

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079028.D
 Acq On : 24 Aug 2023 13:53
 Operator : JC\MD
 Sample : 04047-03
 Misc : 5.17g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB05-Z60-61-Q

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: VN079028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1045	1056	1061	rBV	183766	443056	2.12%	1.050%
2	8.224	1061	1066	1085	rVB	294849	642241	3.07%	1.523%
3	8.588	1116	1128	1139	rBV3	239646	734563	3.51%	1.742%
4	9.100	1207	1215	1228	rBV	437577	907483	4.33%	2.151%
5	10.571	1457	1465	1473	rBV	677210	1234036	5.89%	2.926%
6	11.871	1678	1686	1695	rBV	629650	1122628	5.36%	2.662%
7	11.965	1695	1702	1711	rVV	924287	1589599	7.59%	3.769%
8	12.071	1711	1720	1730	rVB	265432	536400	2.56%	1.272%
9	12.400	1764	1776	1786	rBV	248464	429676	2.05%	1.019%
10	12.853	1846	1853	1862	rVB	534756	896153	4.28%	2.125%
11	13.135	1890	1901	1905	rBV	280872	498432	2.38%	1.182%
12	13.488	1951	1961	1966	rBV	359126	629780	3.01%	1.493%
13	13.794	2007	2013	2022	rBV2	676976	1368995	6.54%	3.246%
14	13.953	2034	2040	2042	rBV2	156819	239478	1.14%	0.568%
15	14.000	2042	2048	2062	rVB	2627243	4836033	23.10%	11.465%
16	14.335	2099	2105	2114	rVB	229431	363953	1.74%	0.863%
17	14.453	2117	2125	2133	rBV3	111169	292442	1.40%	0.693%
18	14.929	2200	2206	2219	rVB	335309	615725	2.94%	1.460%
19	15.041	2219	2225	2233	rBV2	162417	413810	1.98%	0.981%
20	15.123	2233	2239	2246	rVB	374849	665748	3.18%	1.578%
21	15.212	2246	2254	2262	rVB	769902	1406754	6.72%	3.335%
22	15.317	2262	2272	2278	rBV4	165140	393552	1.88%	0.933%
23	15.647	2313	2328	2337	rBV	10832155	20936170	100.00%	49.636%
24	15.747	2339	2345	2354	rBV	215012	428179	2.05%	1.015%
25	15.988	2382	2386	2401	rVB3	97516	317501	1.52%	0.753%
26	16.282	2429	2436	2443	rBV4	83092	237256	1.13%	0.562%

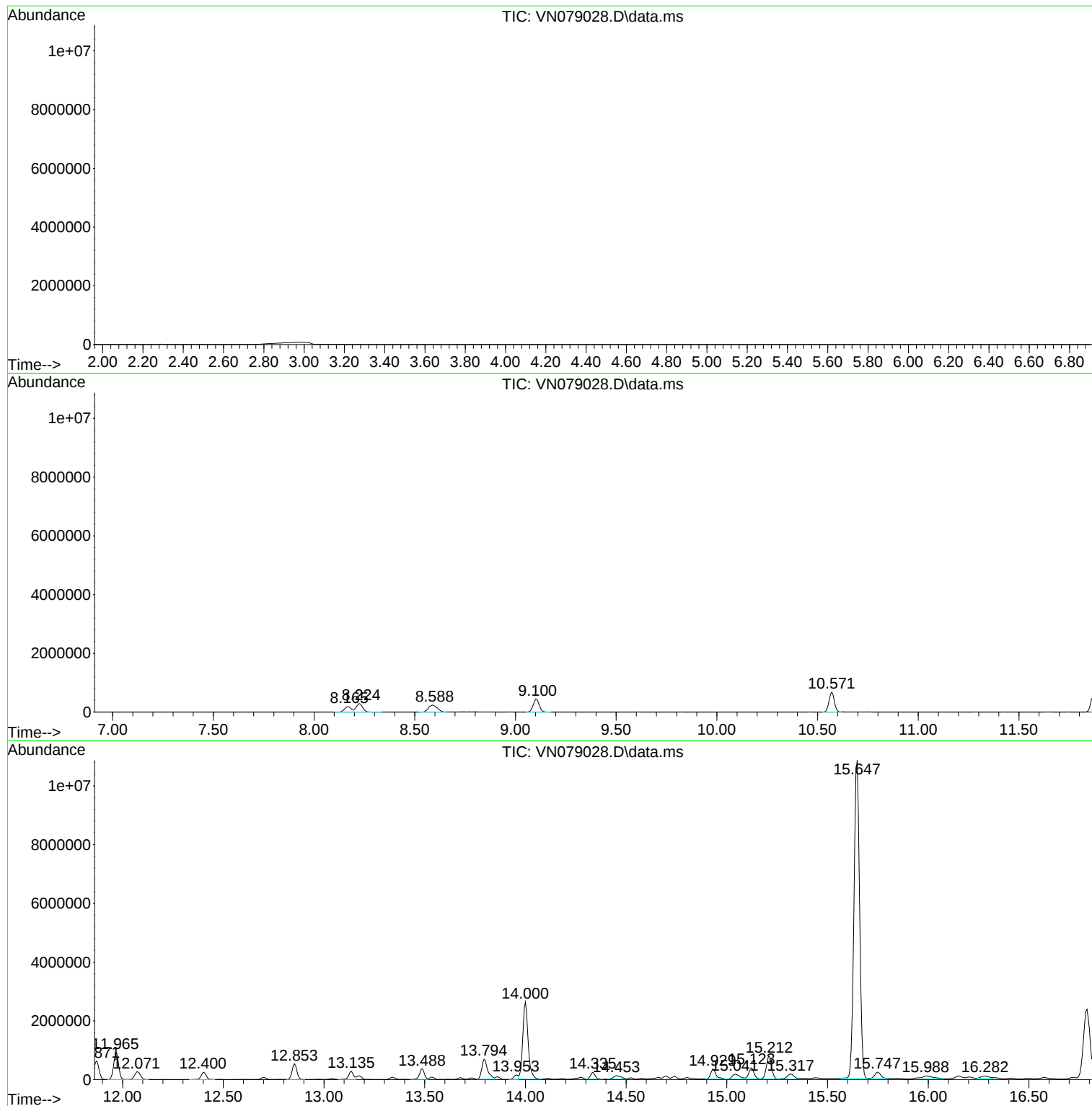
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

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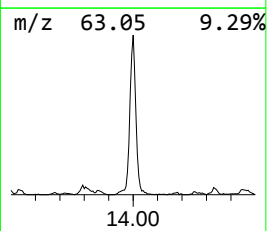
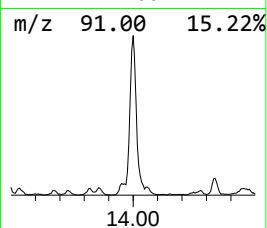
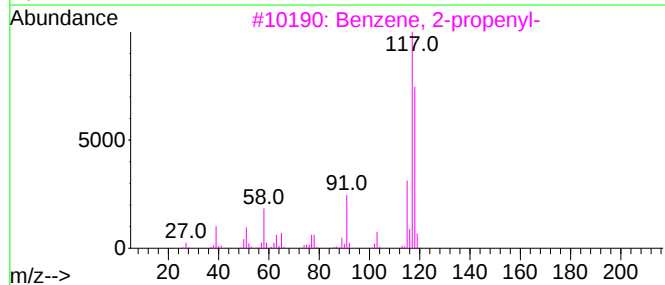
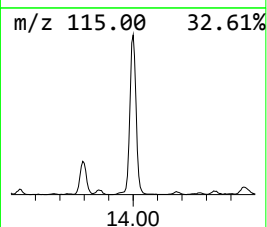
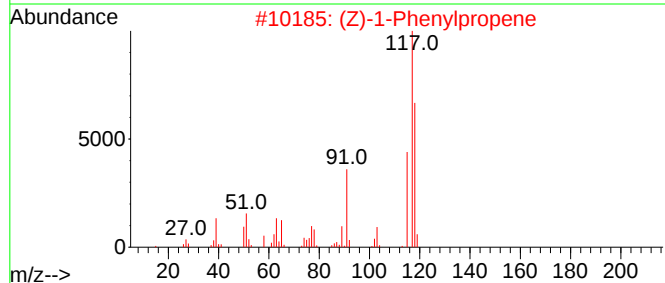
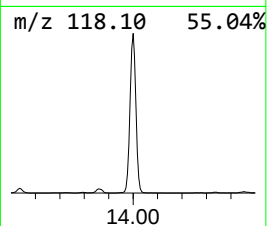
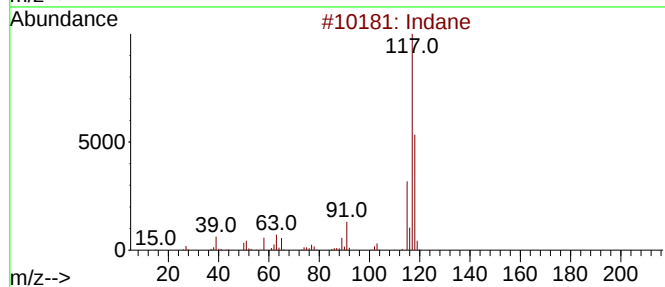
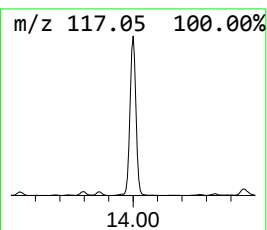
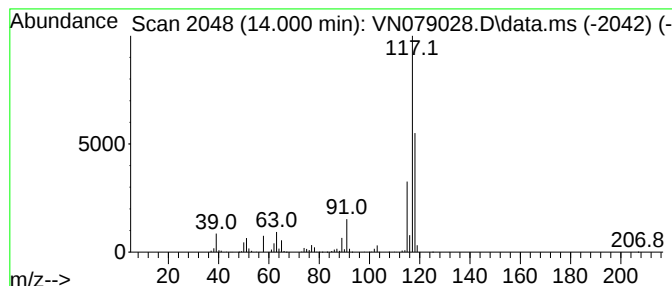
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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	176.63 ug/l	4836030	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	53



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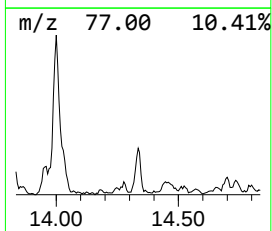
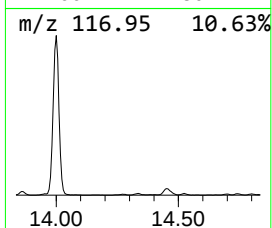
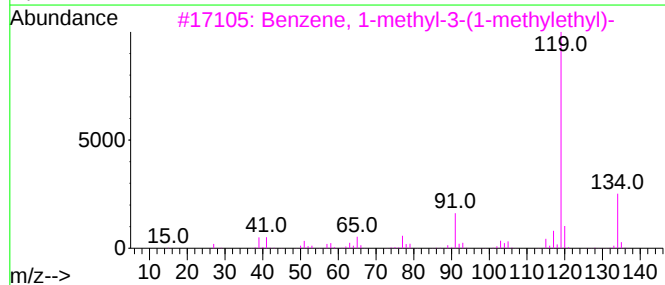
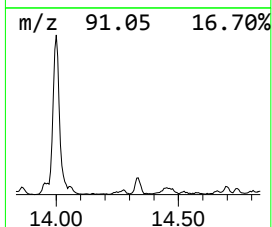
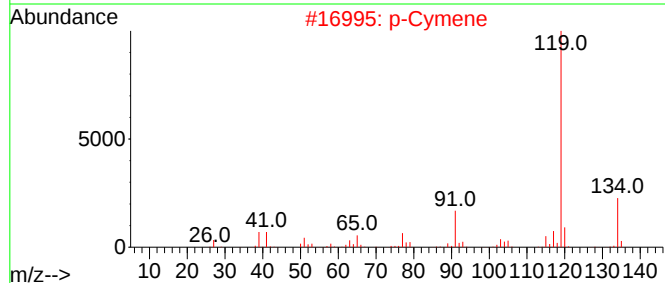
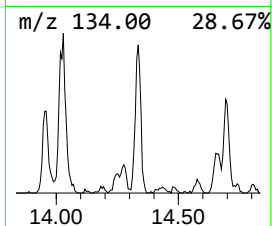
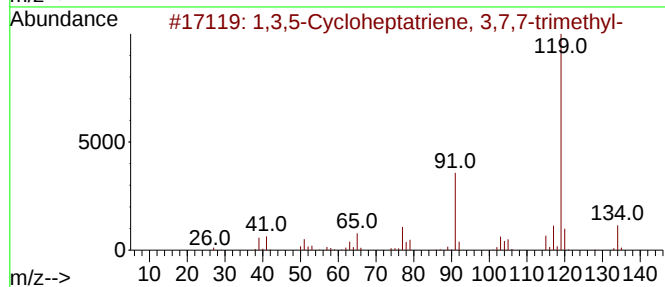
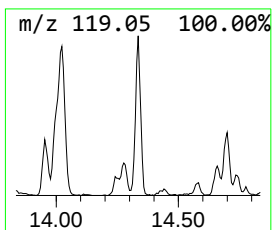
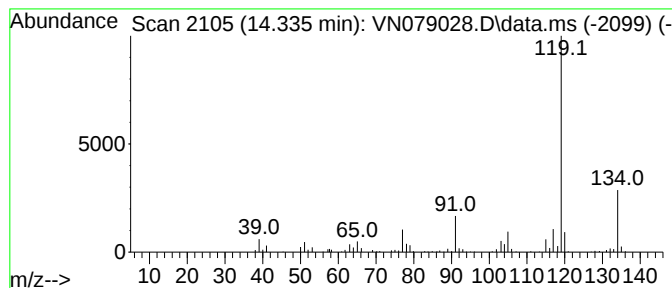
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 2 1,3,5-Cycloheptatriene, 3,7... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	13.29 ug/l	363953	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	95		
2	p-Cymene	134	C10H14	000099-87-6	95		
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95		
4	o-Cymene	134	C10H14	000527-84-4	95		
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93		



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NEVINS-SB05-Z60-61-Q

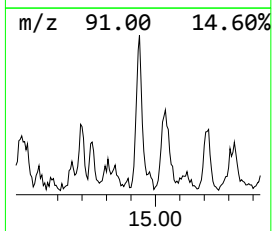
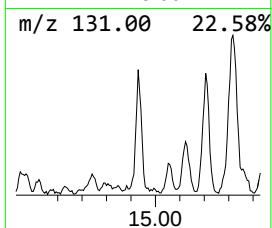
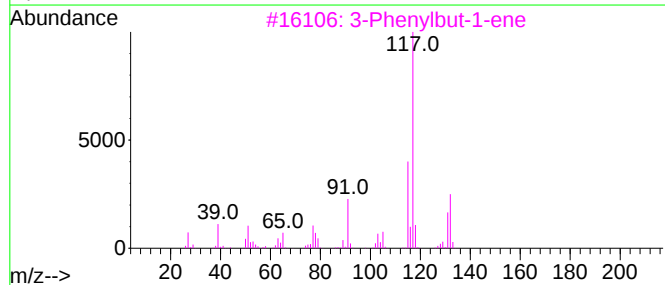
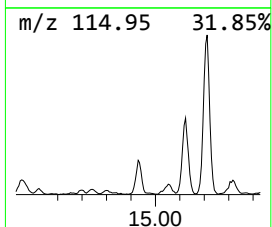
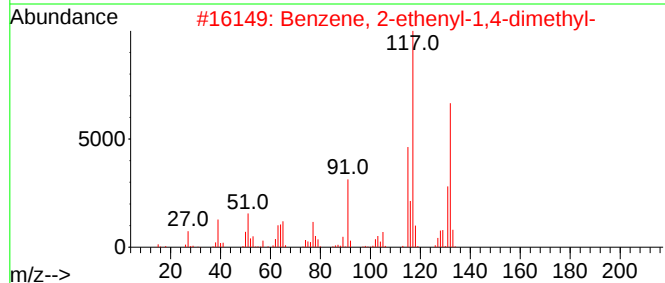
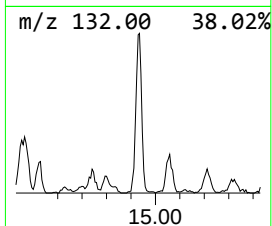
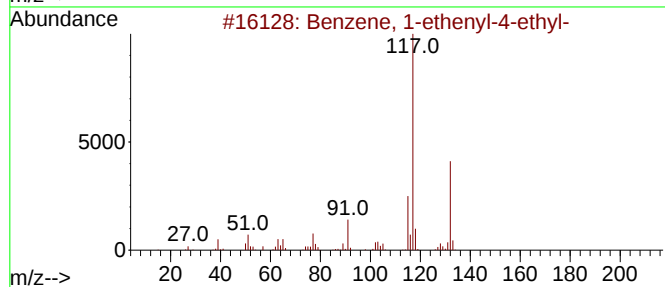
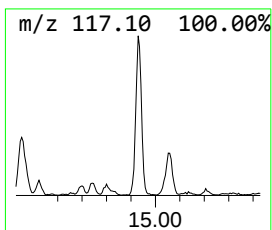
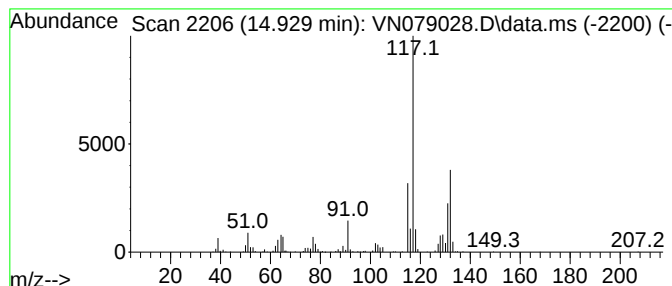
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	22.49 ug/l	615725	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			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



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Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

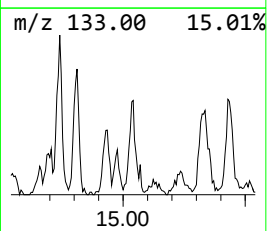
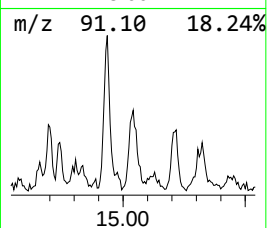
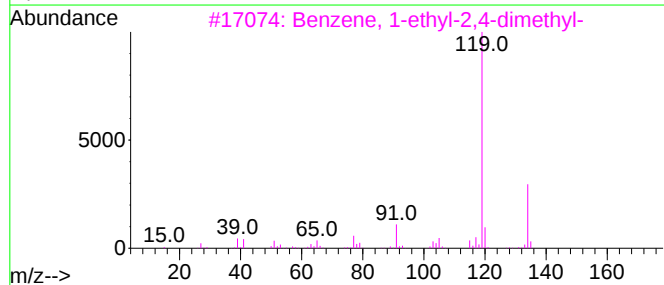
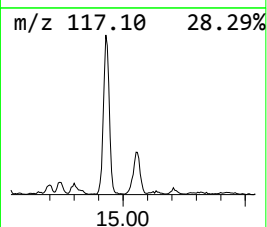
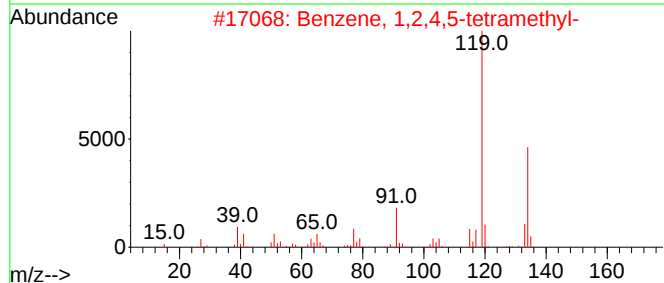
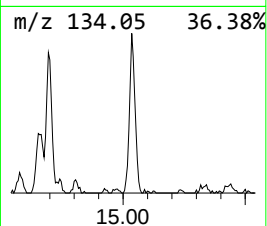
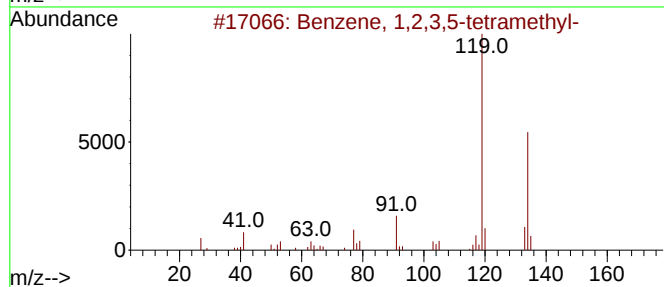
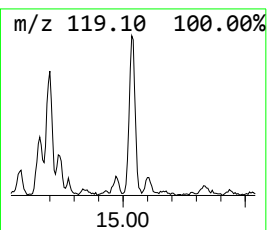
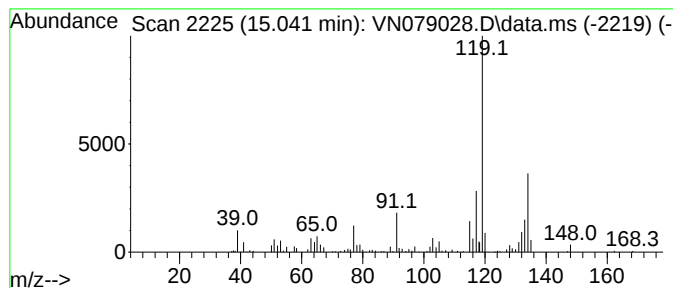
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	15.11 ug/l	413810	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	70
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	70
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	62
5			p-Cymene	134	C10H14	000099-87-6	62



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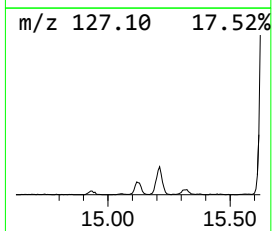
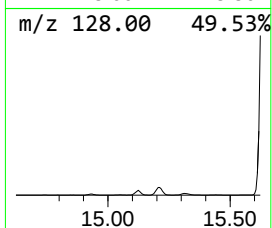
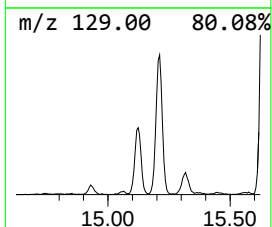
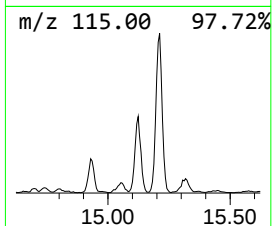
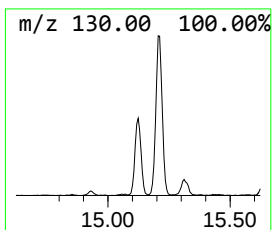
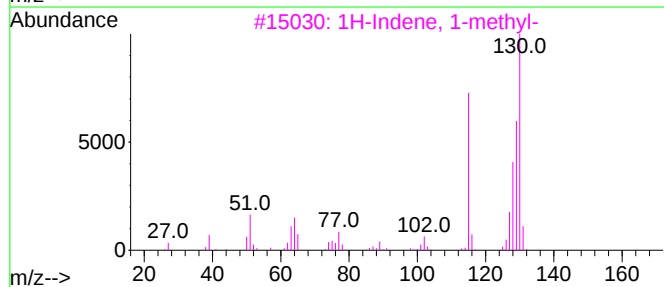
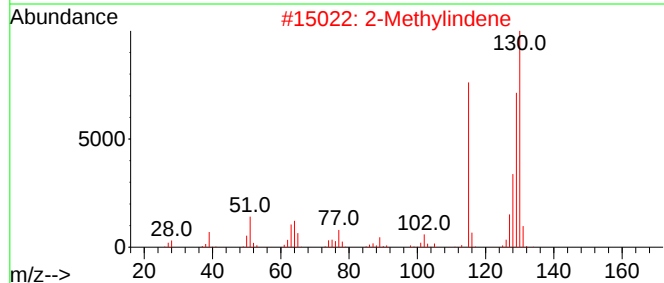
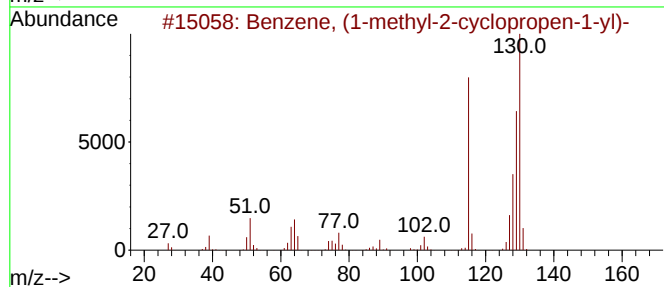
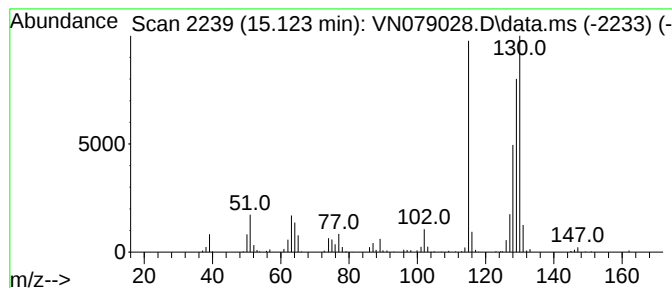
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	24.32 ug/l	665748	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	96
2			2-Methylindene	130	C10H10	002177-47-1	96
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
4			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
5			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95



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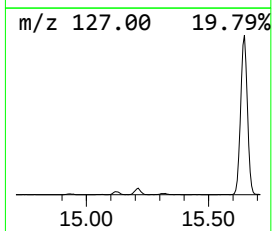
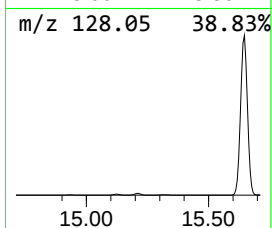
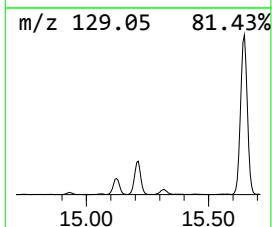
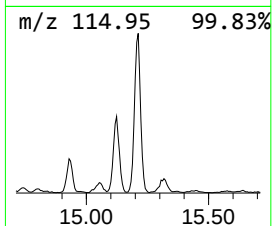
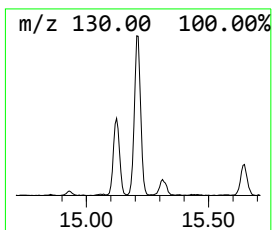
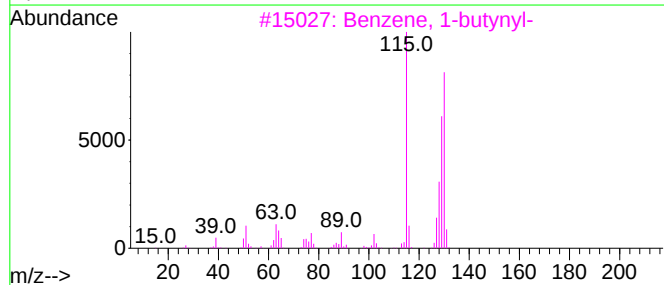
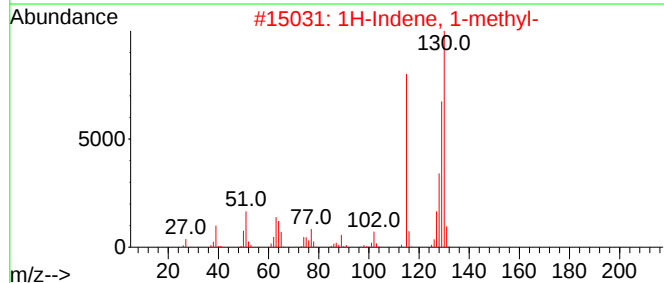
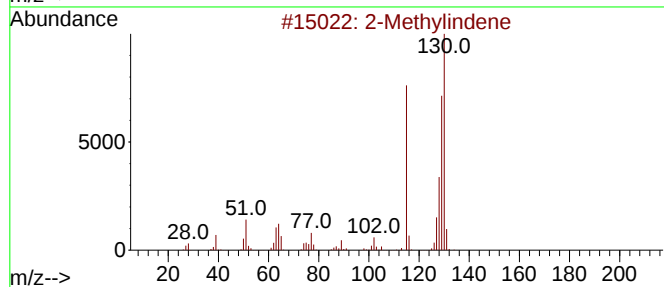
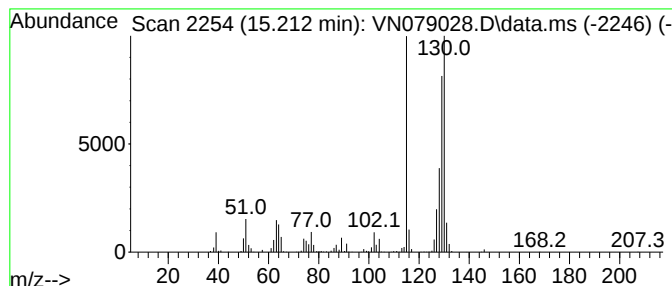
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Quant Title : SW846 8260

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	51.38 ug/l	1406750	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-butynyl-	130	C10H10	000622-76-4	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
5			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079028.D
Acq On : 24 Aug 2023 13:53
Operator : JC\MD
Sample : 04047-03
Misc : 5.17g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

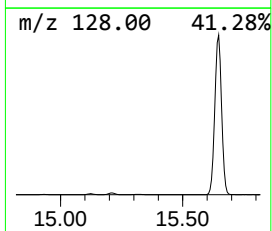
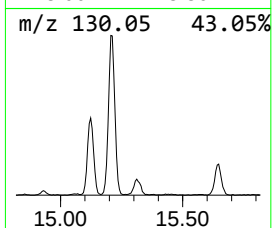
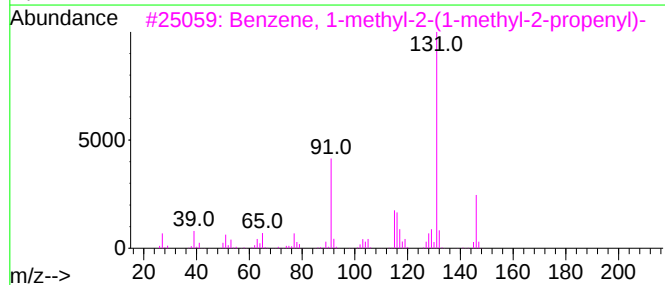
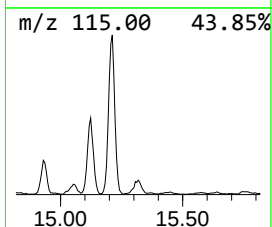
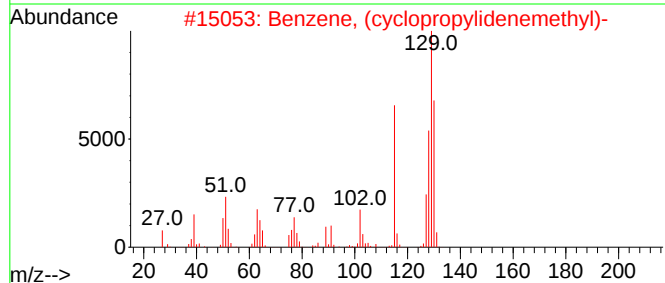
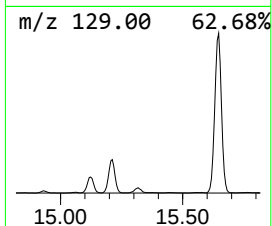
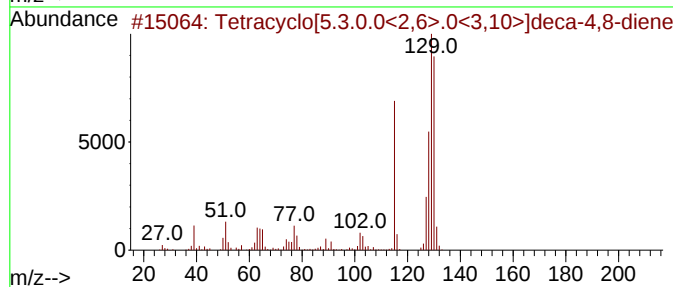
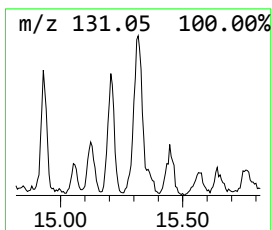
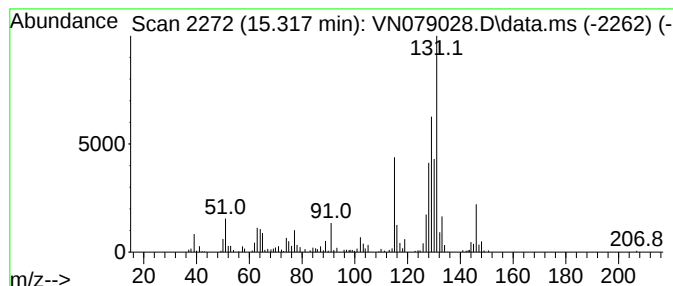
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.318 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	14.37 ug/l	393552	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	42
2			Benzene, (cyclopropylidenemethyl)-	130	C10H10	007555-67-1	42
3			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	38
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	38
5			Benzene, (methylenecyclopropyl)-	130	C10H10	029817-09-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079028.D
Acq On : 24 Aug 2023 13:53
Operator : JC\MD
Sample : 04047-03
Misc : 5.17g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

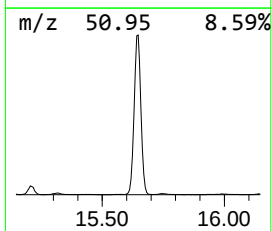
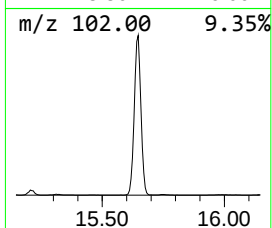
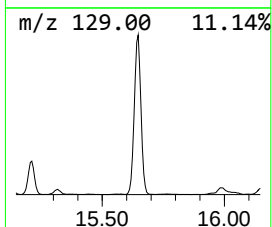
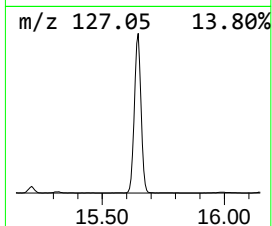
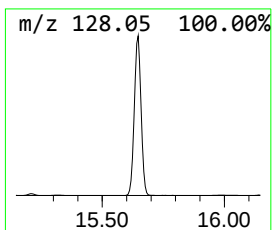
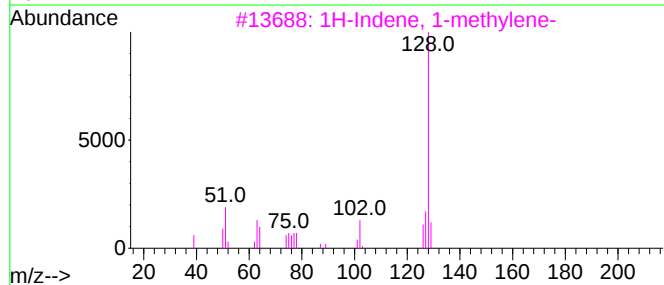
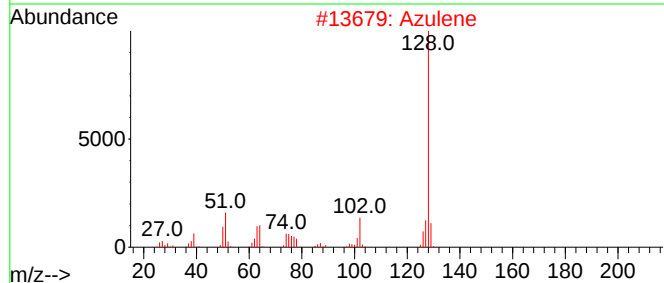
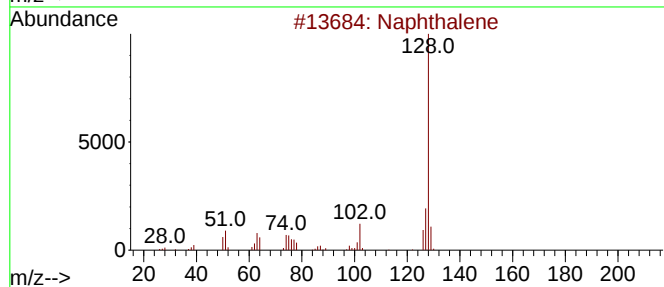
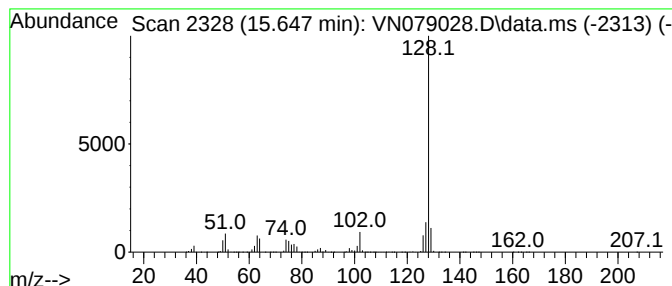
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Quant Title : SW846 8260

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	764.65 ug/l	20936200	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Azulene	128	C10H8	000275-51-4	94
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
5			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079028.D
Acq On : 24 Aug 2023 13:53
Operator : JC\MD
Sample : 04047-03
Misc : 5.17g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

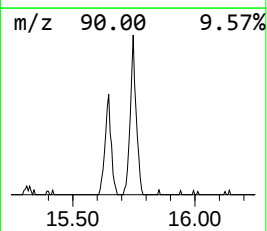
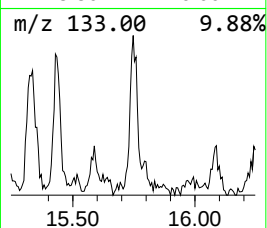
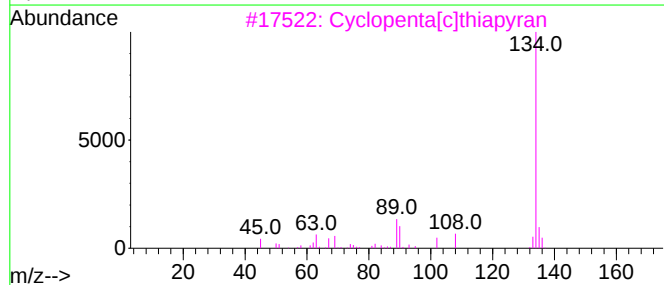
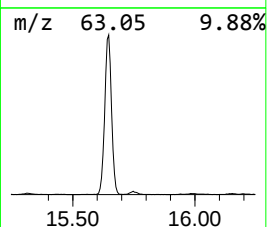
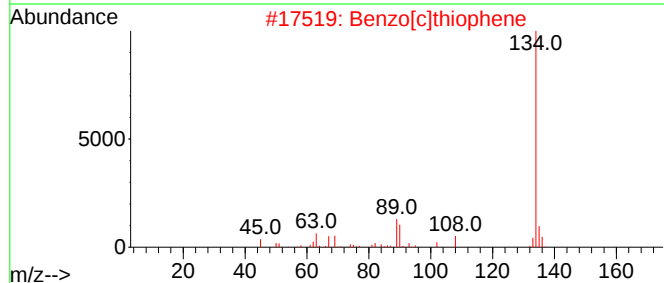
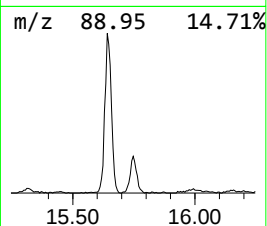
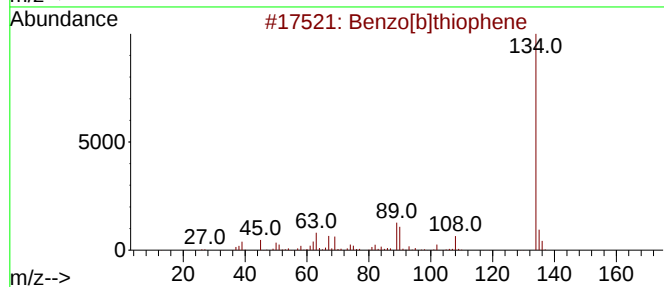
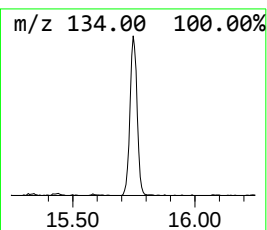
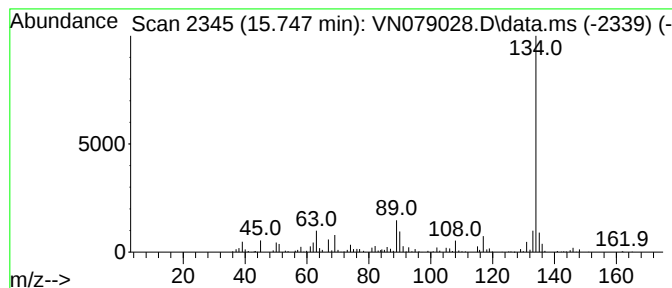
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Quant Title : SW846 8260

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	15.64 ug/l	428179	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	90
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	90
4			3-Deazaadenine	134	C6H6N4	006811-77-4	53
5			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079028.D
Acq On : 24 Aug 2023 13:53
Operator : JC\MD
Sample : 04047-03
Misc : 5.17g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

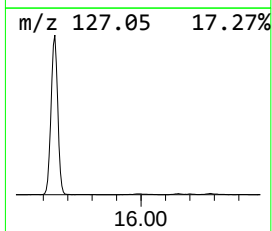
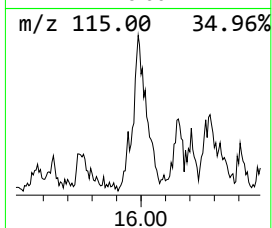
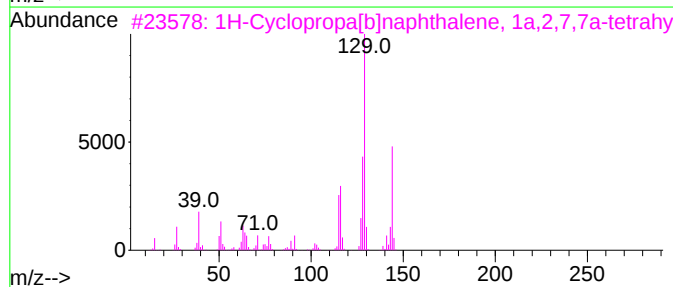
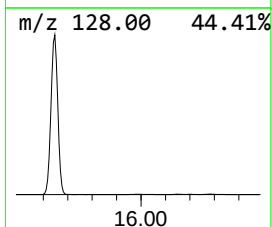
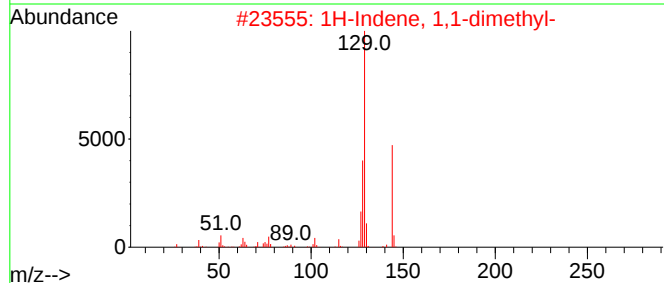
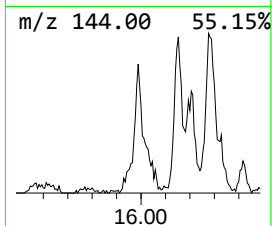
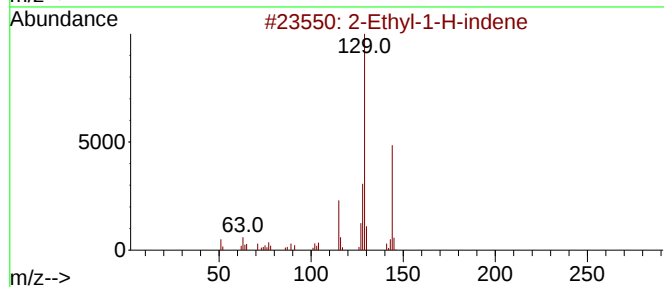
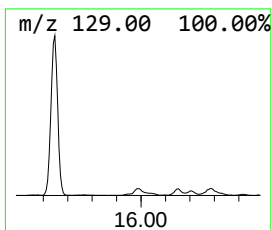
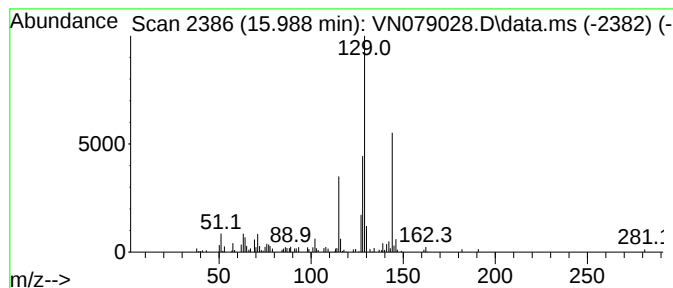
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Quant Title : SW846 8260

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

Peak Number 10 2-Ethyl-1-H-indene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.988	11.60 ug/l	317501	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-1-H-indene	144	C11H12	017059-50-6	91
2			1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	87
3			1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	87
4			5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	87
5			1H-Indene, 2,3-dimethyl-	144	C11H12	004773-82-4	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079028.D
Acq On : 24 Aug 2023 13:53
Operator : JC\MD
Sample : 04047-03
Misc : 5.17g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB05-Z60-61-Q

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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1,3,5-Cyclohept...	14.335	13.3	ug/l	363953	4	13.794	1369000	50.0
Benzene, 1-ethe...	14.929	22.5	ug/l	615725	4	13.794	1369000	50.0
Benzene, 1,2,3,...	15.041	15.1	ug/l	413810	4	13.794	1369000	50.0
Benzene, (1-met...	15.123	24.3	ug/l	665748	4	13.794	1369000	50.0
2-Methylindene	15.212	51.4	ug/l	1406750	4	13.794	1369000	50.0
unknown15.318	15.318	14.4	ug/l	393552	4	13.794	1369000	50.0
Azulene	15.647	764.6	ug/l	20936200	4	13.794	1369000	50.0
Benzo[b]thiophene	15.747	15.6	ug/l	428179	4	13.794	1369000	50.0
2-Ethyl-1-H-indene	15.988	11.6	ug/l	317501	4	13.794	1369000	50.0