

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
 Data File : VN079034.D
 Acq On : 24 Aug 2023 16:18
 Operator : JC\MD
 Sample : 04093-01 20X
 Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 NEVINS-SB04-Z45-46

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: VN079034.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	1062	1067	1081	rVB	377066	837413	1.15%	0.547%
2	9.106	1207	1216	1230	rBV	548759	1129356	1.55%	0.737%
3	10.571	1457	1465	1473	rBV	856392	1594279	2.18%	1.040%
4	11.871	1678	1686	1695	rBV	815463	1443835	1.98%	0.942%
5	11.971	1695	1703	1712	rVV	4512929	7707117	10.54%	5.030%
6	12.077	1712	1721	1731	rVB	1367792	2692942	3.68%	1.758%
7	12.400	1764	1776	1785	rBV	1210290	2168561	2.97%	1.415%
8	12.629	1795	1815	1822	rBV4	204300	1095152	1.50%	0.715%
9	12.700	1822	1827	1835	rVB	413902	751126	1.03%	0.490%
10	12.853	1847	1853	1863	rVB	709468	1236453	1.69%	0.807%
11	13.135	1890	1901	1905	rBV	1169535	2072402	2.84%	1.353%
12	13.335	1916	1935	1951	rVB3	872136	3734617	5.11%	2.437%
13	13.488	1951	1961	1966	rBV	1448359	2553520	3.49%	1.667%
14	13.676	1974	1993	2000	rBV4	604998	2746260	3.76%	1.792%
15	13.794	2008	2013	2016	rBV	822441	1432338	1.96%	0.935%
16	13.959	2034	2041	2042	rBV	582015	886788	1.21%	0.579%
17	14.000	2042	2048	2061	rVV	11957462	21993430	30.09%	14.354%
18	14.118	2061	2068	2084	rVB4	431686	1763477	2.41%	1.151%
19	14.335	2099	2105	2114	rVB	916717	1504566	2.06%	0.982%
20	14.453	2114	2125	2134	rBV	861178	2257792	3.09%	1.474%
21	14.929	2201	2206	2218	rVB	968366	1873527	2.56%	1.223%
22	15.041	2218	2225	2233	rBV3	566288	1643104	2.25%	1.072%
23	15.123	2233	2239	2247	rVB	990380	1863153	2.55%	1.216%
24	15.212	2247	2254	2261	rVB	2358877	4365627	5.97%	2.849%
25	15.317	2263	2272	2280	rBV3	590350	1354407	1.85%	0.884%
26	15.523	2298	2307	2319	rVV2	755660	3002222	4.11%	1.959%
27	15.647	2319	2328	2338	rVV2	38776360	73096576	100.00%	47.706%
28	15.747	2339	2345	2358	rVB	984795	2105282	2.88%	1.374%
29	15.994	2382	2387	2401	rVB4	238025	847999	1.16%	0.553%
30	16.282	2428	2436	2453	rVB3	377168	1471286	2.01%	0.960%

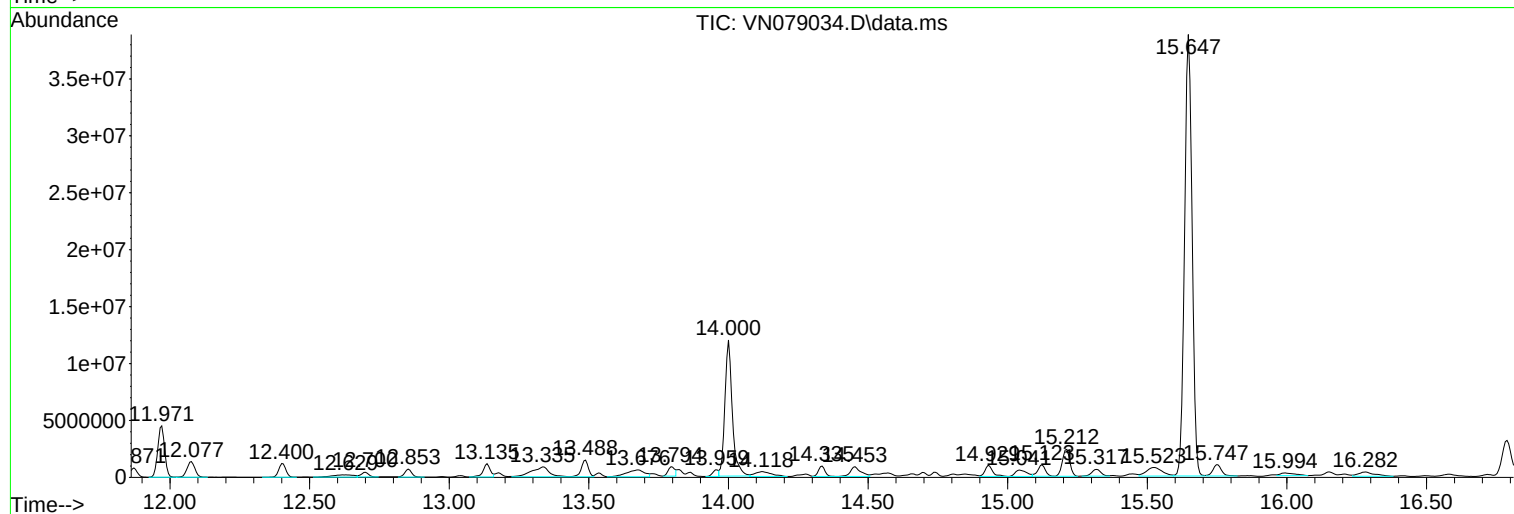
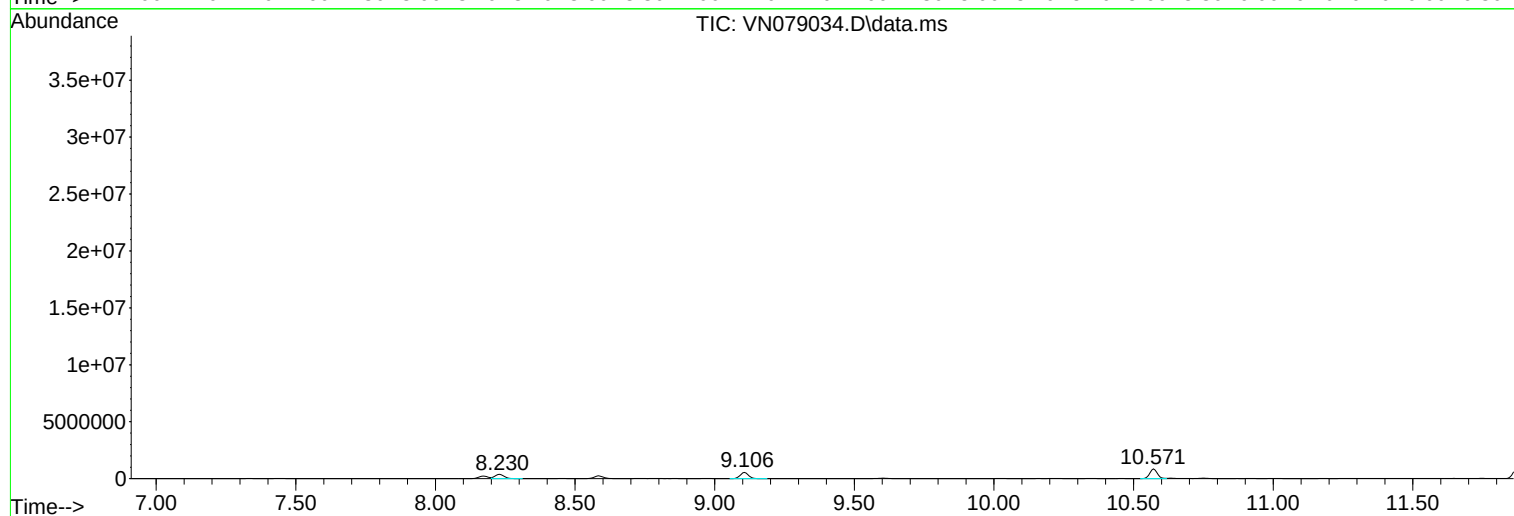
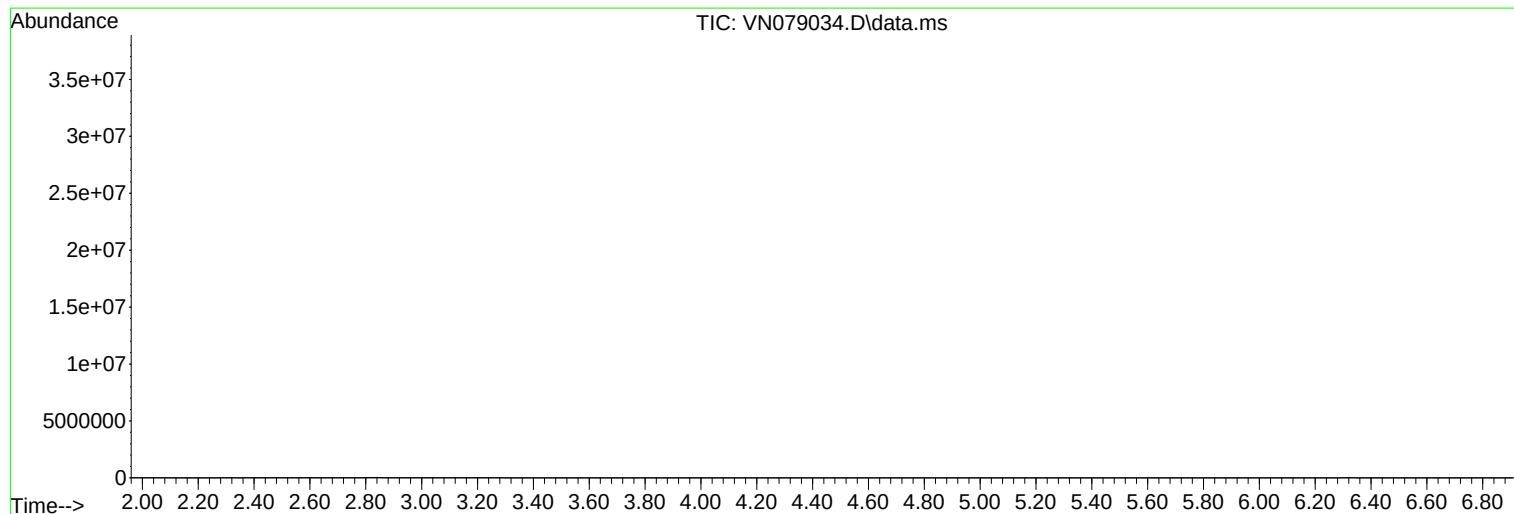
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NEVINS-SB04-Z45-46

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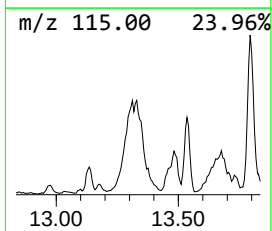
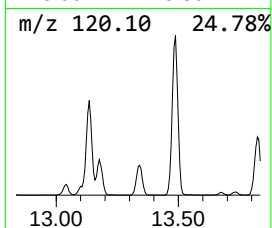
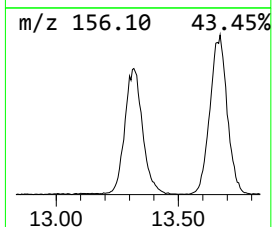
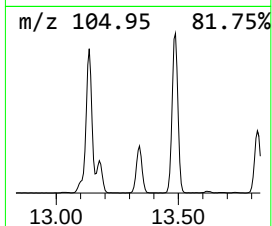
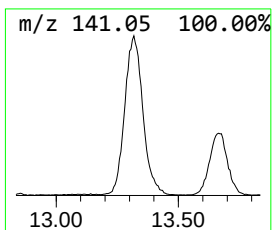
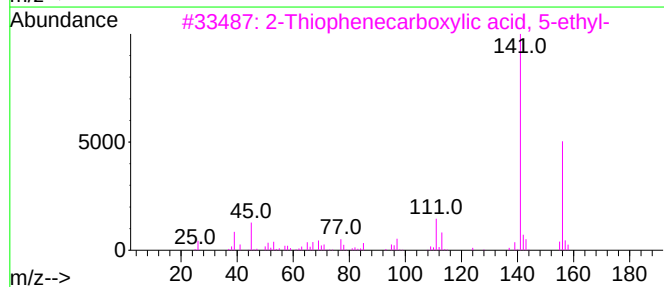
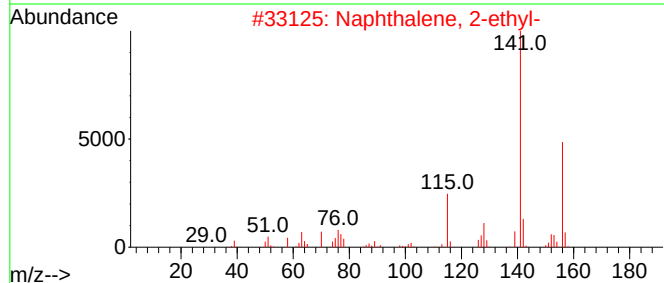
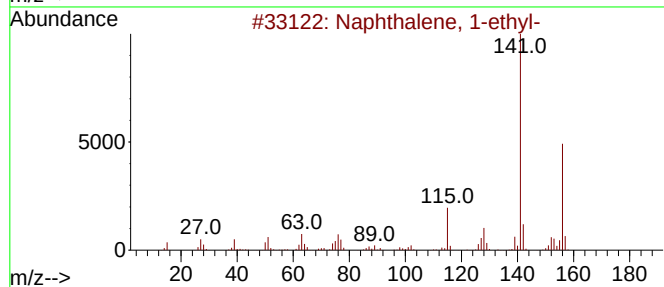
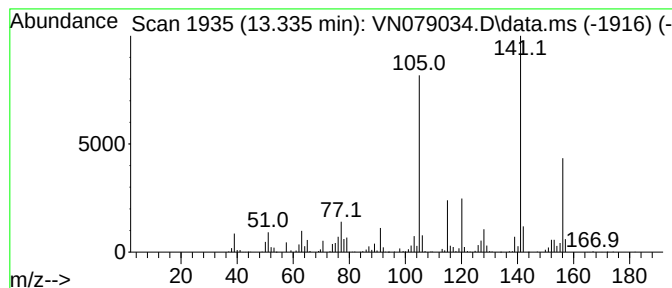
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, 1-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	130.37 ug/l	3734620	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
3			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	50
4			4-Chloro-3-ethylphenol	156	C8H9ClO	014143-32-9	49
5			3',4'-Difluoroacetophenone	156	C8H6F2O	000369-33-5	47



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

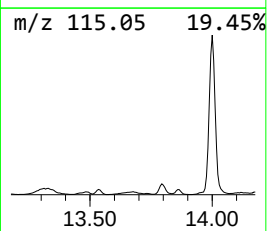
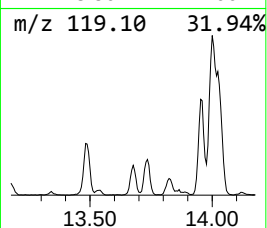
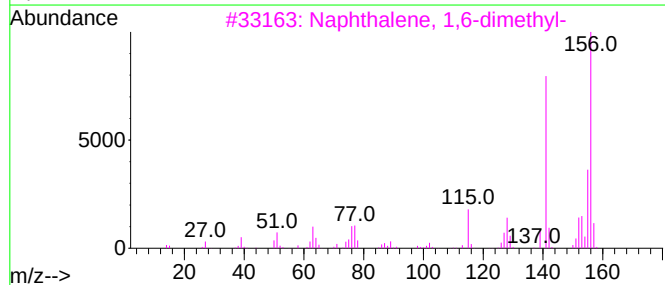
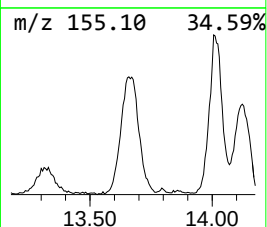
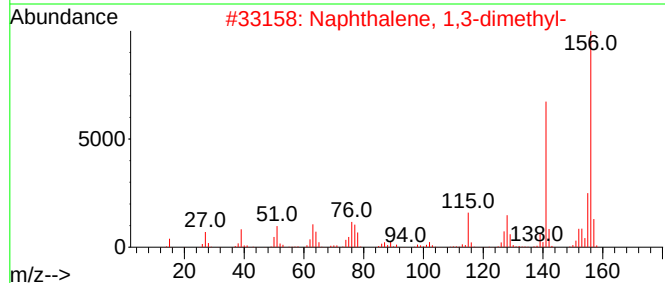
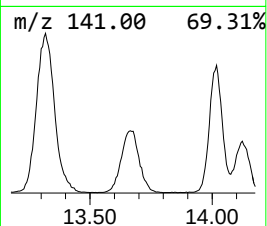
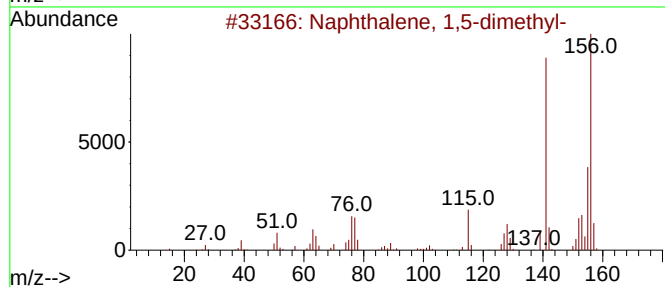
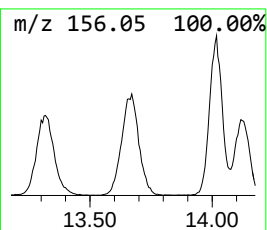
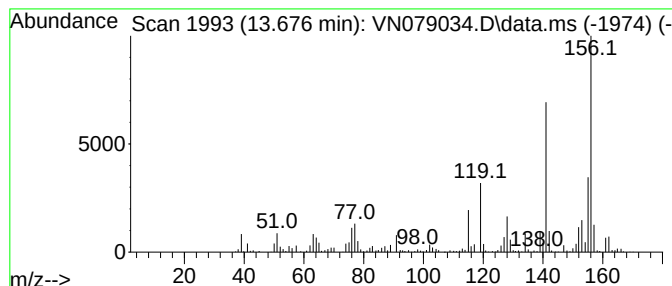
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 1,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	95.87 ug/l	2746260	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	98
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96



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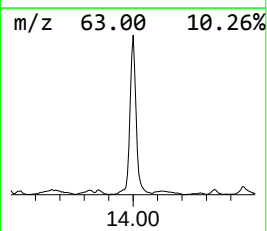
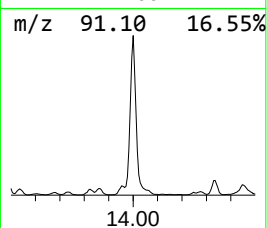
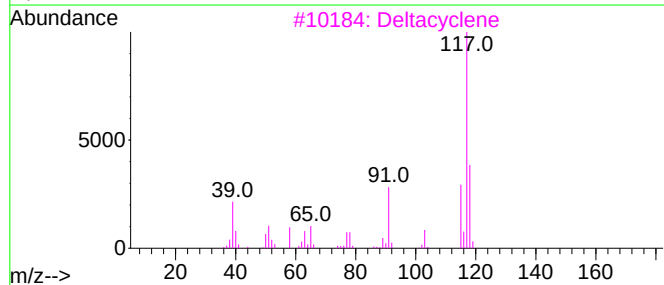
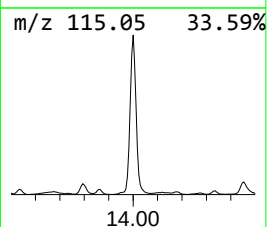
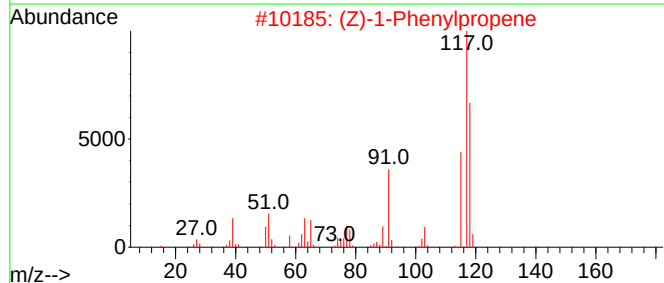
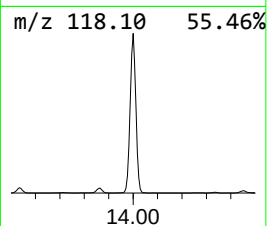
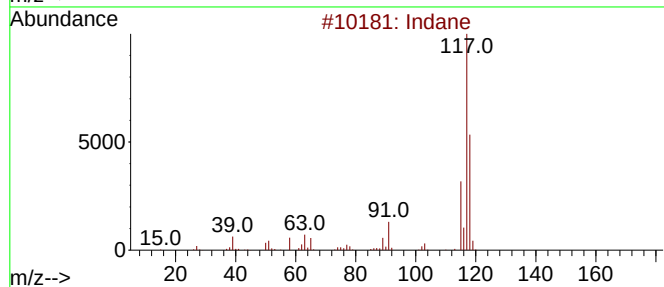
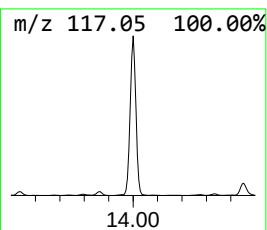
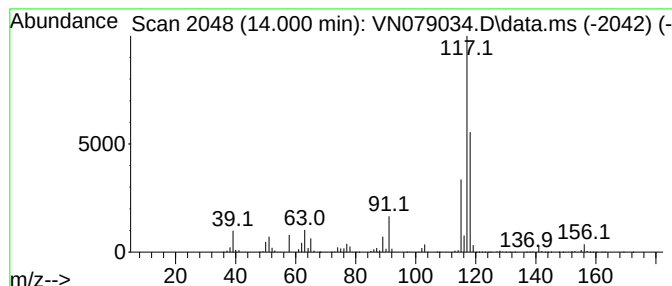
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081523W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	767.75 ug/l	21993400	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72
3			Deltacyclene	118	C9H10	007785-10-6	68
4			Benzene, 1-(chloromethyl)-3-ethe...	152	C9H9Cl	039833-65-3	53
5			Benzene, 1-(chloromethyl)-4-ethe...	152	C9H9Cl	001592-20-7	53



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

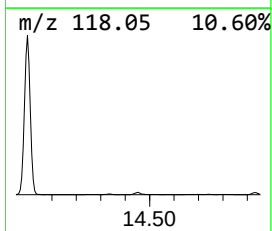
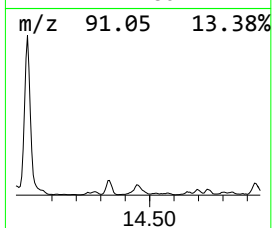
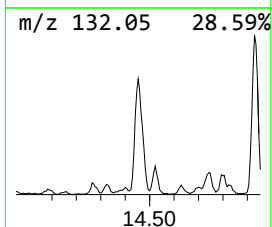
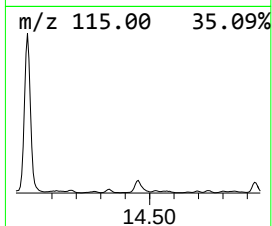
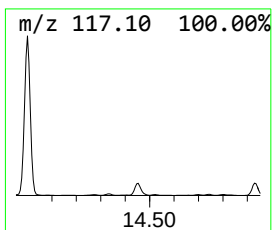
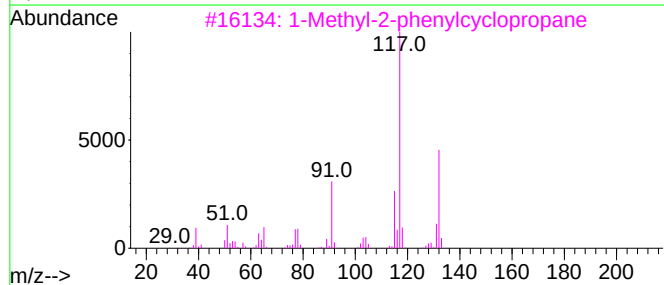
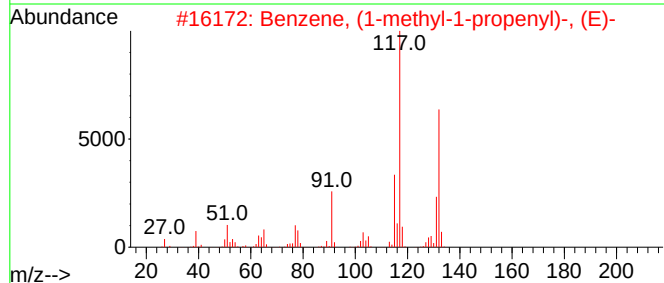
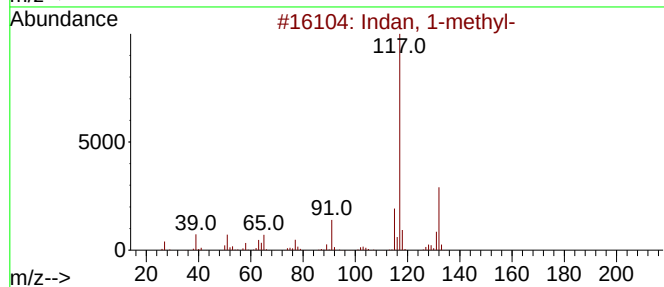
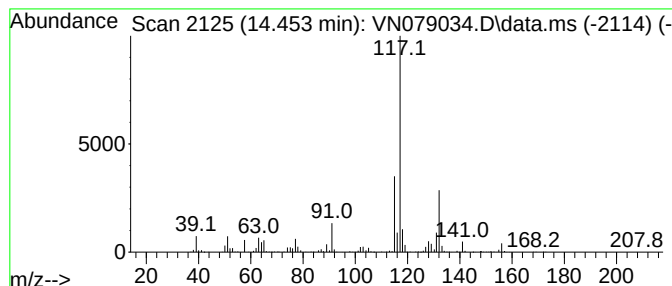
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Quant Title : SW846 8260

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

Peak Number 4 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.453	78.81 ug/l	2257790	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86



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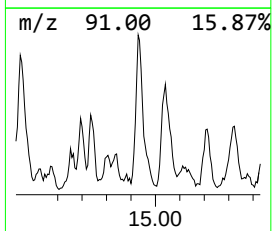
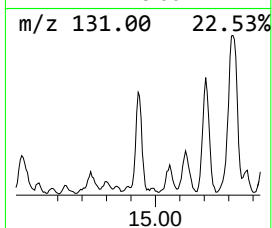
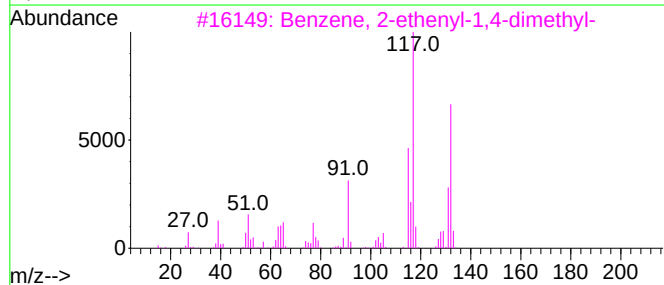
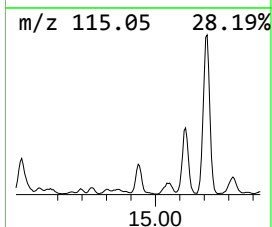
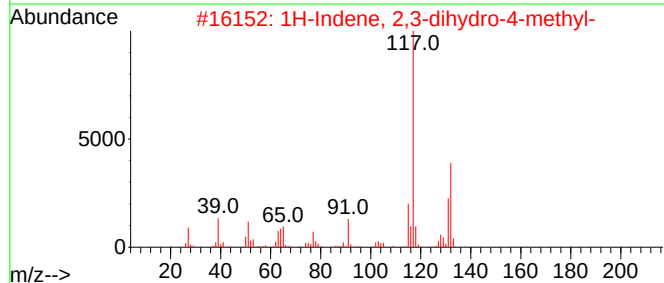
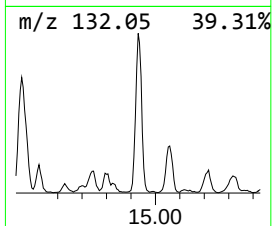
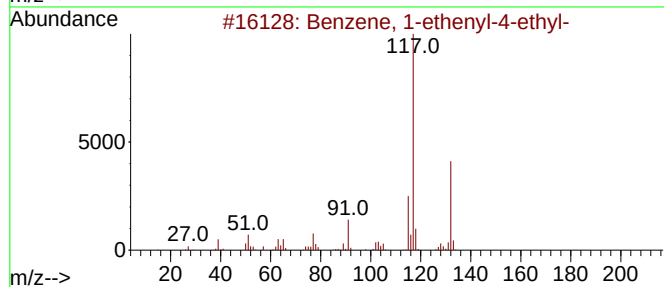
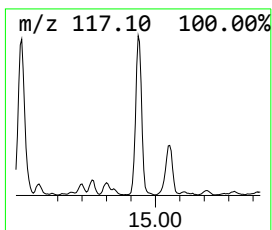
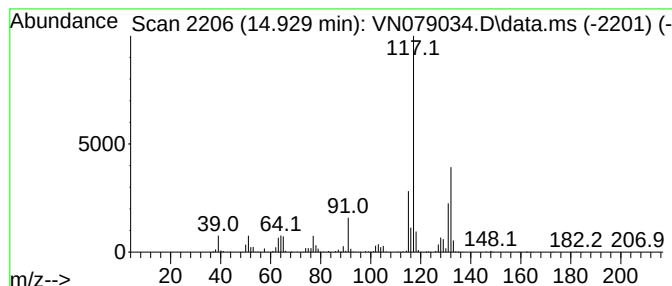
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	65.40 ug/l	1873530	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			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	92
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



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Operator : JC\MD
Sample : 04093-01 20X
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

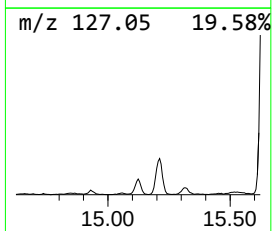
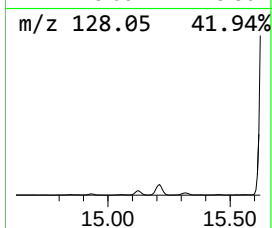
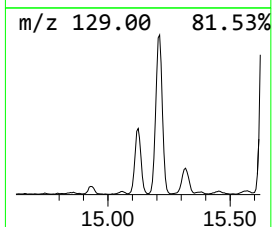
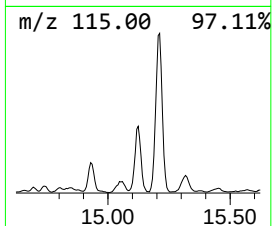
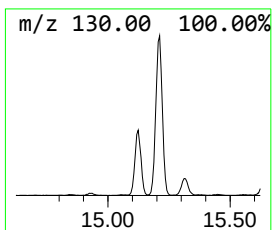
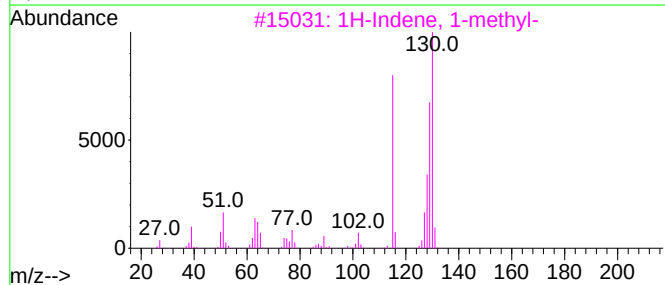
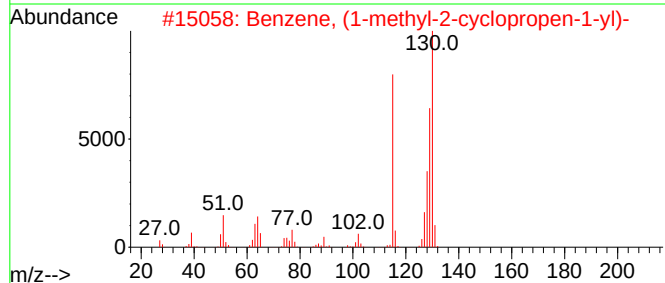
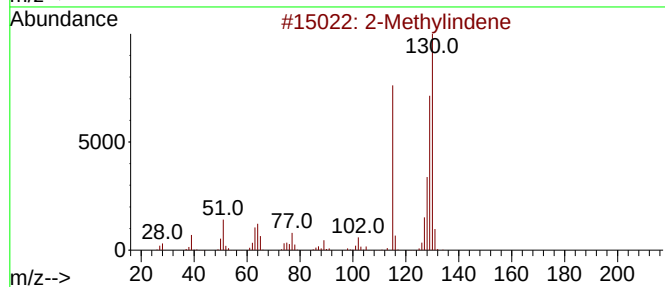
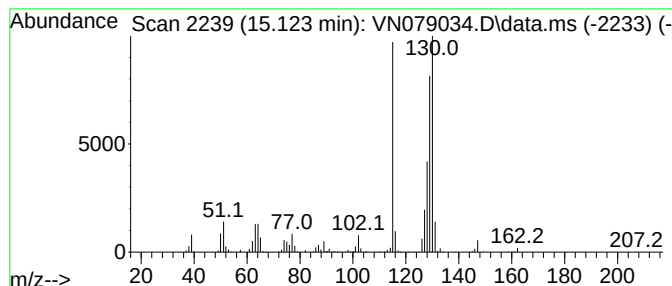
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Quant Title : SW846 8260

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

Peak Number 6 2-Methylindene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	65.04 ug/l	1863150	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	97
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			Benzene, 1-butynyl-	130	C10H10	000622-76-4	94
5			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079034.D
Acq On : 24 Aug 2023 16:18
Operator : JC\MD
Sample : 04093-01 20X
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

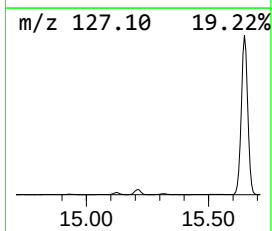
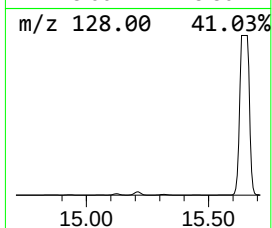
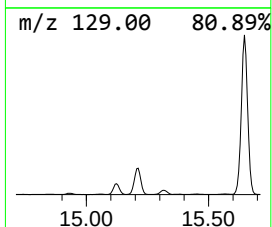
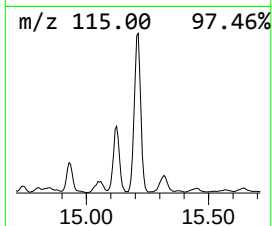
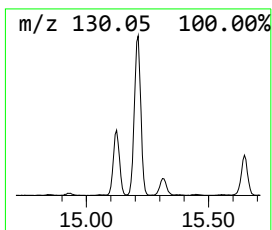
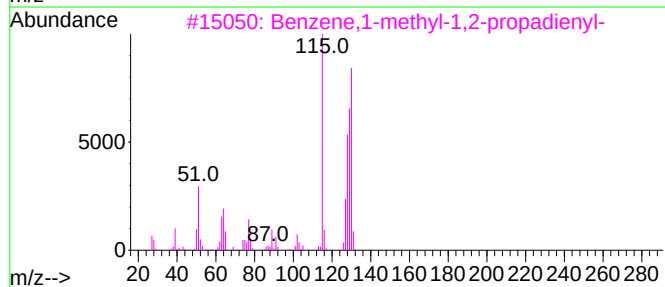
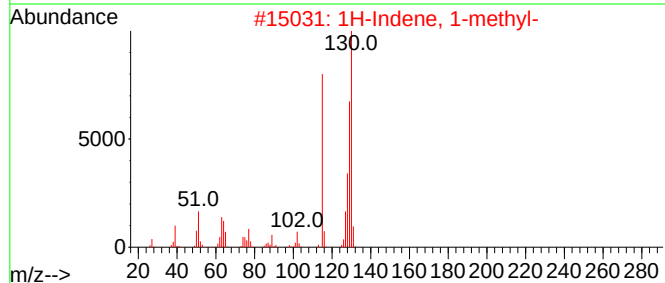
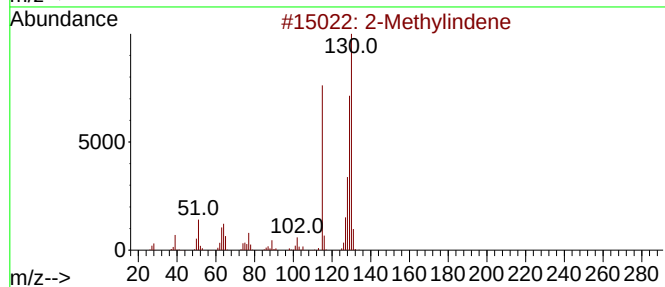
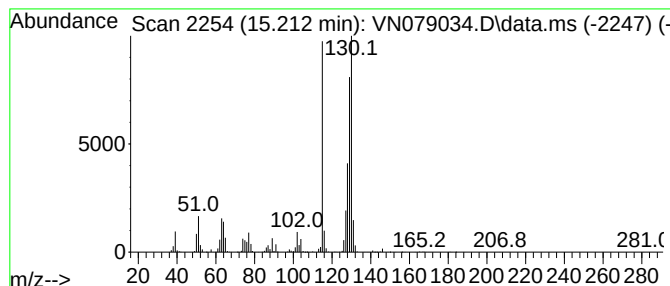
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	152.40 ug/l	4365630	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	96
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
4			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	94
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 : VN079034.D
Acq On : 24 Aug 2023 16:18
Operator : JC\MD
Sample : 04093-01 20X
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

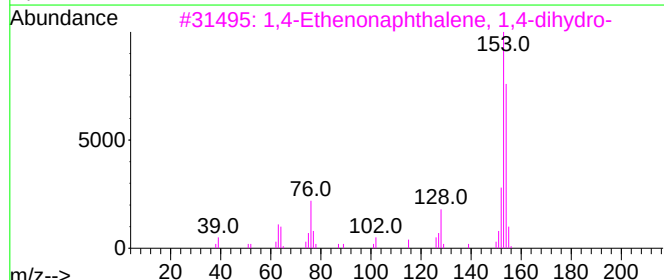
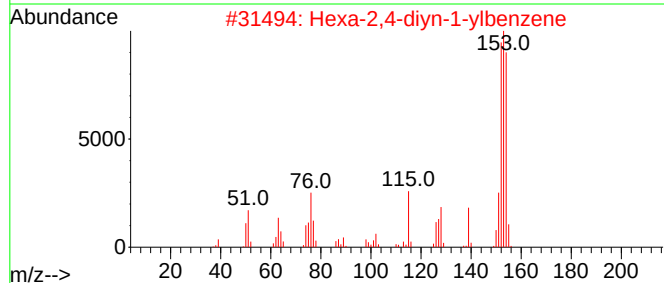
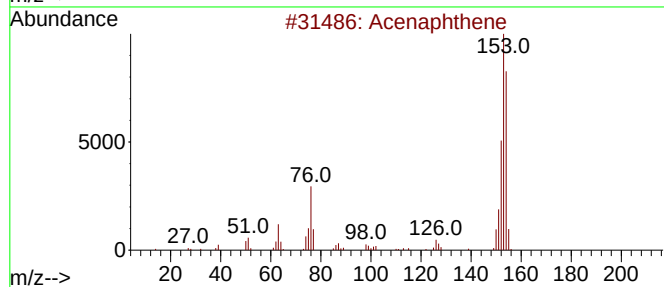
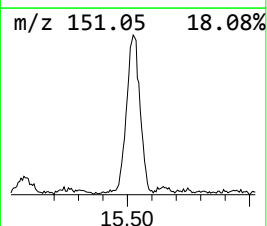
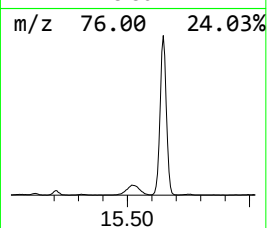
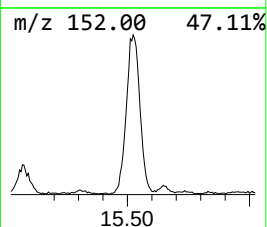
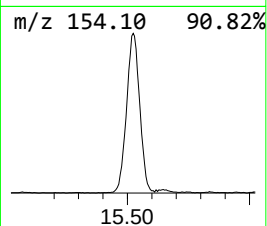
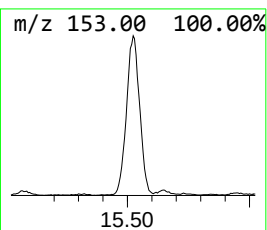
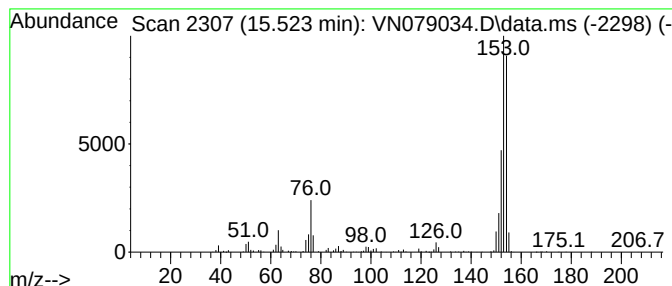
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Quant Title : SW846 8260

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

Peak Number 8 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.523	104.80 ug/l	3002220	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	89
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
3			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079034.D
Acq On : 24 Aug 2023 16:18
Operator : JC\MD
Sample : 04093-01 20X
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

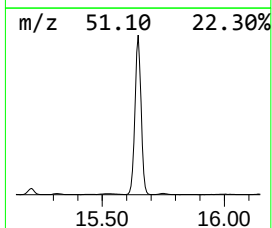
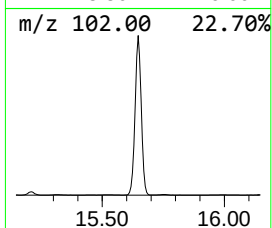
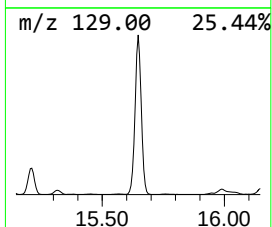
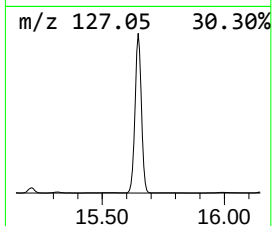
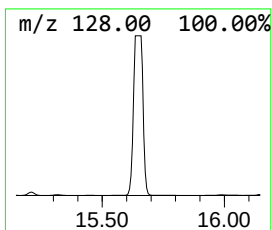
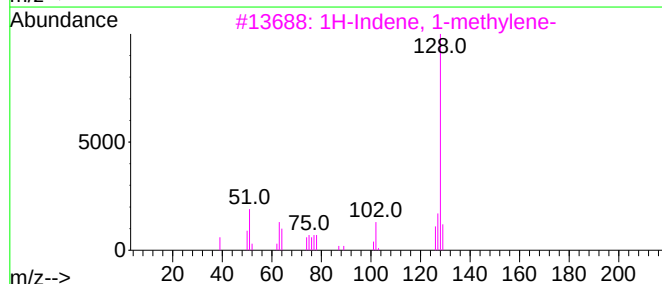
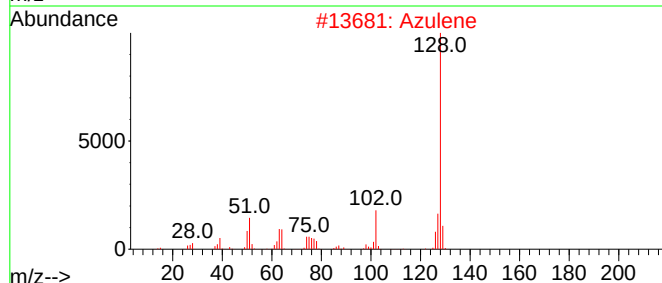
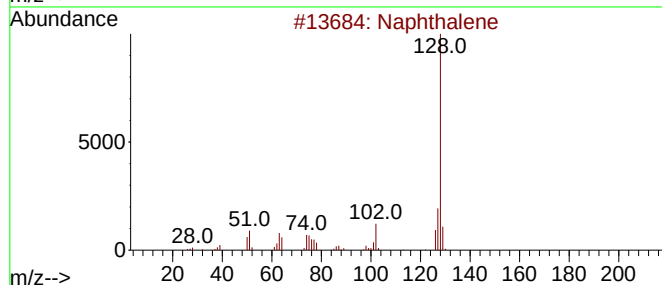
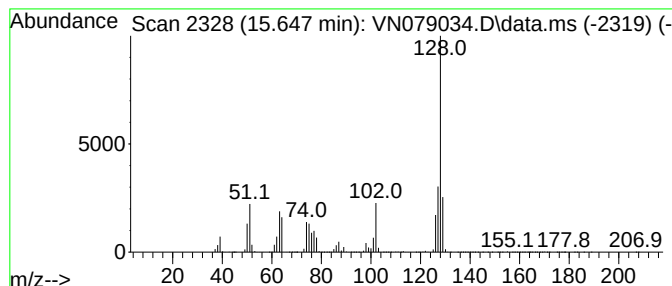
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Quant Title : SW846 8260

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	2551.65 ug/l	73096600	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	89
2			Azulene	128	C10H8	000275-51-4	87
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	64
5			4-Phenylbut-3-ene-1-yne	128	C10H8	100022-12-0	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079034.D
Acq On : 24 Aug 2023 16:18
Operator : JC\MD
Sample : 04093-01 20X
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

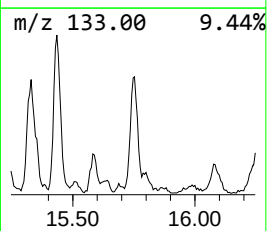
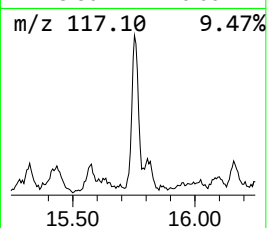
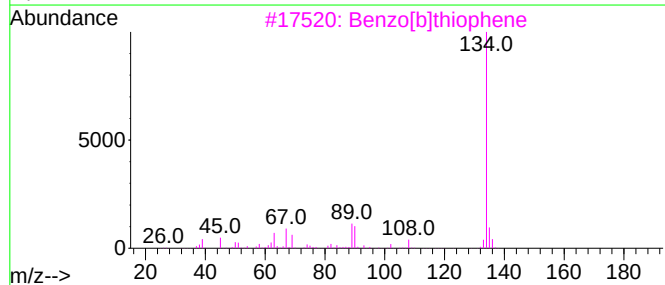
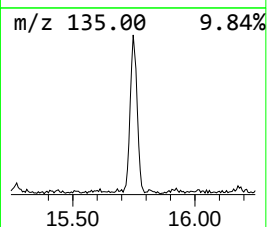
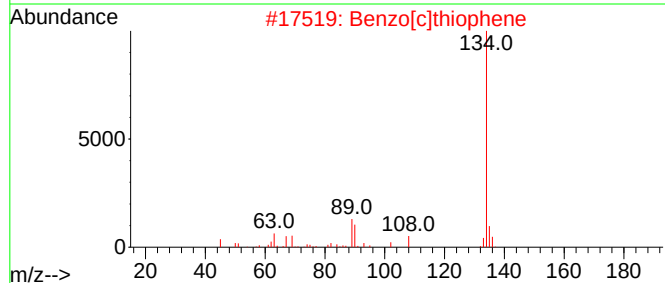
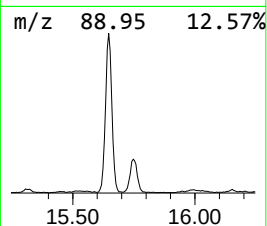
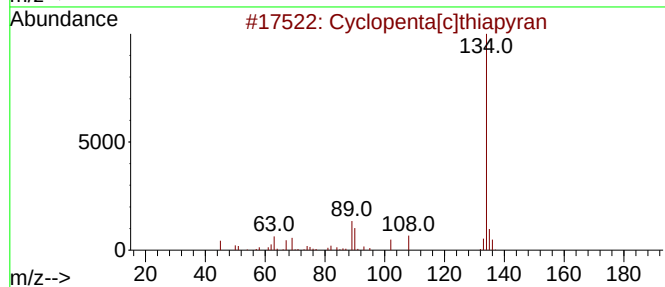
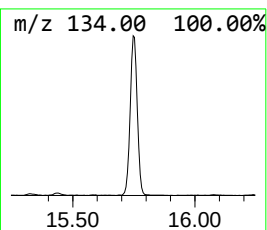
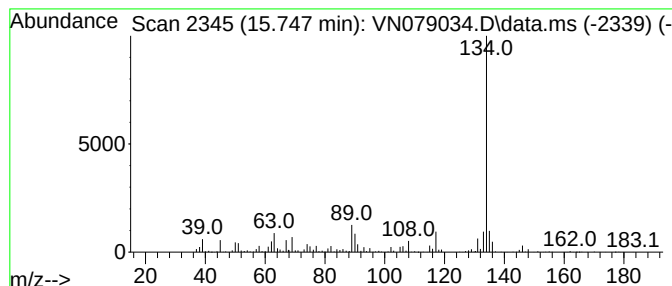
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Quant Title : SW846 8260

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

Peak Number 10 Cyclopenta[c]thiapyran Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.747	73.49 ug/l	2105280	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	90
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	87
3			Benzo[b]thiophene	134	C8H6S	000095-15-8	81
4			5-Phenyl-1,2,3-thiadiazole	162	C8H6N2S	018212-29-8	64
5			Phenol, 4-(2-propenyl)-	134	C9H10O	000501-92-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN082423\
Data File : VN079034.D
Acq On : 24 Aug 2023 16:18
Operator : JC\MD
Sample : 04093-01 20X
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NEVINS-SB04-Z45-46

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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Naphthalene, 1,...	13.676	95.9	ug/l	2746260	4	13.794	1432340	50.0
Indane	14.000	767.8	ug/l	21993400	4	13.794	1432340	50.0
Indan, 1-methyl-	14.453	78.8	ug/l	2257790	4	13.794	1432340	50.0
Benzene, 1-ethe...	14.929	65.4	ug/l	1873530	4	13.794	1432340	50.0
2-Methylindene	15.123	65.0	ug/l	1863150	4	13.794	1432340	50.0
1H-Indene, 1-me...	15.212	152.4	ug/l	4365630	4	13.794	1432340	50.0
Hexa-2,4-diyne-1...	15.523	104.8	ug/l	3002220	4	13.794	1432340	50.0
Azulene	15.647	2551.7	ug/l	73096600	4	13.794	1432340	50.0
Cyclopenta[c]th...	15.747	73.5	ug/l	2105280	4	13.794	1432340	50.0