

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
 Data File : VN074958.D
 Acq On : 21 Oct 2022 13:47
 Operator : JC\MD
 Sample : N5222-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-12

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\82N102022W.M

Title : SW846 8260

Signal : TIC: VN074958.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.106	1189	1199	1213	rBV	1323105	2790363	1.01%	0.243%
2	10.565	1438	1447	1454	rBV	3823414	7393236	2.67%	0.643%
3	11.865	1662	1668	1675	rBV	2291651	4262862	1.54%	0.371%
4	11.965	1678	1685	1695	rVV	27191469	44951292	16.24%	3.907%
5	12.076	1696	1704	1722	rVB	1532228	3362273	1.21%	0.292%
6	12.400	1749	1759	1768	rBV	1907349	3452985	1.25%	0.300%
7	12.694	1802	1809	1825	rVB	9816856	16735144	6.04%	1.455%
8	12.847	1825	1835	1847	rBV	2944455	5240157	1.89%	0.455%
9	13.035	1859	1867	1873	rBV	10117721	16140582	5.83%	1.403%
10	13.129	1873	1883	1887	rVV	6223245	11020250	3.98%	0.958%
11	13.176	1887	1891	1897	rVB	7538313	11756545	4.25%	1.022%
12	13.335	1911	1918	1927	rBV	20000605	33093872	11.95%	2.877%
13	13.482	1931	1943	1949	rBV2	56151219	94258626	34.05%	8.193%
14	13.676	1970	1976	1981	rBV	3231115	5114710	1.85%	0.445%
15	13.735	1981	1986	1991	rBV2	2084715	3229113	1.17%	0.281%
16	13.823	1991	2001	2006	rBV	25356012	48201296	17.41%	4.190%
17	13.953	2016	2023	2025	rBV	7118031	11247883	4.06%	0.978%
18	13.994	2025	2030	2043	rVB4	58273988	111714935	40.35%	9.711%
19	14.182	2055	2062	2067	rVB2	2115046	3810361	1.38%	0.331%
20	14.247	2067	2073	2075	rBV	4061660	6753700	2.44%	0.587%
21	14.270	2075	2077	2082	rVV2	3912779	5591264	2.02%	0.486%
22	14.329	2082	2087	2094	rVV	7597227	12612814	4.56%	1.096%
23	14.447	2101	2107	2117	rVB	30921513	56119174	20.27%	4.878%
24	14.576	2123	2129	2134	rBV	2509145	3912749	1.41%	0.340%
25	14.653	2134	2142	2145	rBV	4640083	7692246	2.78%	0.669%
26	14.694	2145	2149	2154	rVV	10031095	14967765	5.41%	1.301%
27	14.794	2161	2166	2170	rBV2	2027115	3624394	1.31%	0.315%
28	14.929	2182	2189	2200	rVB	19083187	32206101	11.63%	2.799%
29	15.035	2200	2207	2215	rBV2	16776717	38555703	13.93%	3.351%
30	15.117	2215	2221	2229	rVV	19004855	33499180	12.10%	2.912%
31	15.206	2229	2236	2245	rVV	56011640	101708683	36.74%	8.841%
32	15.312	2246	2254	2261	rVV	10043841	20756573	7.50%	1.804%
33	15.447	2269	2277	2286	rVB4	1930160	4897948	1.77%	0.426%
34	15.576	2288	2299	2302	rBV6	1063519	3064325	1.11%	0.266%
35	15.647	2302	2311	2323	rVV3	134124728	276855928	100.00%	24.065%
36	15.753	2323	2329	2352	rVB5	1281403	4422812	1.60%	0.384%

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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\82N102022W.M
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37	15.988	2365	2369	2384	rVV	1812771	6612965	2.39%	0.575%
38	16.147	2384	2396	2401	rVV	3496217	8530243	3.08%	0.741%
39	16.200	2401	2405	2410	rVV	2508138	5579499	2.02%	0.485%
40	16.282	2410	2419	2436	rVB2	4663120	16942008	6.12%	1.473%
41	16.576	2462	2469	2485	rVB	2229443	6236926	2.25%	0.542%
42	16.782	2496	2504	2505	rBV	27406546	41531993	15.00%	3.610%

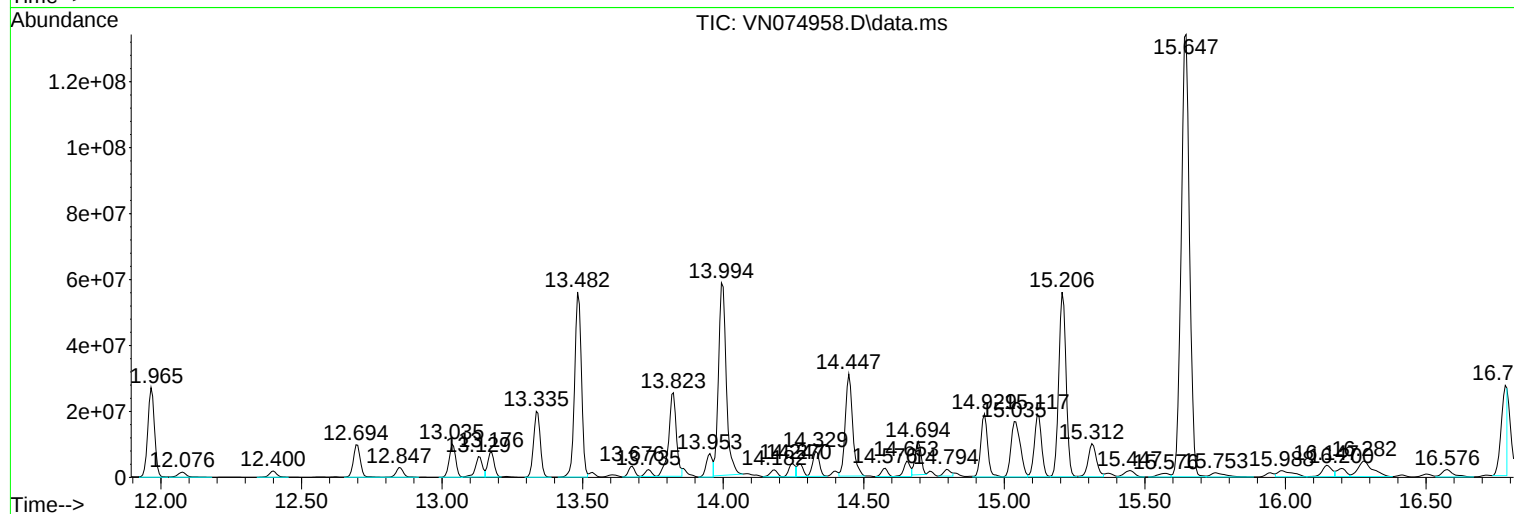
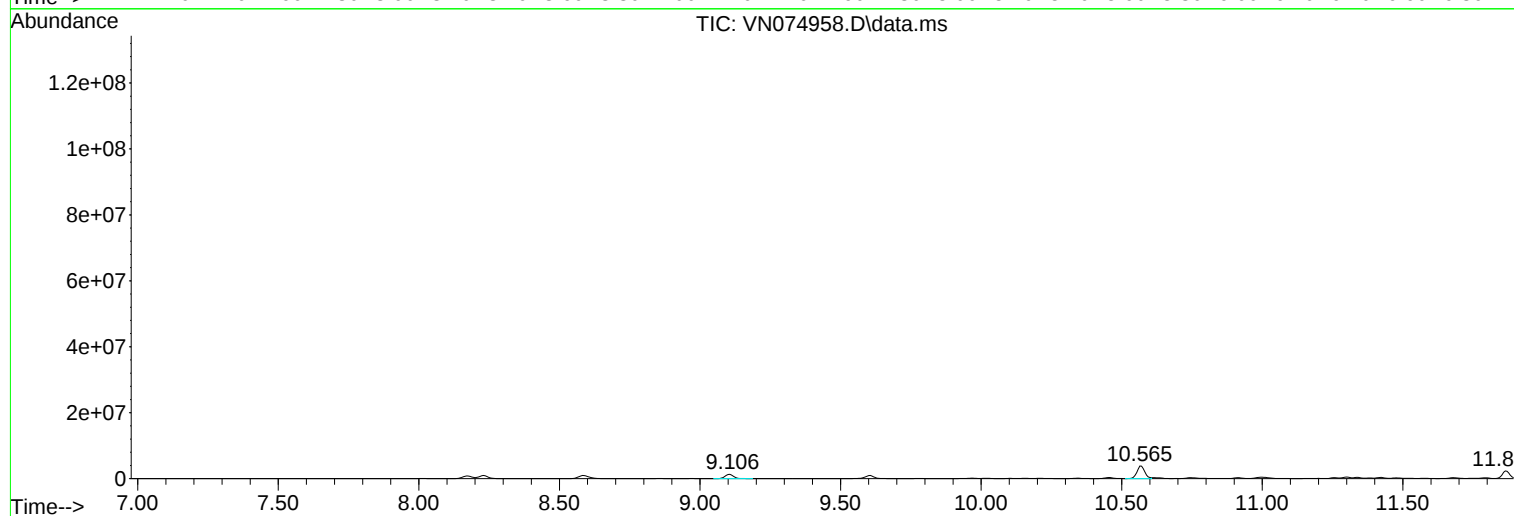
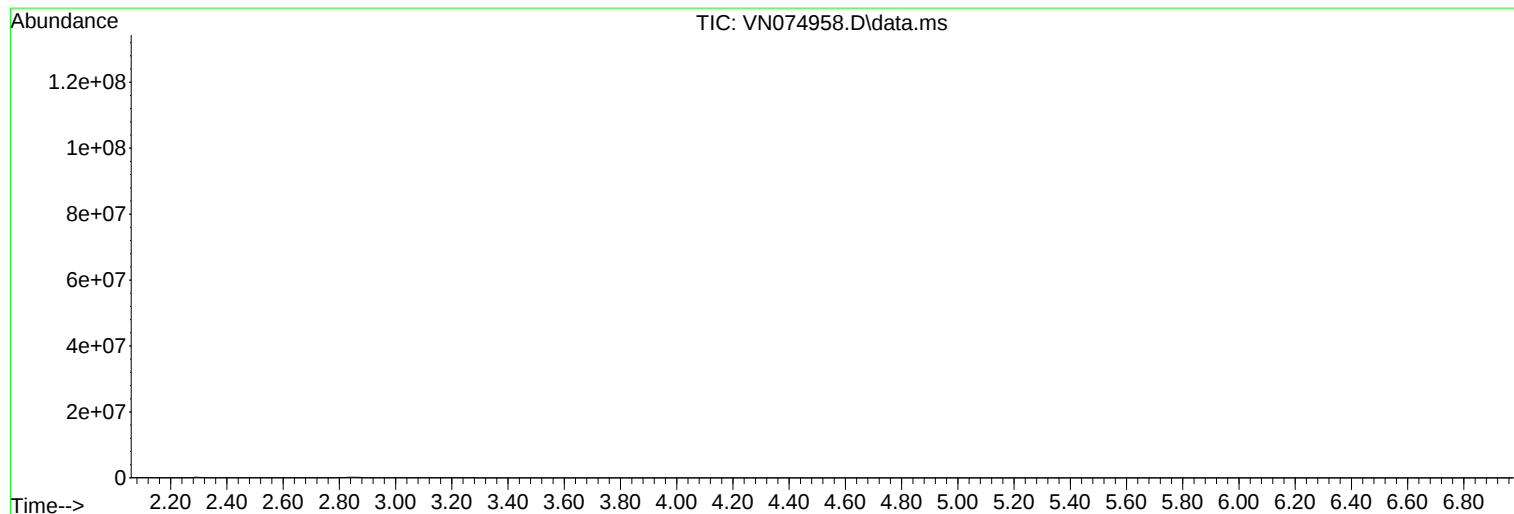
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

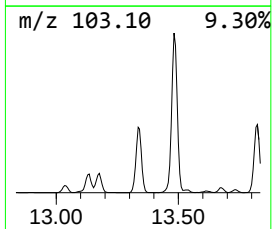
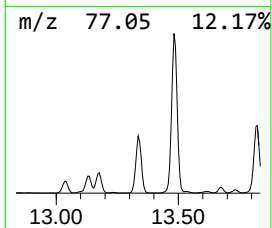
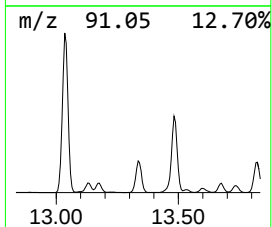
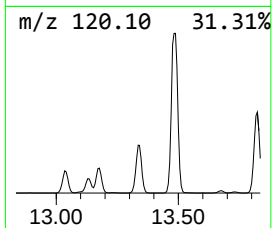
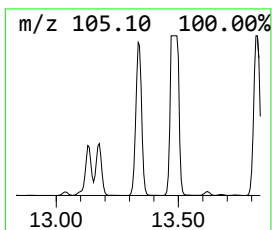
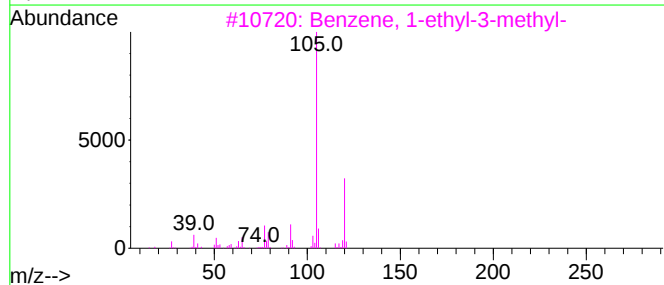
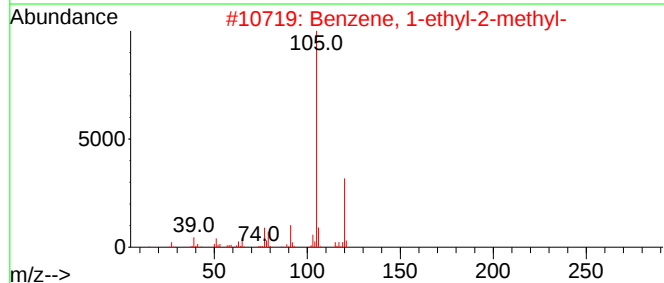
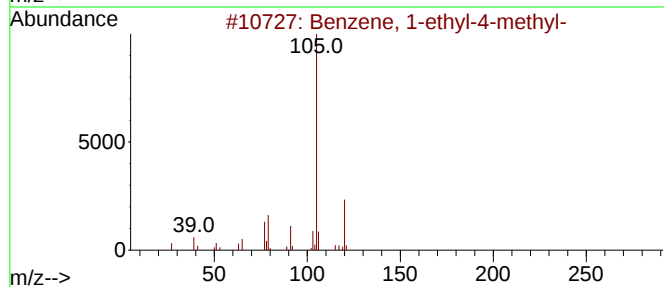
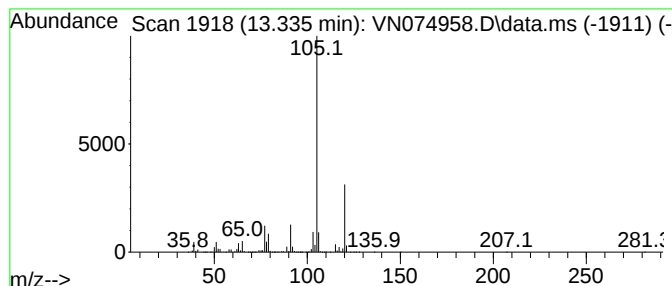
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	34.33 ug/l	33093900	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

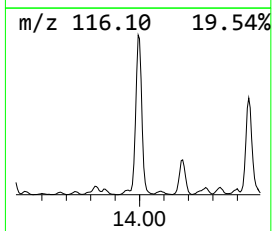
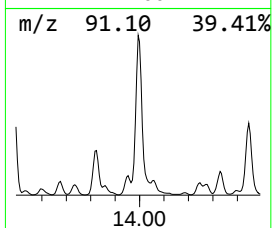
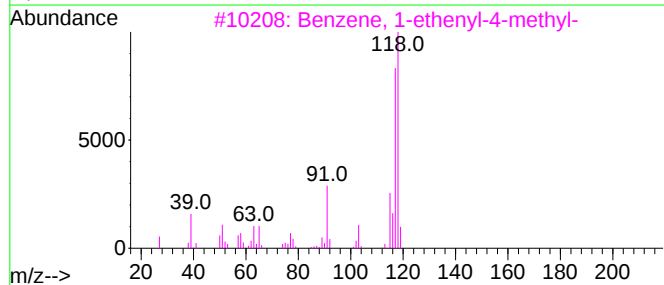
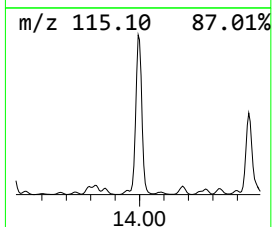
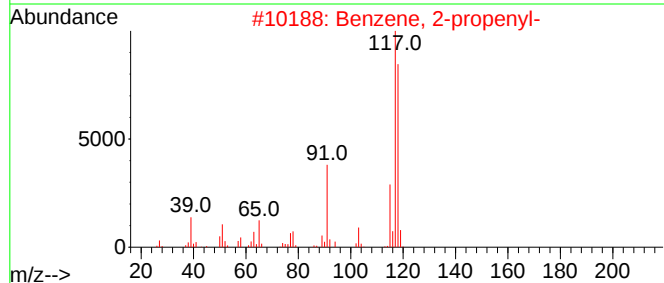
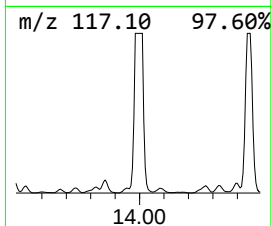
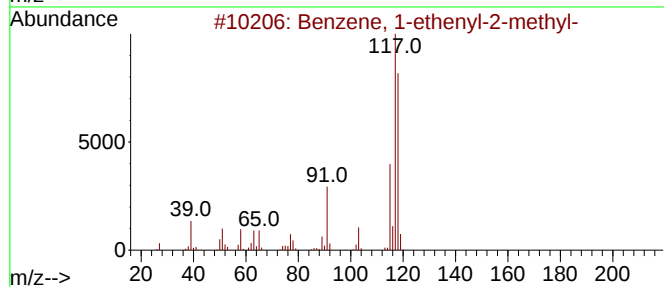
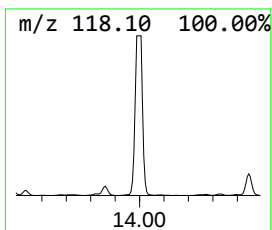
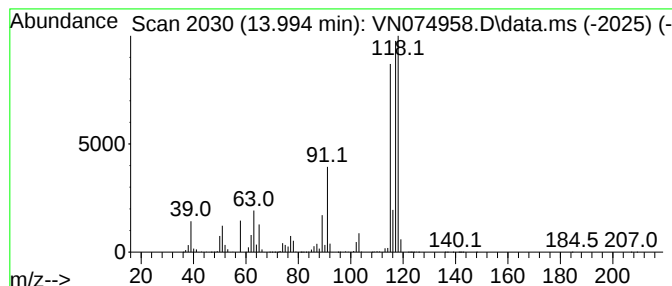
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethenyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	115.88 ug/l	111715000	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	58
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	52
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	52
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	52



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Instrument :
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ClientSampleId :
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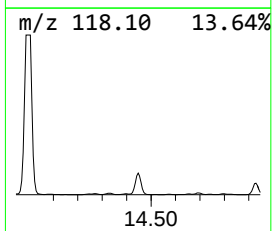
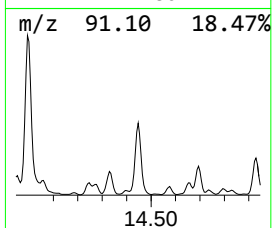
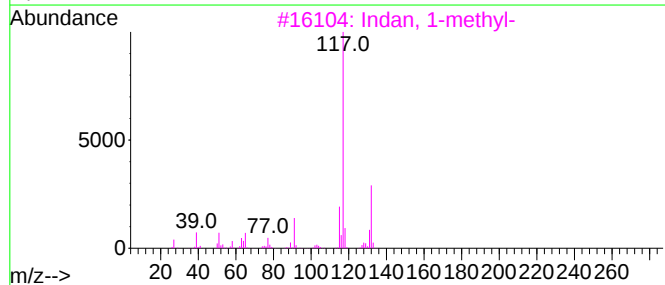
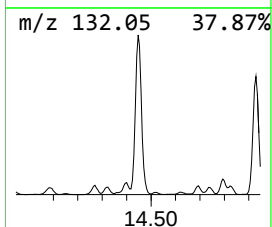
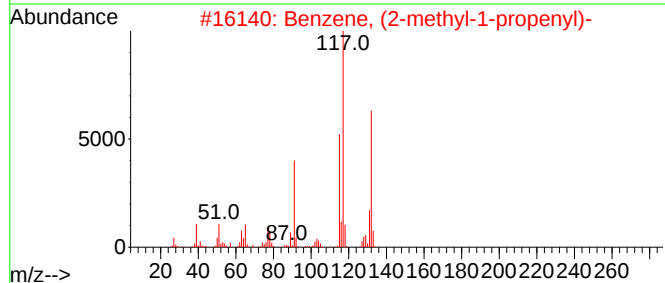
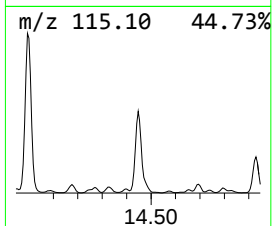
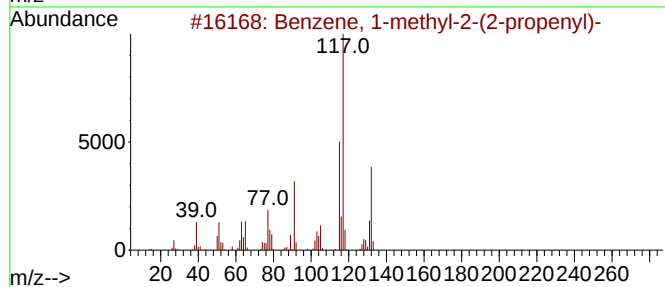
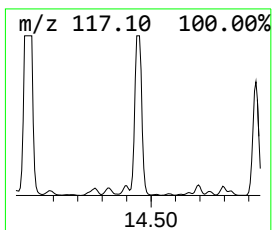
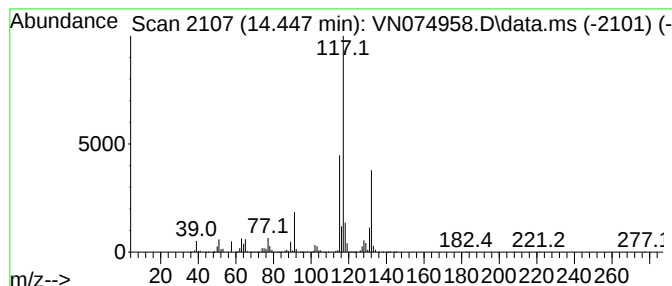
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-methyl-2-(2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	58.21 ug/l	56119200	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3			Indan, 1-methyl-	132	C10H12	000767-58-8	87
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	83
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83



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ClientSampleId :
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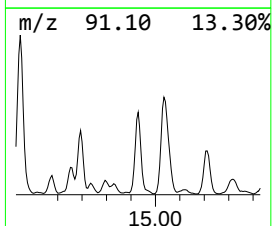
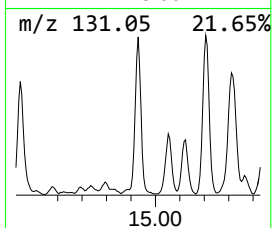
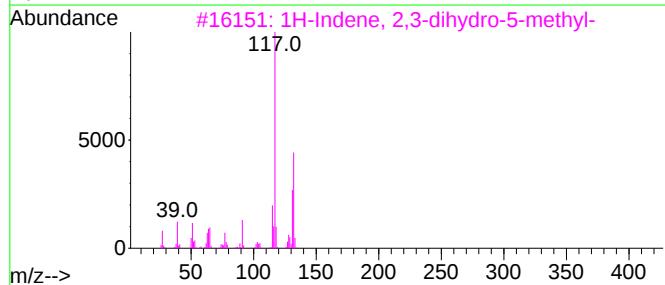
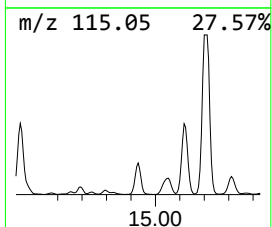
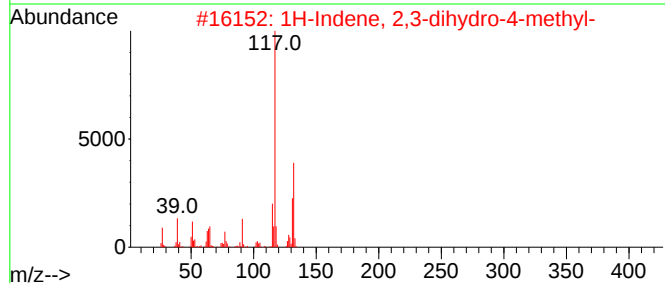
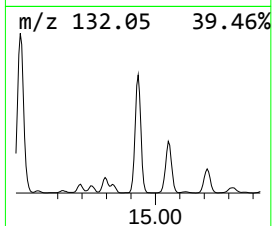
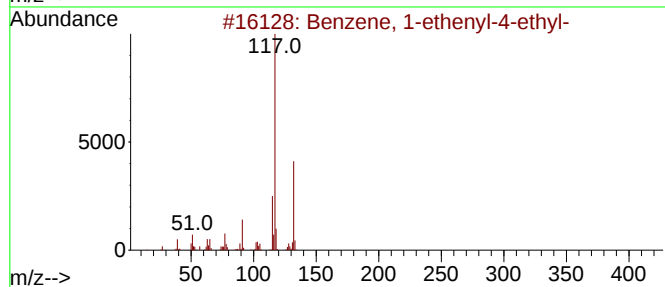
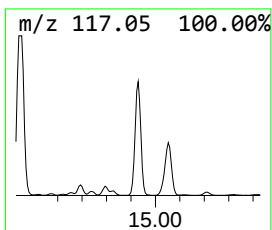
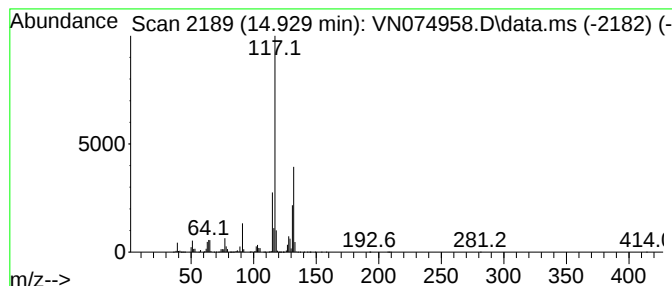
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	33.41 ug/l	32206100	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			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



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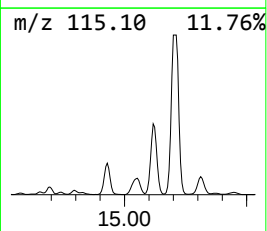
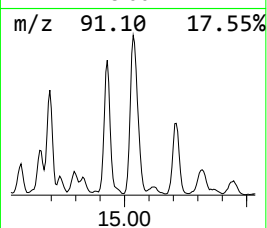
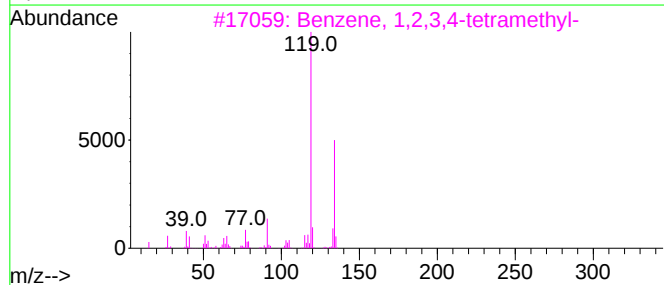
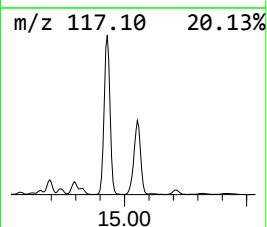
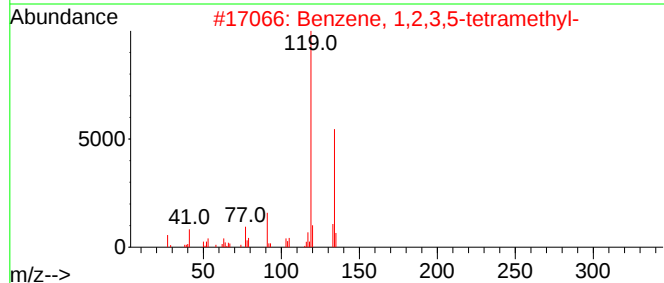
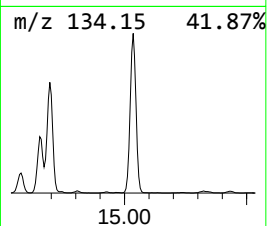
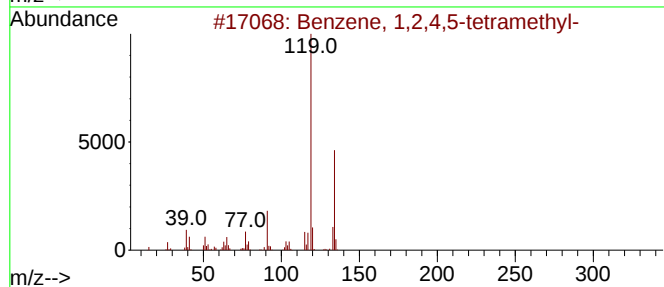
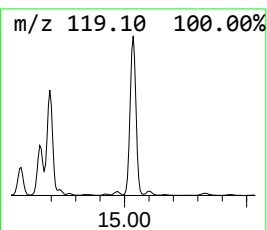
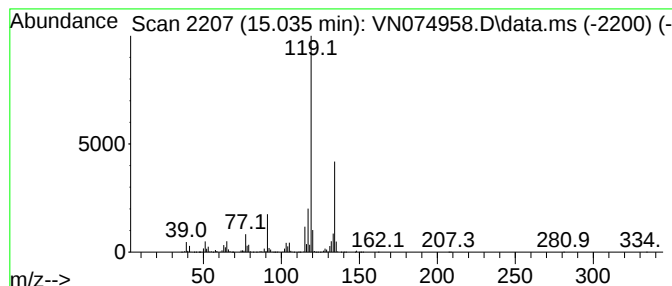
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	39.99 ug/l	38555700	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	94
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	93
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90
5			p-Cymene	134	C10H14	000099-87-6	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074958.D
Acq On : 21 Oct 2022 13:47
Operator : JC\MD
Sample : N5222-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

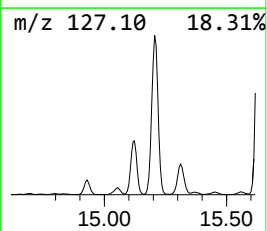
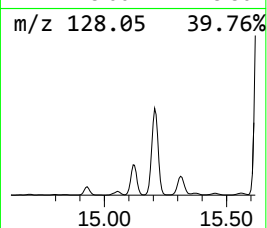
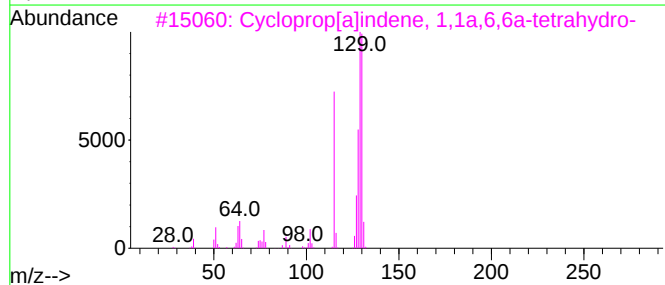
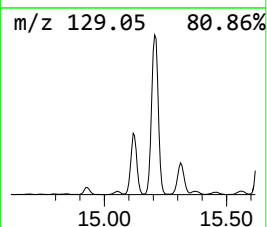
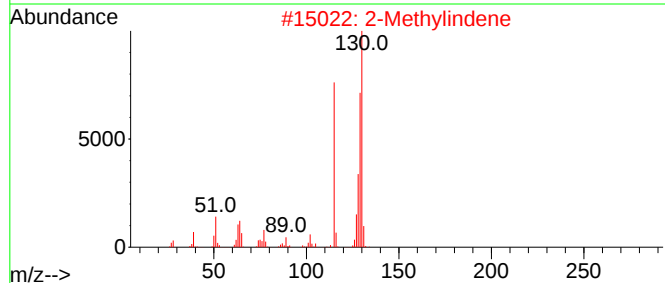
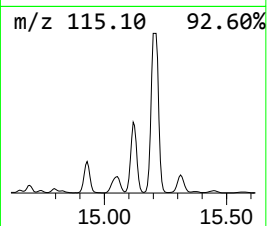
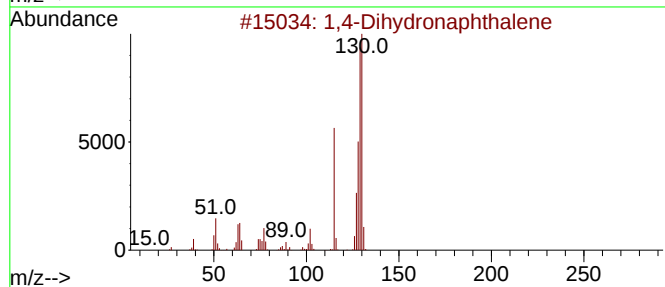
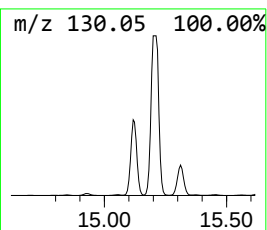
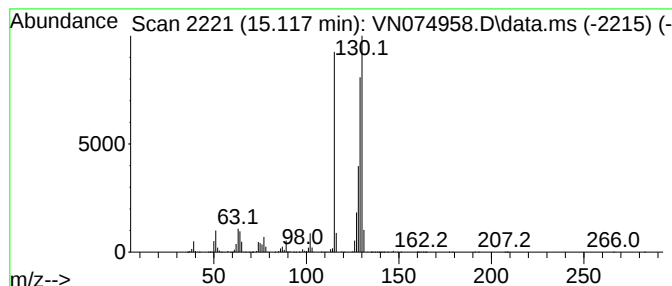
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Quant Title : SW846 8260

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

Peak Number 6 1,4-Dihydronaphthalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.117	34.75 ug/l	33499200	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
2			2-Methylindene	130	C10H10	002177-47-1	94
3			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	93
5			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074958.D
Acq On : 21 Oct 2022 13:47
Operator : JC\MD
Sample : N5222-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

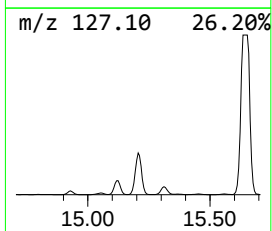
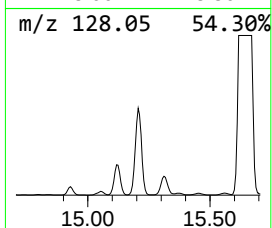
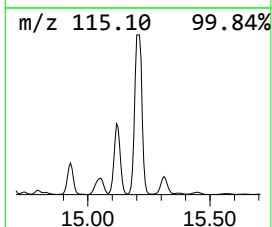
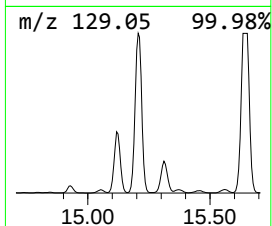
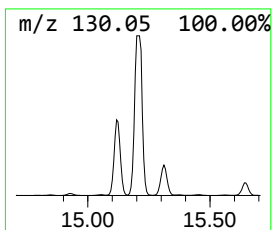
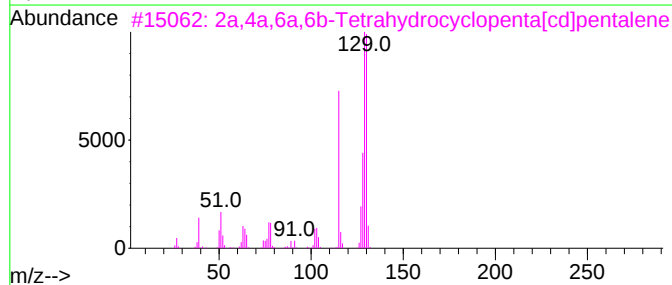
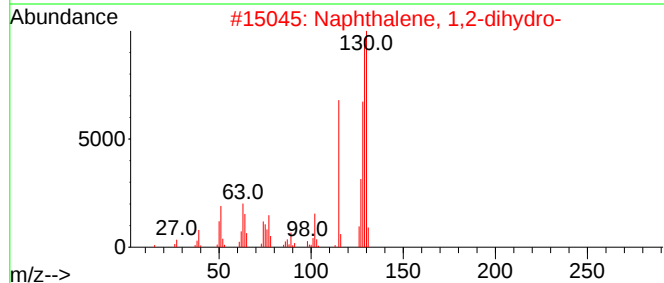
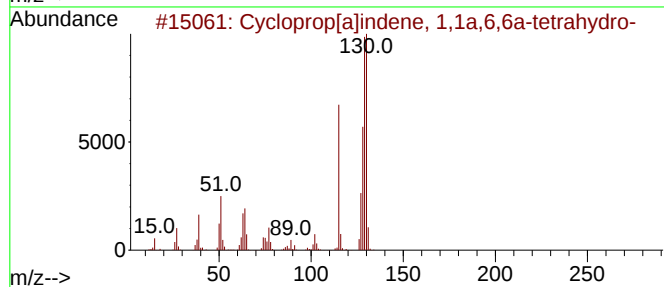
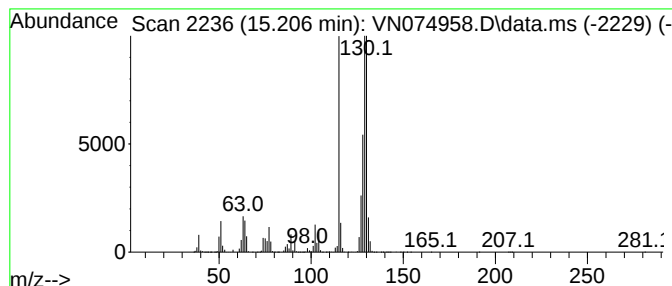
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Quant Title : SW846 8260

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

Peak Number 7 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	105.50 ug/l	101709000	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	97
2			Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	93
3			2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	91
4			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	91
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074958.D
Acq On : 21 Oct 2022 13:47
Operator : JC\MD
Sample : N5222-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

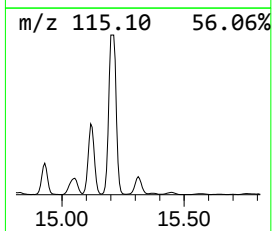
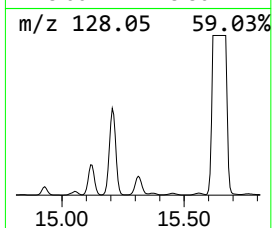
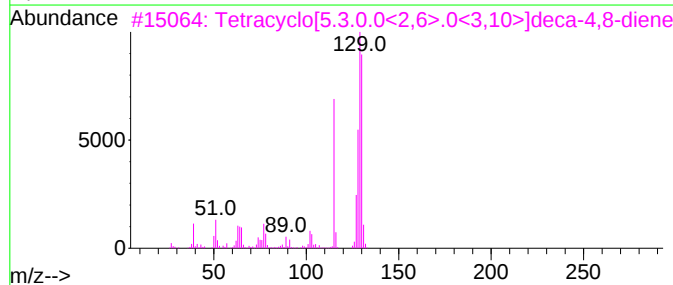
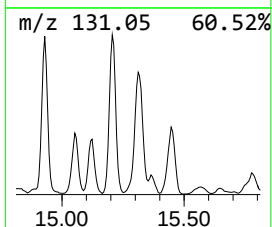
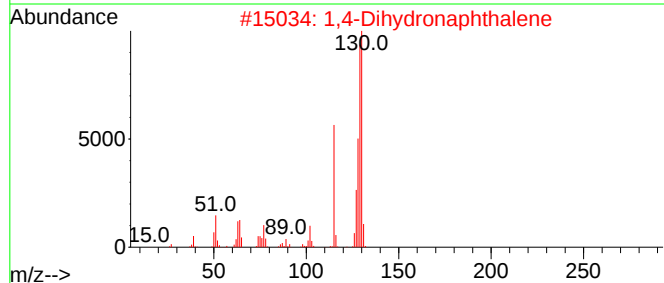
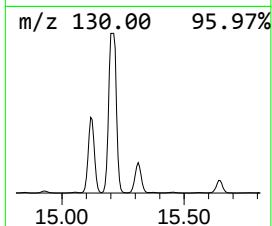
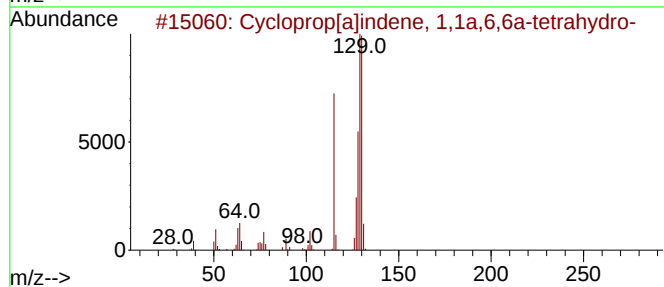
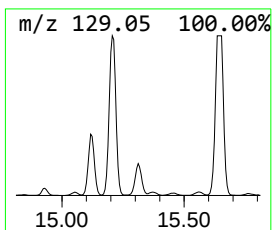
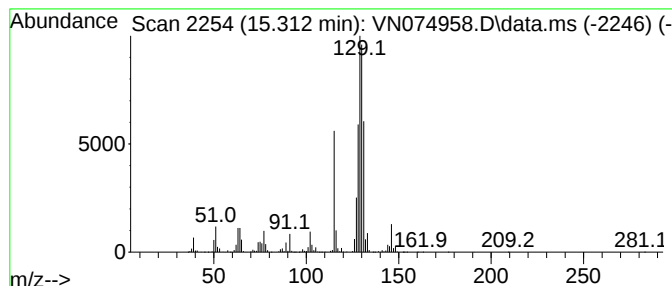
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Quant Title : SW846 8260

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

Peak Number 8 Tetracyclo[5.3.0.0<2,6>.0<3... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.312	21.53 ug/l	20756600	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	95
2			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93
3			Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	86
4			2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	70
5			Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074958.D
Acq On : 21 Oct 2022 13:47
Operator : JC\MD
Sample : N5222-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

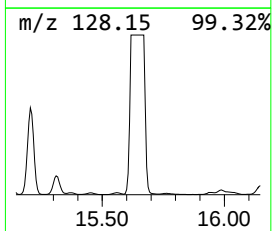
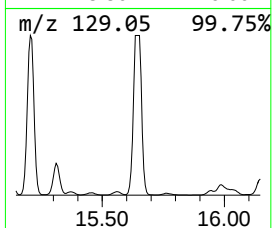
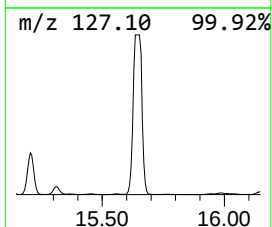
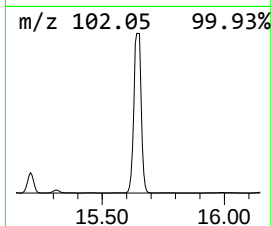
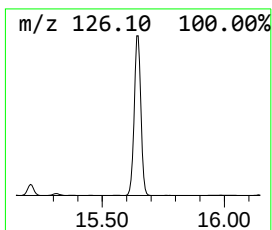
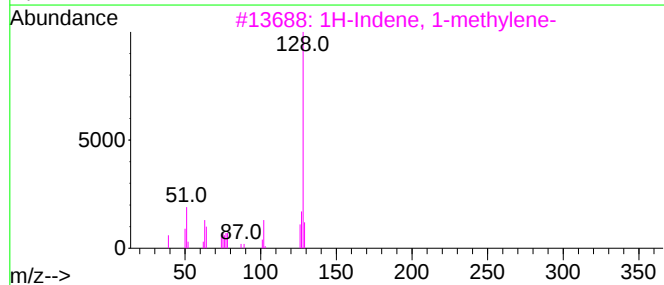
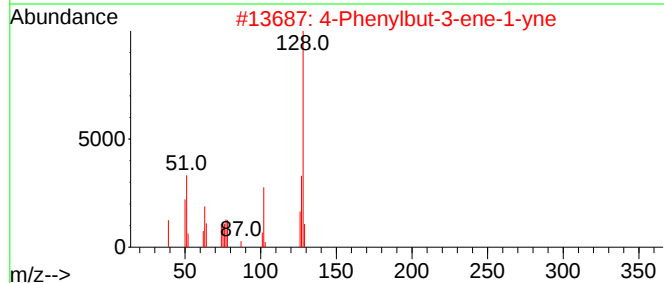
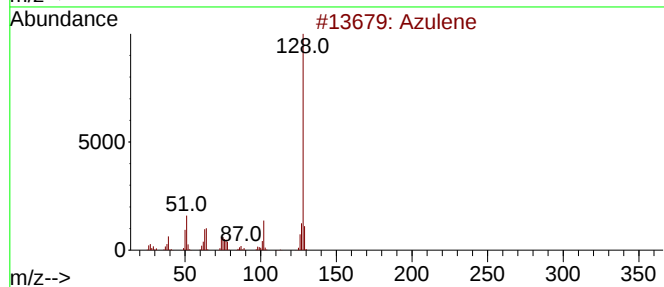
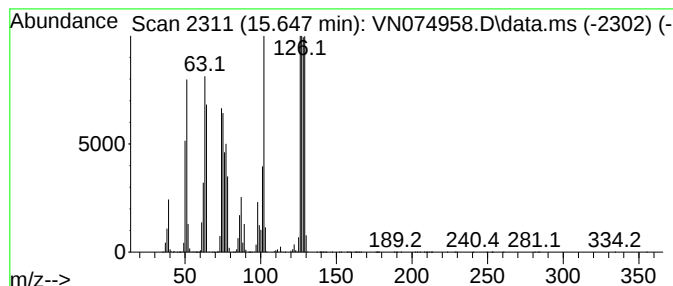
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Quant Title : SW846 8260

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

Peak Number 9 4-Phenylbut-3-ene-1-yne Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	287.19 ug/l	276856000	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	96
2			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	89
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	86
4			Naphthalene	128	C10H8	000091-20-3	86
5			Isoquinoline	129	C9H7N	000119-65-3	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074958.D
Acq On : 21 Oct 2022 13:47
Operator : JC\MD
Sample : N5222-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

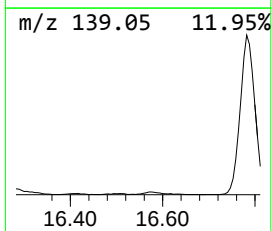
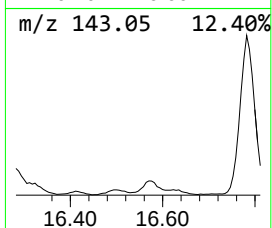
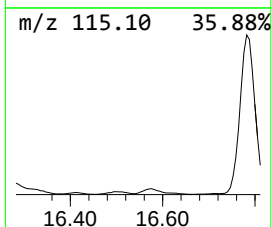
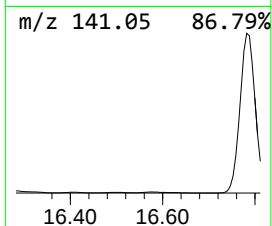
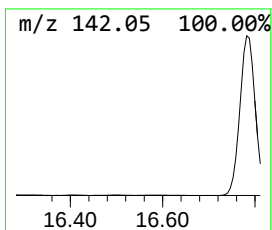
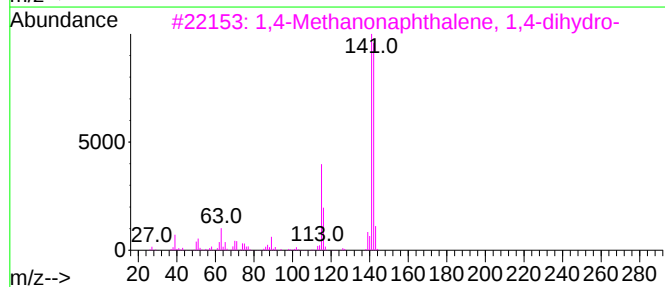
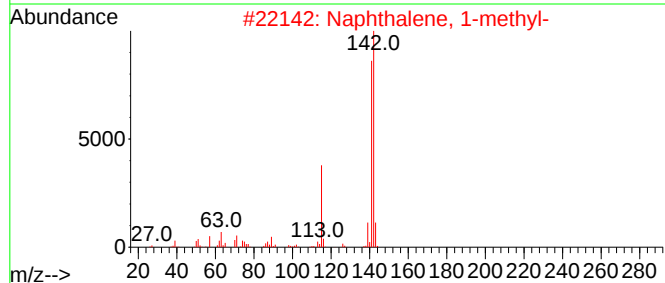
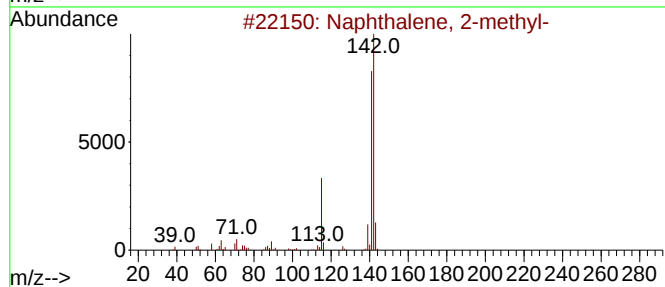
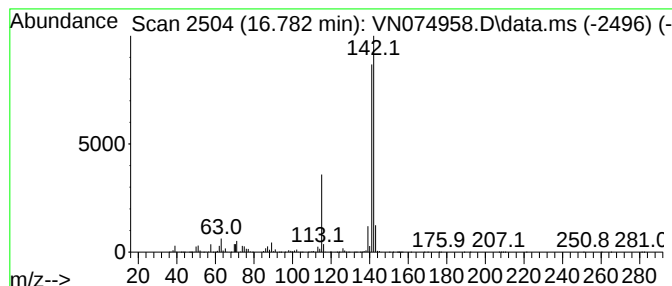
Instrument :
MSVOA_N
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.782	43.08 ug/l	41532000	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5	Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
Data File : VN074958.D
Acq On : 21 Oct 2022 13:47
Operator : JC\MD
Sample : N5222-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.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, 1-ethe...	13.994	115.9	ug/l	111715000	4	13.794	48201300	50.0
Benzene, 1-meth...	14.447	58.2	ug/l	56119200	4	13.794	48201300	50.0
Benzene, 1-ethe...	14.929	33.4	ug/l	32206100	4	13.794	48201300	50.0
Benzene, 1,2,4,...	15.035	40.0	ug/l	38555700	4	13.794	48201300	50.0
1,4-Dihydronaph...	15.117	34.8	ug/l	33499200	4	13.794	48201300	50.0
Cycloprop[a]ind...	15.206	105.5	ug/l	101709000	4	13.794	48201300	50.0
Tetracyclo[5.3....	15.312	21.5	ug/l	20756600	4	13.794	48201300	50.0
4-Phenylbut-3-e...	15.647	287.2	ug/l	276856000	4	13.794	48201300	50.0
1,4-Methanonaph...	16.782	43.1	ug/l	41532000	4	13.794	48201300	50.0