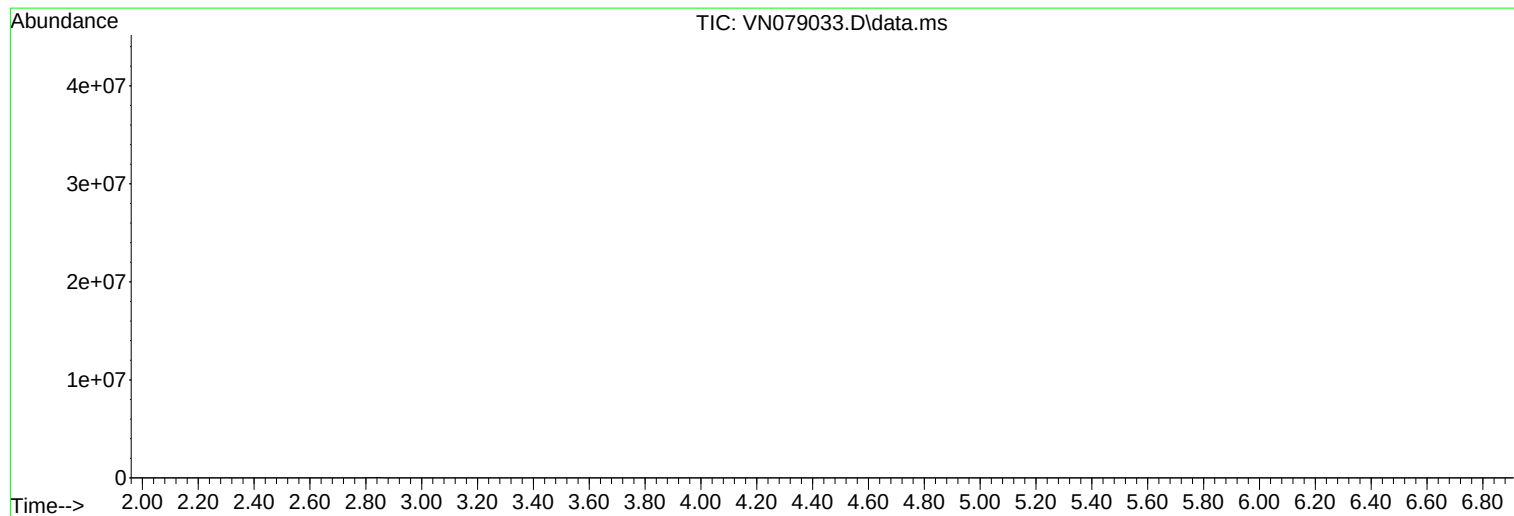
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB04-Z23-24

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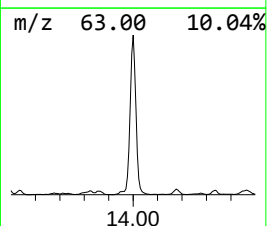
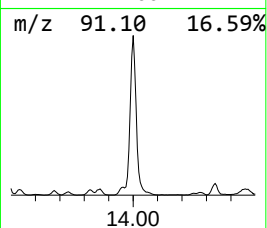
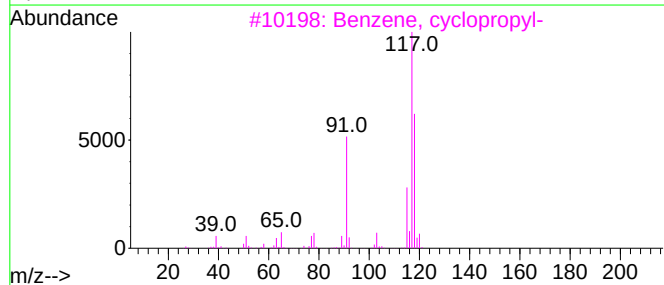
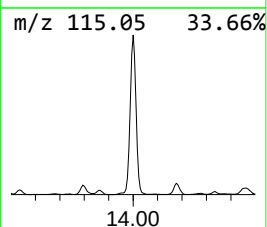
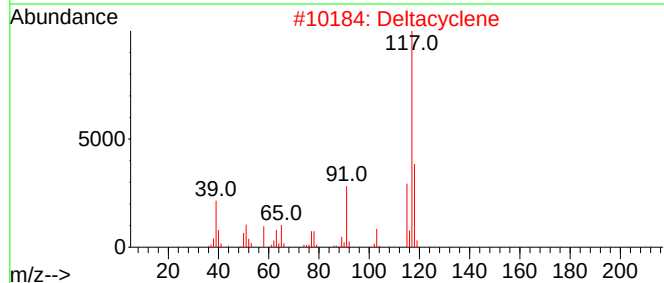
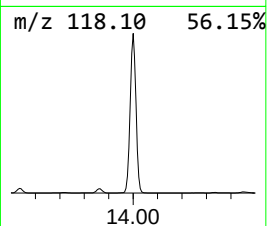
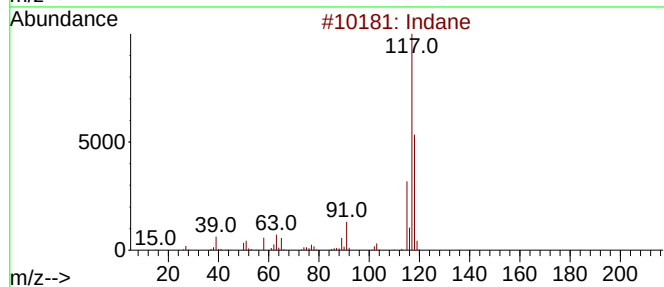
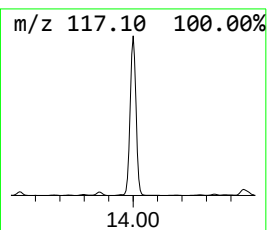
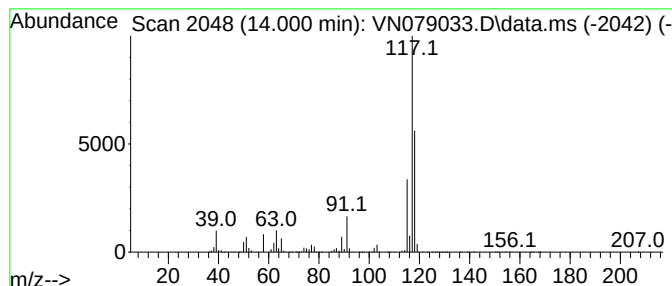
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	802.36 ug/l	23215000	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	68
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	59
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59



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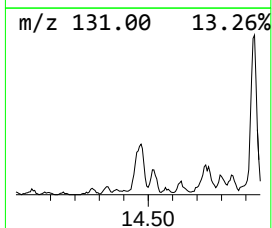
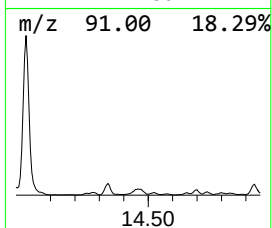
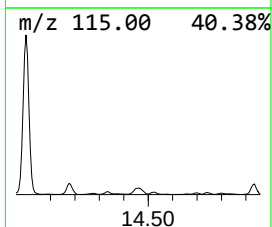
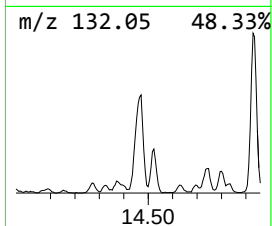
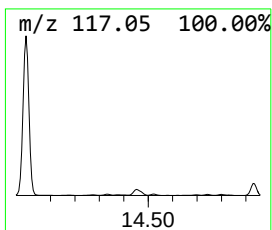
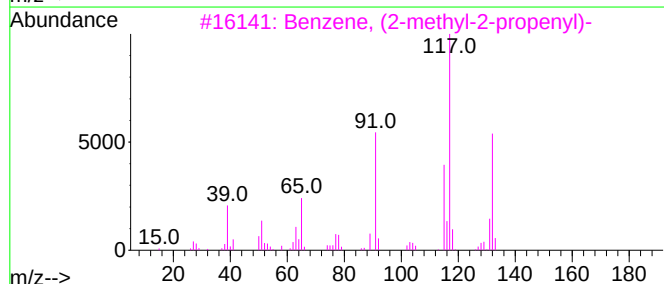
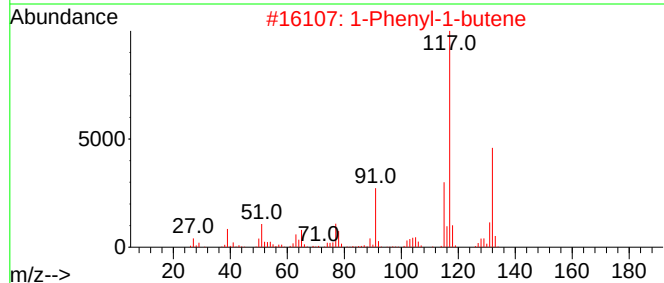
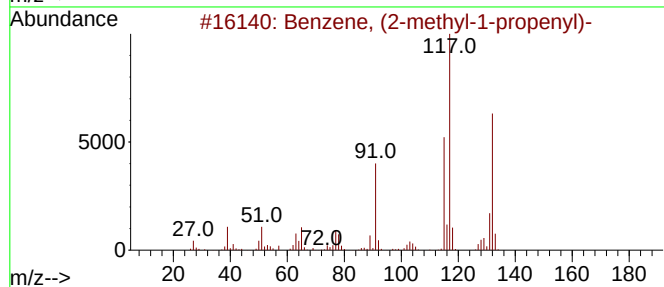
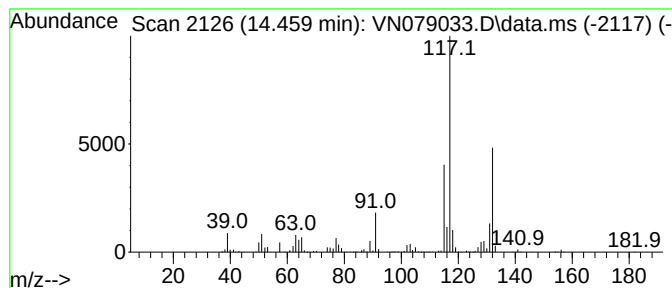
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, (2-methyl-1-propen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.459	46.36 ug/l	1341440	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	91
4			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	91
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

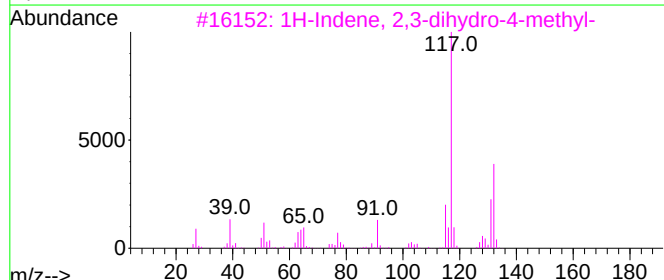
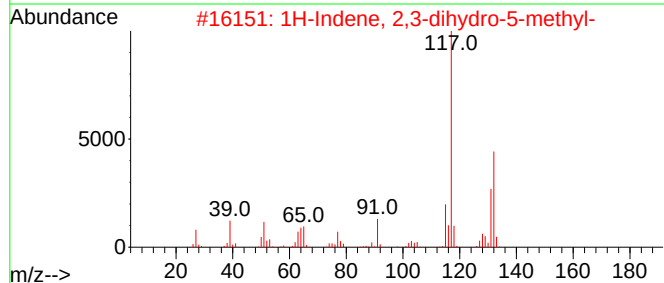
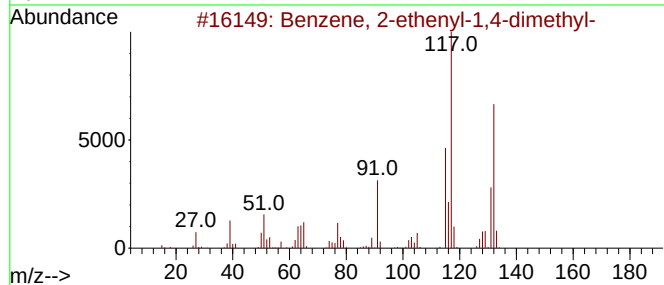
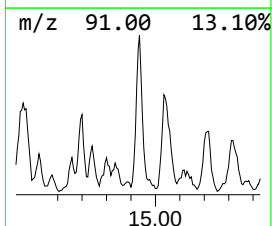
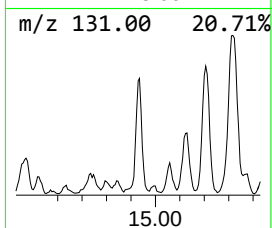
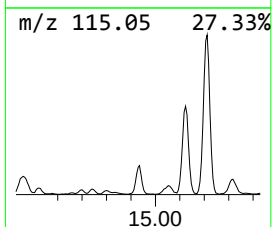
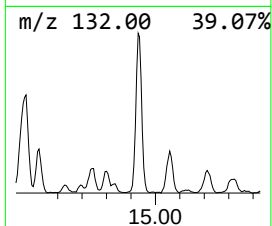
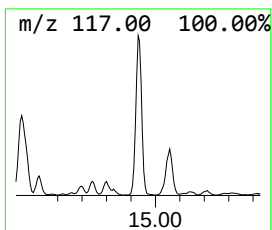
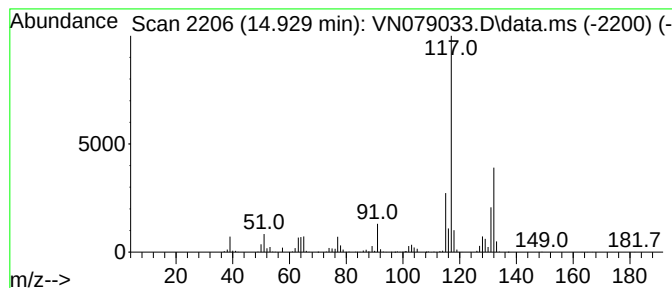
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	67.75 ug/l	1960130	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	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	96
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90



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Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

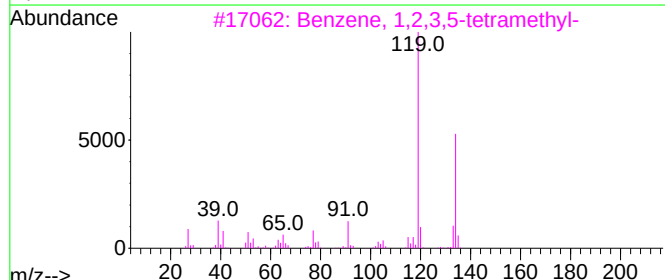
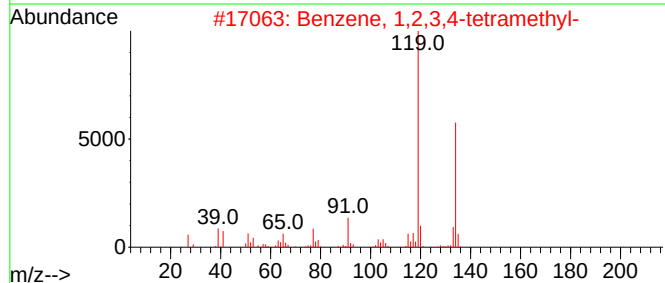
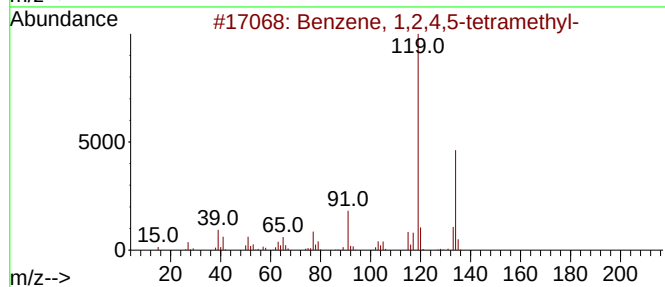
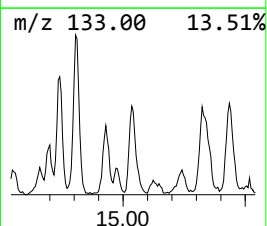
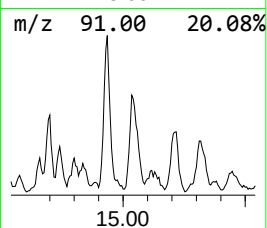
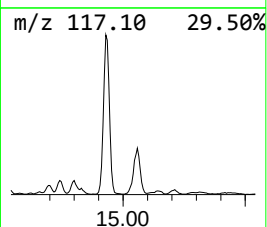
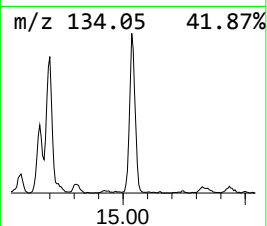
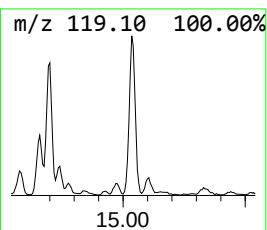
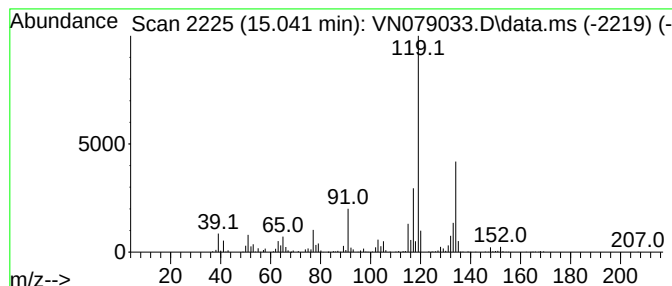
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	46.41 ug/l	1342760	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	90
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87
4			o-Cymene	134	C10H14	000527-84-4	87
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	87



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Instrument :
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ClientSampleId :
NEVINS-SB04-Z23-24

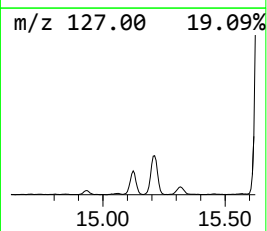
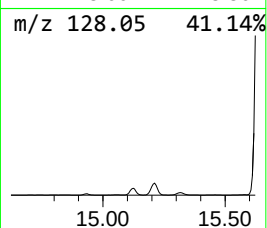
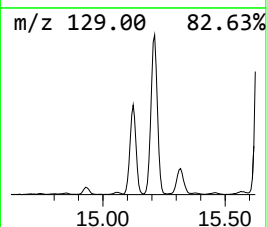
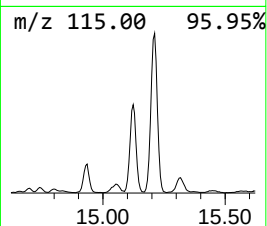
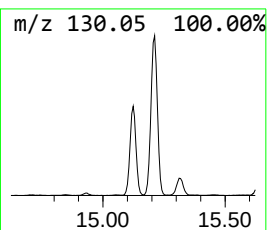
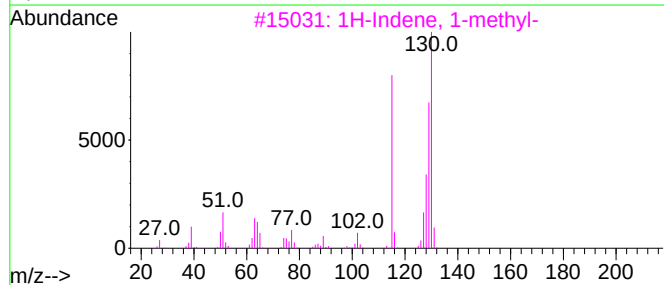
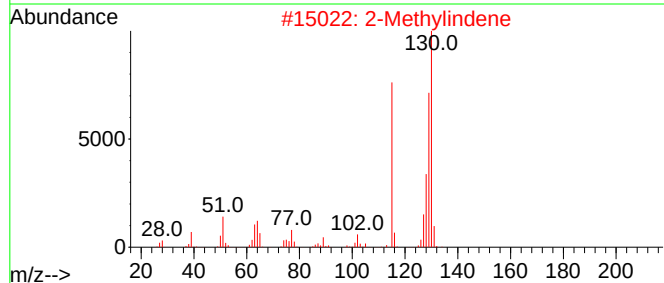
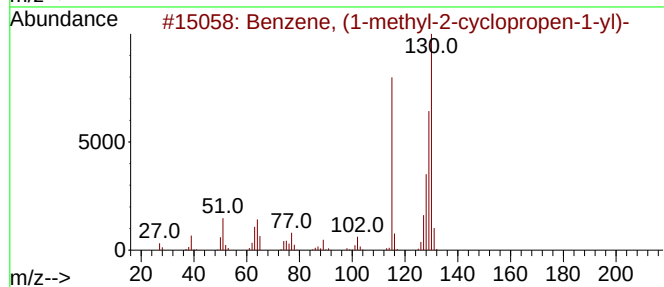
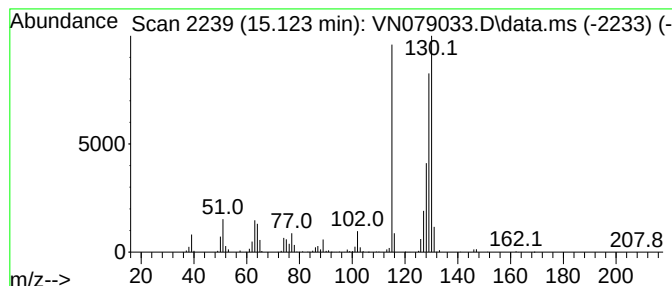
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, (1-methyl-2-cyclop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	94.91 ug/l	2746090	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			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
5			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93



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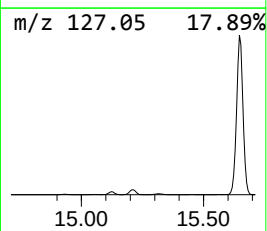
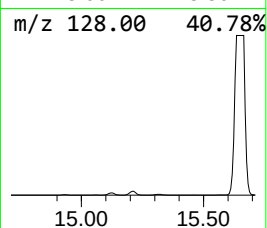
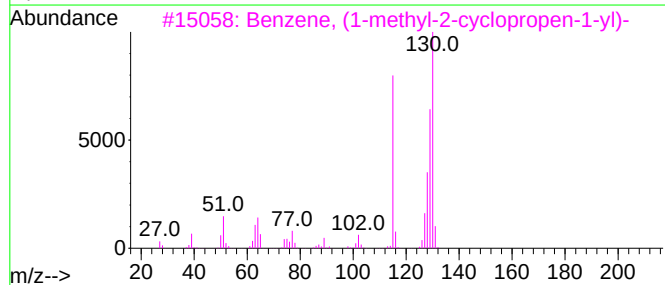
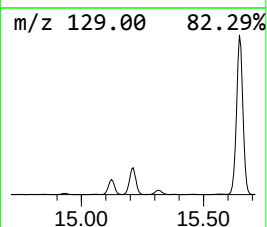
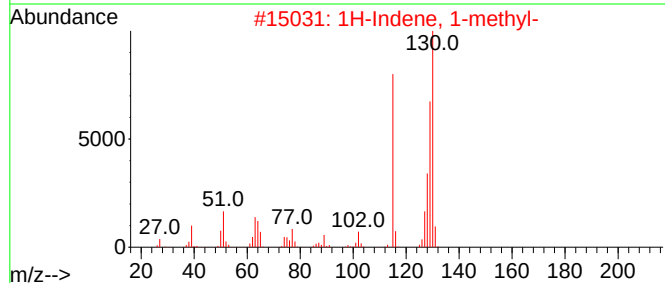
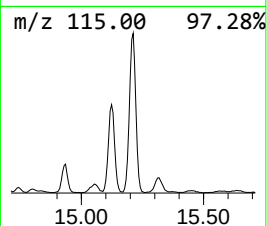
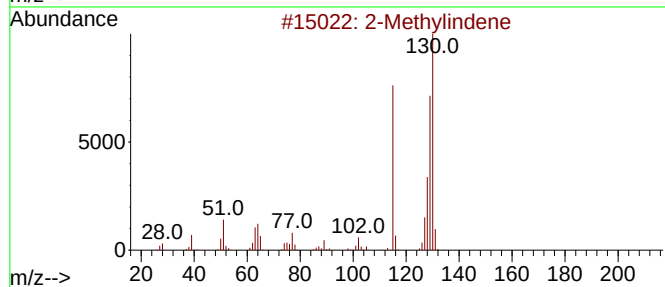
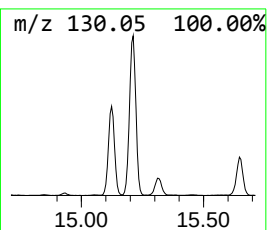
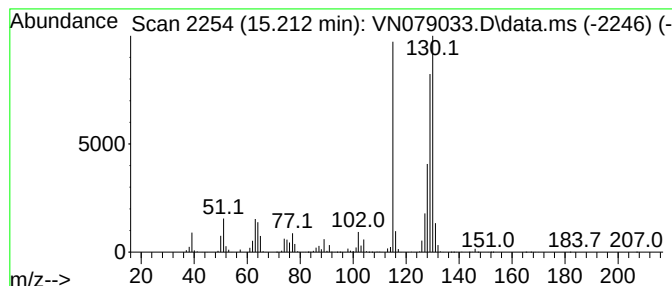
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Quant Title : SW846 8260

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

Peak Number 6 2-Methylindene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	179.10 ug/l	5182110	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			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
5			Benzene, 1-butylnyl-	130	C10H10	000622-76-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079033.D
Acq On : 24 Aug 2023 15:54
Operator : JC\MD
Sample : 04075-02 20X
Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

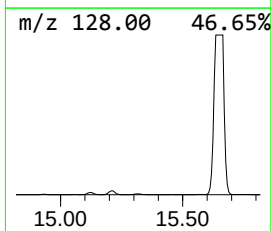
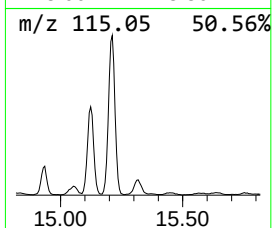
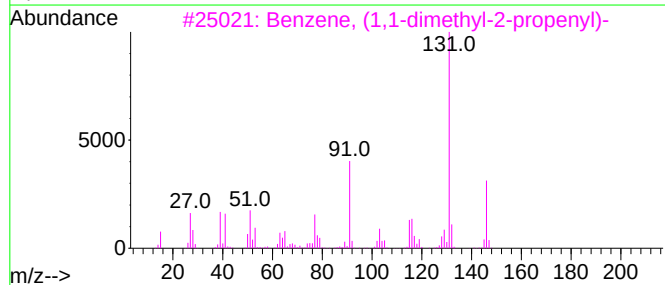
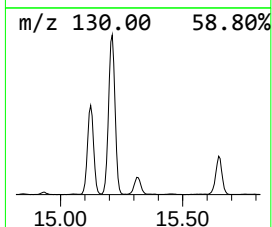
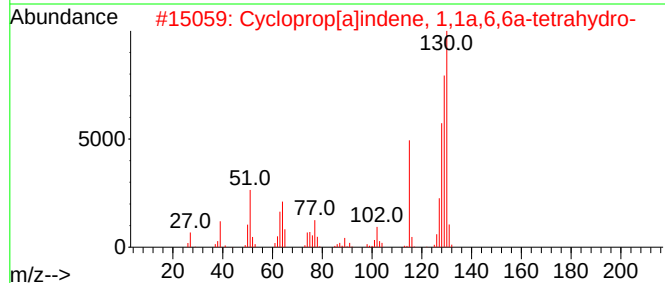
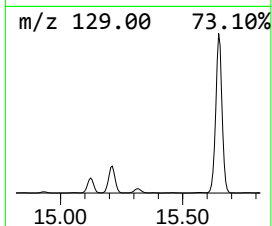
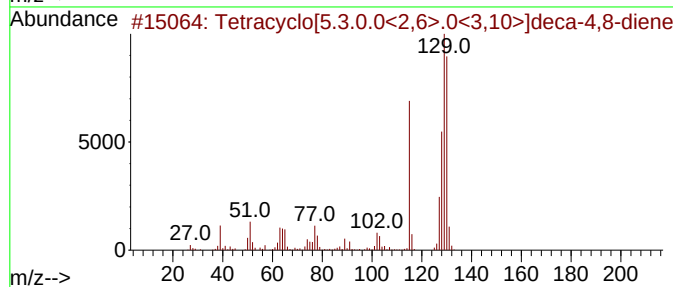
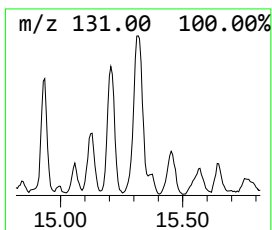
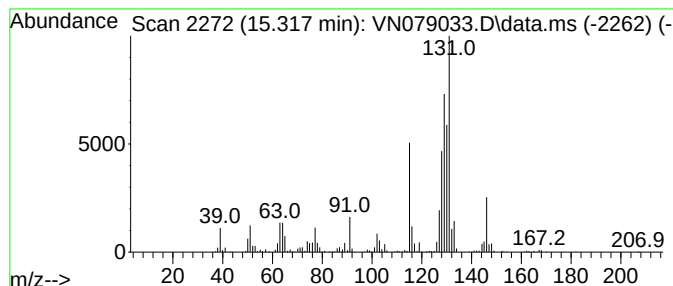
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Quant Title : SW846 8260

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

Peak Number 7 Tetracyclo[5.3.0.0<2,6>.0<3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	47.13 ug/l	1363630	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	86
2			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	42
3			Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	41
4			2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	41
5			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079033.D
Acq On : 24 Aug 2023 15:54
Operator : JC\MD
Sample : 04075-02 20X
Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

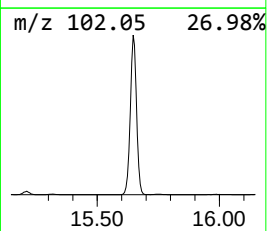
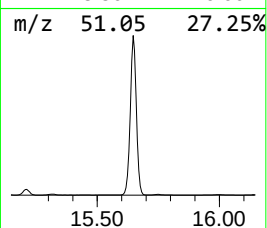
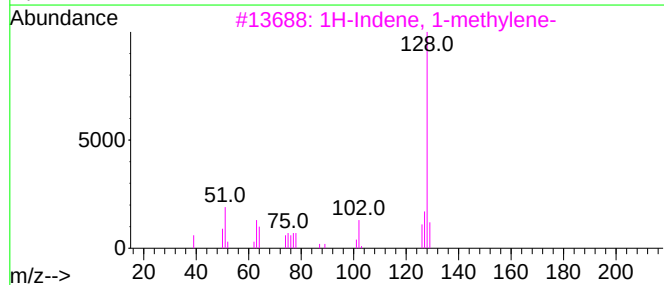
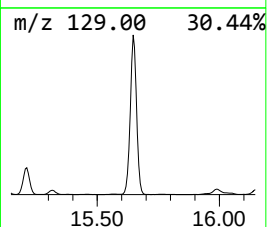
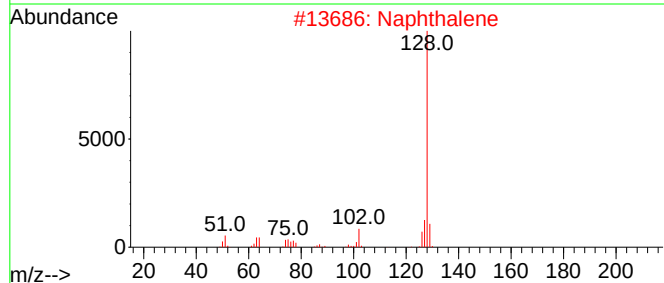
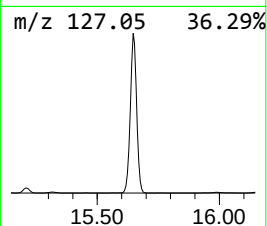
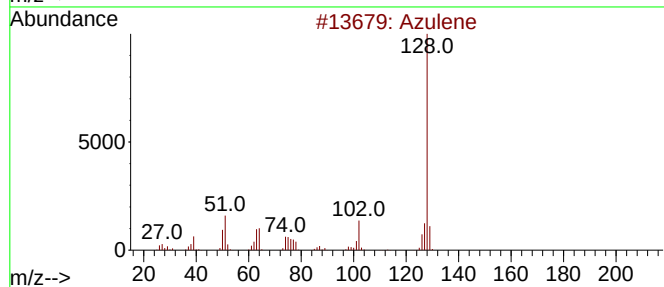
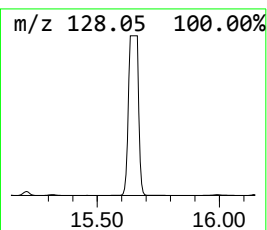
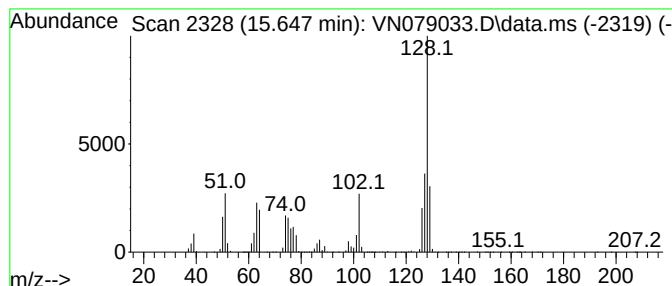
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Quant Title : SW846 8260

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	2940.98 ug/l	85093000	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	81
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	80
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	53
5			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079033.D
Acq On : 24 Aug 2023 15:54
Operator : JC\MD
Sample : 04075-02 20X
Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

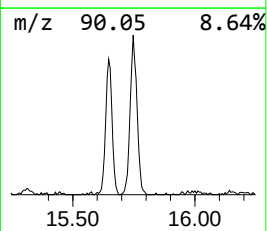
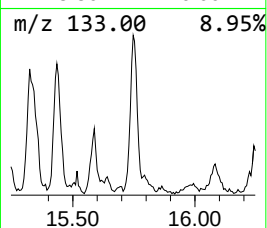
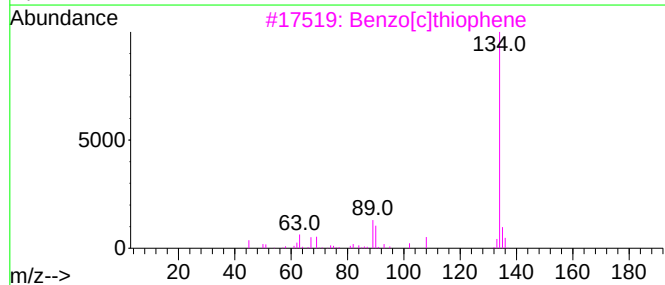
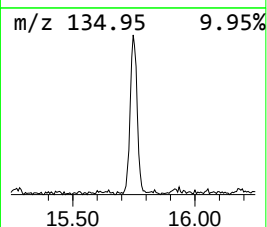
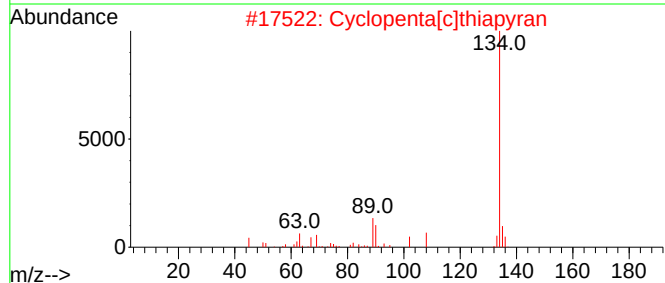
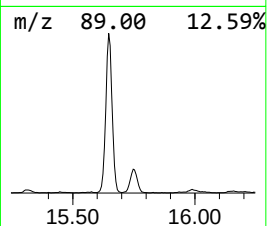
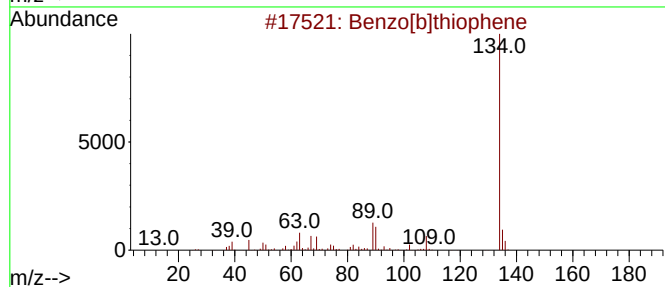
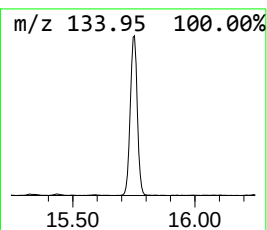
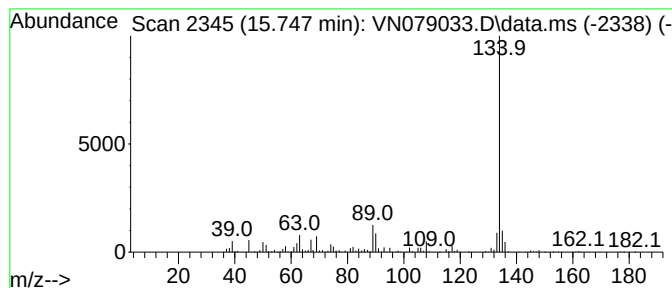
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[b]thiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.747	53.80 ug/l	1556610	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	91
3			Benzo[c]thiophene	134	C8H6S	000270-82-6	91
4			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	72
5			3-Deazaadenine	134	C6H6N4	006811-77-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079033.D
Acq On : 24 Aug 2023 15:54
Operator : JC\MD
Sample : 04075-02 20X
Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

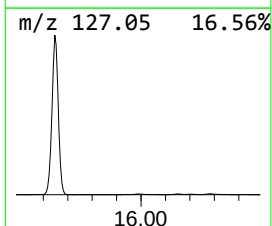
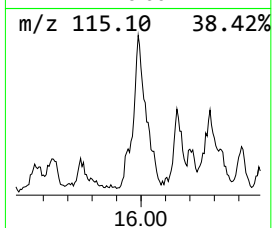
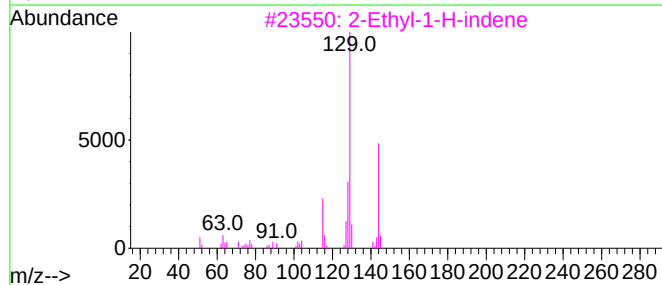
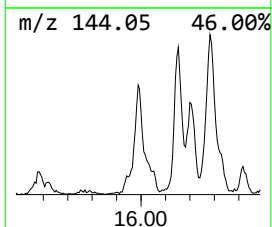
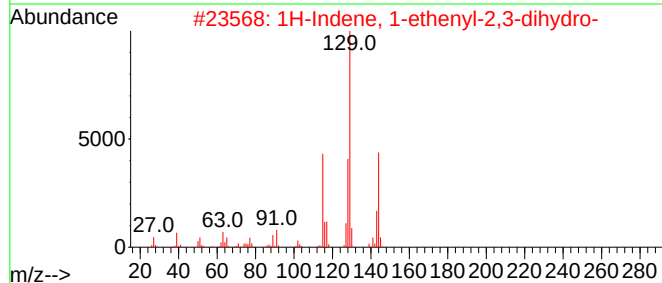
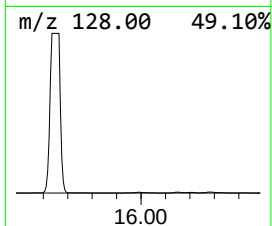
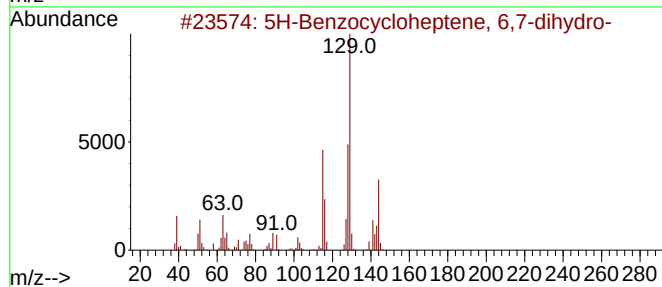
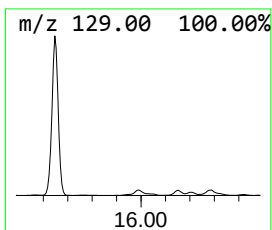
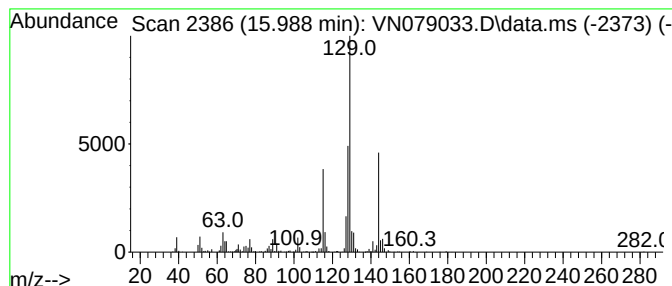
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 10 5H-Benzocycloheptene, 6,7-d... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.988	48.04 ug/l	1390040	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	91
2		1H-Indene, 1-ethenyl-2,3-dihydro-	144	C11H12	051783-46-1	87
3		2-Ethyl-1-H-indene	144	C11H12	017059-50-6	87
4		1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	81
5		1H-Indene, 2,3-dimethyl-	144	C11H12	004773-82-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079033.D
Acq On : 24 Aug 2023 15:54
Operator : JC\MD
Sample : 04075-02 20X
Misc : 7.22g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z23-24

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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Benzene, (2-met...	14.459	46.4	ug/l	1341440	4	13.794	1446680	50.0
Benzene, 2-ethe...	14.929	67.8	ug/l	1960130	4	13.794	1446680	50.0
Benzene, 1,2,4,...	15.041	46.4	ug/l	1342760	4	13.794	1446680	50.0
Benzene, (1-met...	15.123	94.9	ug/l	2746090	4	13.794	1446680	50.0
2-Methylindene	15.212	179.1	ug/l	5182110	4	13.794	1446680	50.0
Tetracyclo[5.3....	15.317	47.1	ug/l	1363630	4	13.794	1446680	50.0
Azulene	15.647	2941.0	ug/l	85093000	4	13.794	1446680	50.0
Benzo[b]thiophene	15.747	53.8	ug/l	1556610	4	13.794	1446680	50.0
5H-Benzocyclohe...	15.988	48.0	ug/l	1390040	4	13.794	1446680	50.0