

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
 Data File : VN075352.D
 Acq On : 21 Nov 2022 19:30
 Operator : JC\MD
 Sample : N5557-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-14

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\82N112122W.M
 Title : SW846 8260

Signal : TIC: VN075352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	34	40	49	rBV	16113	40556	1.87%	0.184%
2	2.824	123	131	133	rBV3	14132	30110	1.39%	0.137%
3	4.436	395	405	418	rBV	34469	106302	4.91%	0.484%
4	8.053	1013	1020	1029	rBB3	10501	23953	1.11%	0.109%
5	8.171	1030	1040	1044	rBV2	70526	166044	7.66%	0.755%
6	8.230	1044	1050	1063	rVB2	181262	418575	19.32%	1.904%
7	8.606	1102	1114	1129	rVB2	160415	456506	21.07%	2.077%
8	8.965	1169	1175	1187	rVB2	13462	31560	1.46%	0.144%
9	9.100	1190	1198	1210	rBV	266646	539551	24.90%	2.454%
10	9.600	1274	1283	1289	rVB3	12013	26027	1.20%	0.118%
11	10.447	1420	1427	1433	rBV	22148	40245	1.86%	0.183%
12	10.565	1439	1447	1454	rBV	174651	323874	14.95%	1.473%
13	10.659	1459	1463	1470	rVV2	11569	22620	1.04%	0.103%
14	11.418	1583	1592	1598	rBV4	10698	23879	1.10%	0.109%
15	11.865	1658	1668	1677	rBV	362619	650475	30.02%	2.959%
16	11.965	1677	1685	1695	rVB	670949	1147325	52.95%	5.219%
17	12.394	1747	1758	1763	rBV4	13990	37640	1.74%	0.171%
18	12.694	1802	1809	1817	rVB	154602	256923	11.86%	1.169%
19	12.847	1829	1835	1847	rBV	254073	434075	20.03%	1.975%
20	13.035	1860	1867	1874	rVB	176156	284292	13.12%	1.293%
21	13.335	1911	1918	1925	rBV2	24666	49408	2.28%	0.225%
22	13.429	1925	1934	1938	rVV7	13708	42407	1.96%	0.193%
23	13.482	1938	1943	1954	rVB2	23806	54297	2.51%	0.247%
24	13.617	1959	1966	1971	rVB2	94249	158922	7.33%	0.723%
25	13.729	1980	1985	1990	rVB	27572	41368	1.91%	0.188%
26	13.794	1990	1996	2006	rVB	389356	695838	32.11%	3.165%
27	13.882	2006	2011	2016	rBV	33831	56963	2.63%	0.259%
28	13.953	2016	2023	2025	rBV	179431	266932	12.32%	1.214%
29	13.994	2025	2030	2036	rVV	1371311	2166795	100.00%	9.857%
30	14.117	2045	2051	2057	rVB	127192	205703	9.49%	0.936%
31	14.176	2057	2061	2066	rVB4	16774	25818	1.19%	0.117%
32	14.247	2066	2073	2077	rBV	34424	64353	2.97%	0.293%
33	14.329	2081	2087	2093	rVV	459011	712185	32.87%	3.240%
34	14.400	2093	2099	2102	rVV	155731	289796	13.37%	1.318%
35	14.447	2102	2107	2114	rVB	537211	907351	41.88%	4.128%
36	14.517	2114	2119	2123	rBV3	38256	69784	3.22%	0.317%

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Peak Location: TOP

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37	14.576	2125	2129	2134	rVV2	51247	86128	3.97%	0.392%
38	14.653	2134	2142	2148	rVV	304044	543089	25.06%	2.471%
39	14.735	2152	2156	2160	rVV	67855	90184	4.16%	0.410%
40	14.806	2160	2168	2171	rVV2	43687	87022	4.02%	0.396%
41	14.876	2171	2180	2184	rVV3	65176	181275	8.37%	0.825%
42	14.929	2184	2189	2194	rVV	291465	524215	24.19%	2.385%
43	14.970	2194	2196	2201	rVB	78055	99206	4.58%	0.451%
44	15.053	2201	2210	2215	rBV	614029	1161768	53.62%	5.285%
45	15.106	2215	2219	2226	rVB3	86425	206970	9.55%	0.942%
46	15.211	2230	2237	2243	rBV	657530	1131449	52.22%	5.147%
47	15.317	2244	2255	2260	rVV2	307279	782074	36.09%	3.558%
48	15.364	2260	2263	2268	rVV	152390	269922	12.46%	1.228%
49	15.441	2268	2276	2283	rVB3	320126	795744	36.72%	3.620%
50	15.594	2296	2302	2304	rBV4	32911	60355	2.79%	0.275%
51	15.641	2304	2310	2315	rVV	259280	491462	22.68%	2.236%
52	15.700	2315	2320	2324	rVV	197058	392798	18.13%	1.787%
53	15.747	2324	2328	2331	rVV2	184412	374540	17.29%	1.704%
54	15.782	2331	2334	2354	rVB4	208106	634640	29.29%	2.887%
55	15.947	2354	2362	2370	rBV	188665	406311	18.75%	1.848%
56	16.029	2372	2376	2380	rVV5	18747	35788	1.65%	0.163%
57	16.123	2384	2392	2395	rVV2	160848	373007	17.21%	1.697%
58	16.164	2395	2399	2409	rVV3	233117	550841	25.42%	2.506%
59	16.258	2409	2415	2421	rVV2	74389	169460	7.82%	0.771%
60	16.341	2421	2429	2435	rVV3	121873	336780	15.54%	1.532%
61	16.400	2436	2439	2447	rVB3	55261	110680	5.11%	0.503%
62	16.505	2447	2457	2468	rBV2	284786	694005	32.03%	3.157%
63	16.711	2480	2492	2499	rBV2	140516	386207	17.82%	1.757%
64	16.782	2499	2504	2505	rBV2	95094	138451	6.39%	0.630%

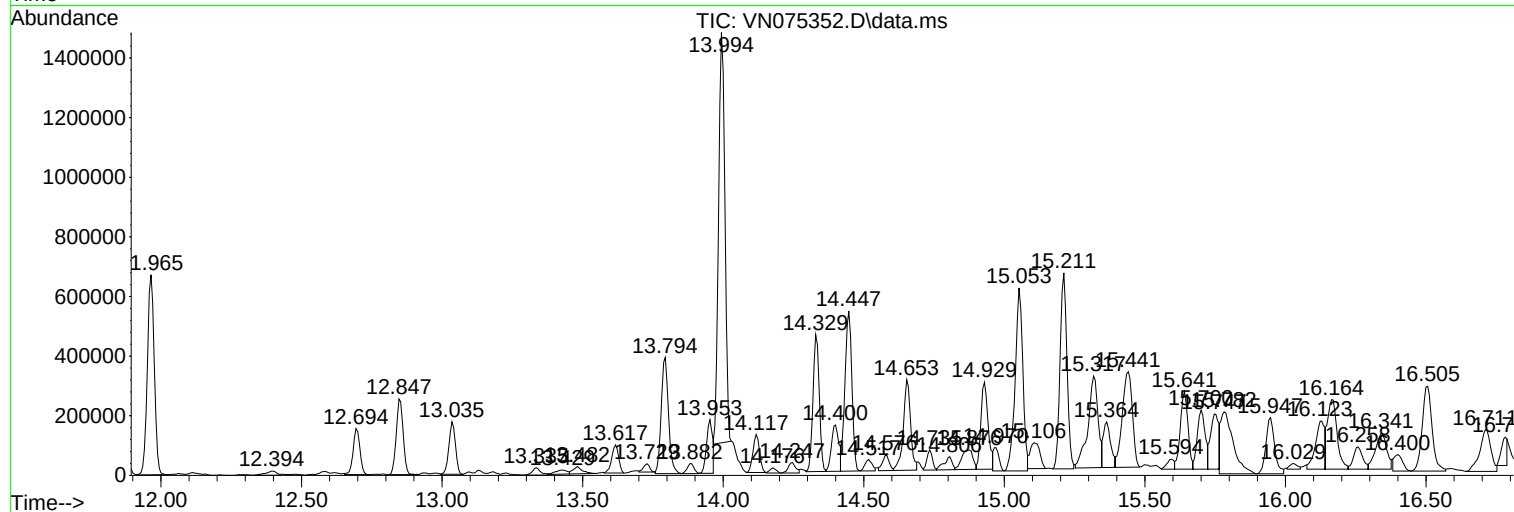
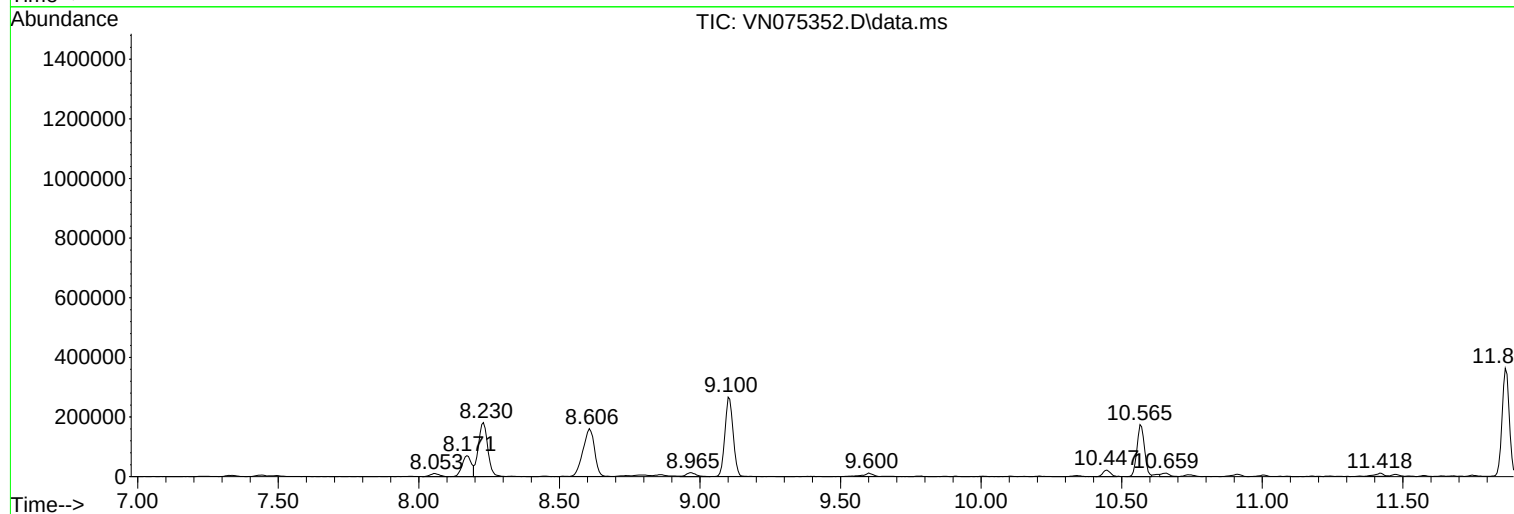
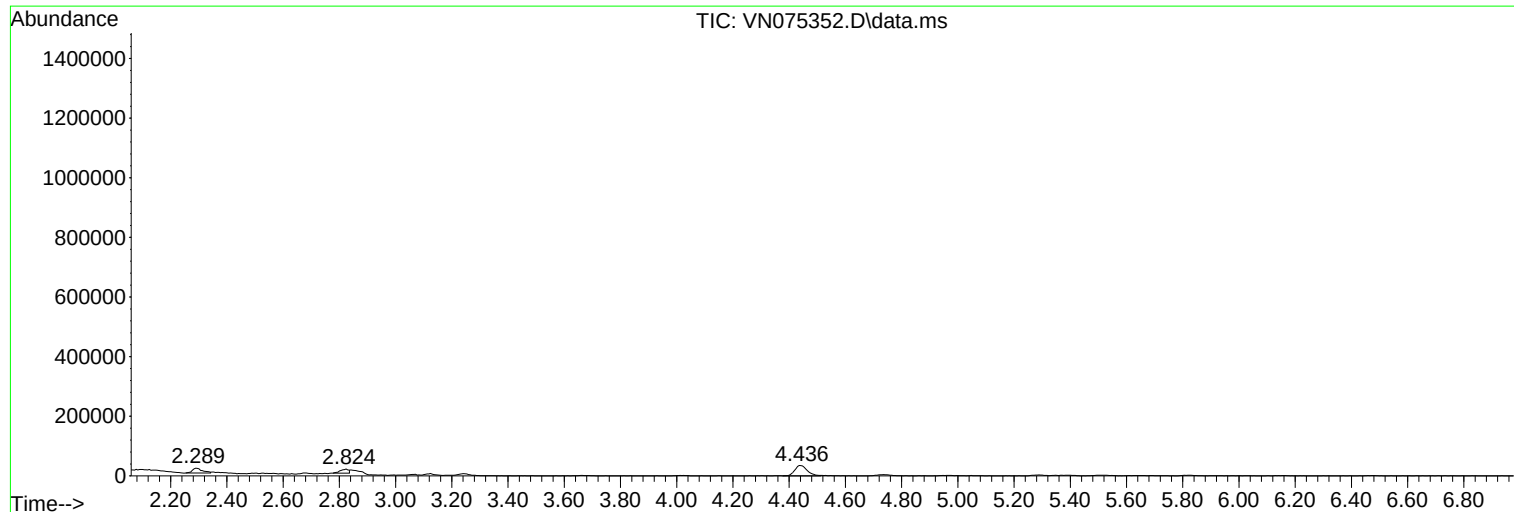
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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Instrument :
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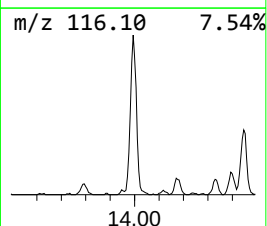
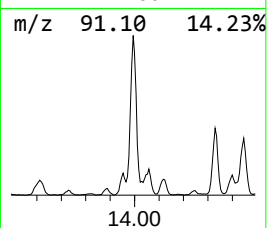
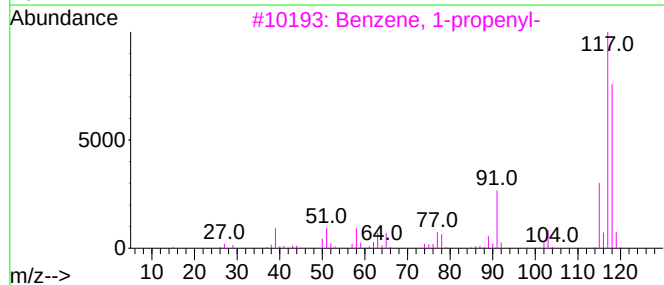
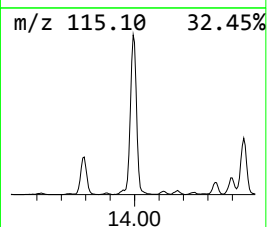
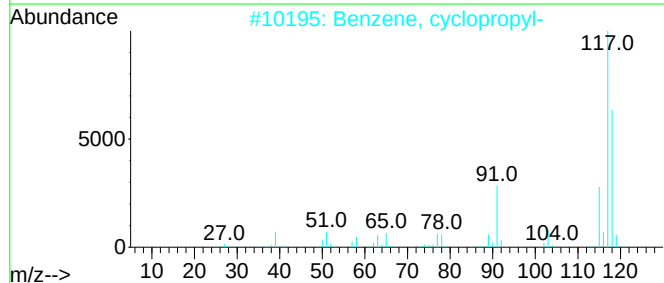
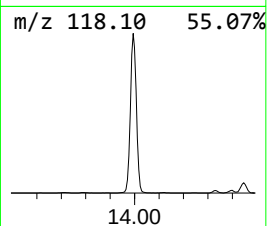
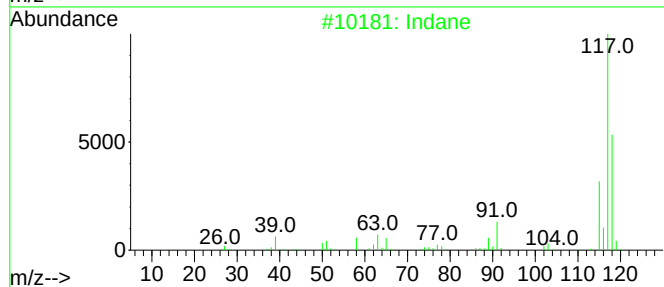
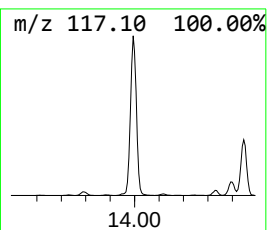
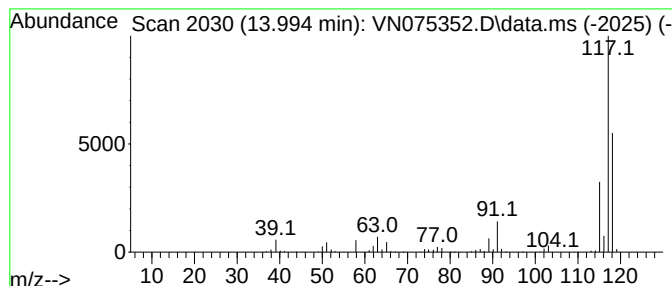
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	155.70 ug/l	2166800	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indane	118	C9H10	000496-11-7	91
2		Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3		Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
4		(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
5		Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59



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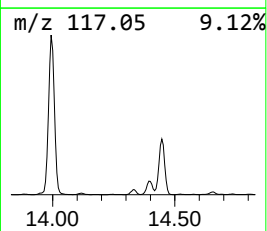
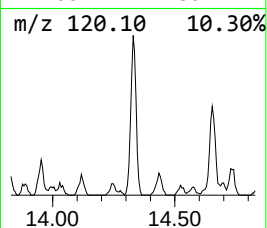
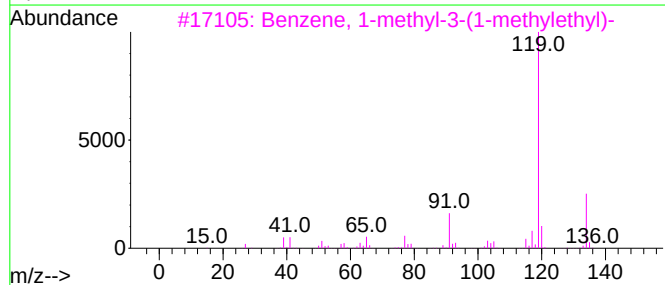
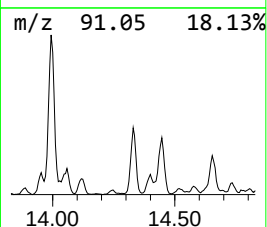
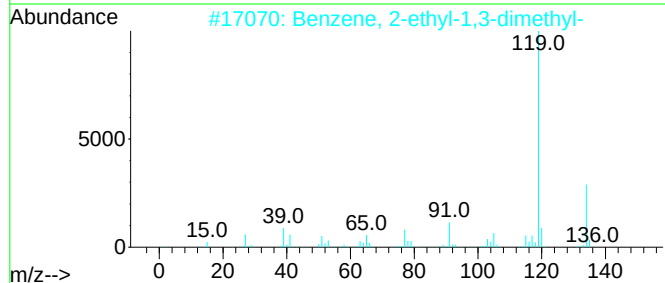
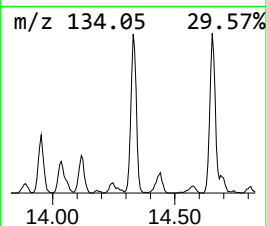
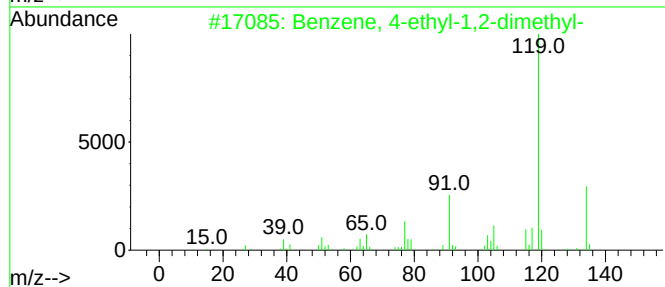
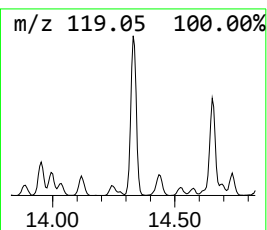
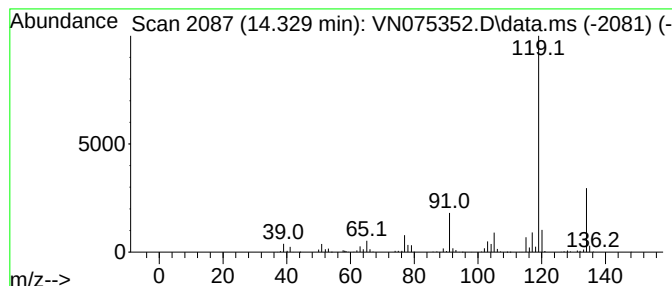
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	51.17 ug/l	712185	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			o-Cymene	134	C10H14	000527-84-4	95



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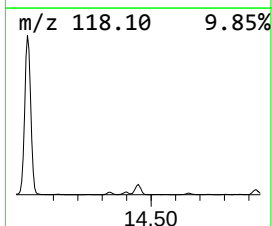
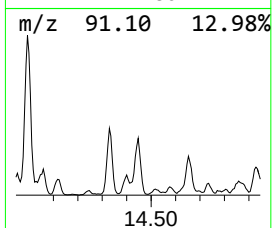
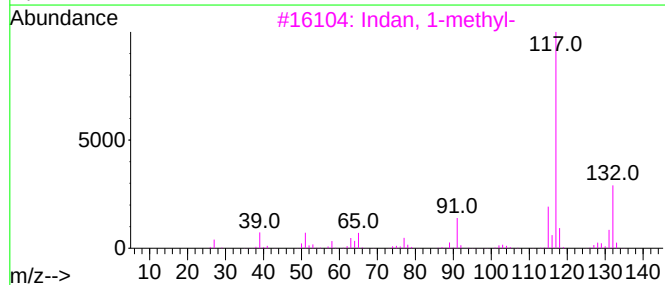
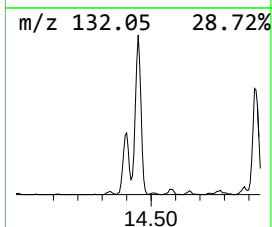
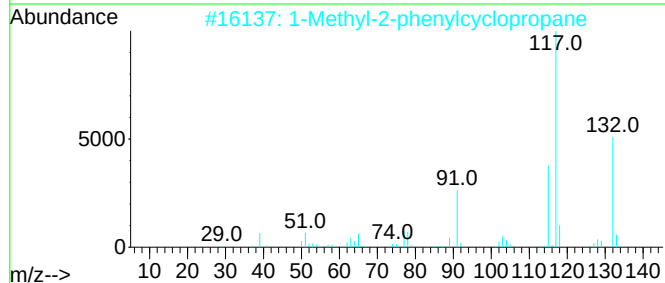
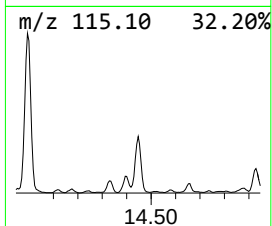
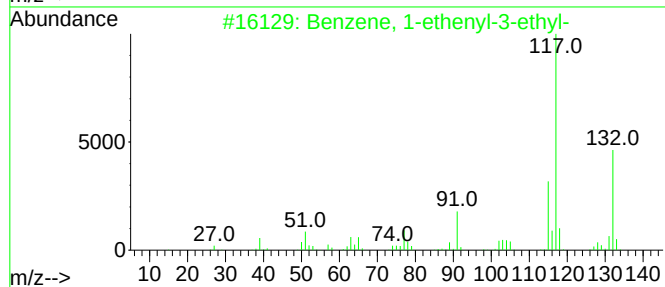
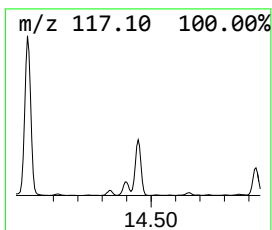
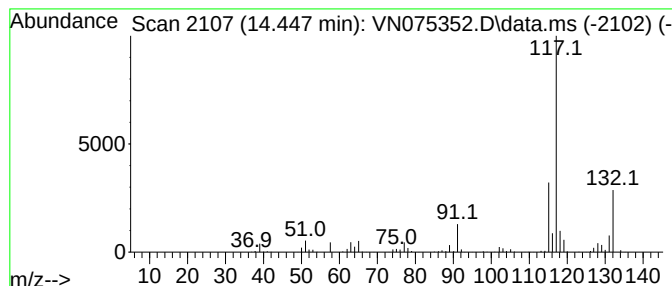
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	65.20 ug/l	907351	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
3			Indan, 1-methyl-	132	C10H12	000767-58-8	87
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	83



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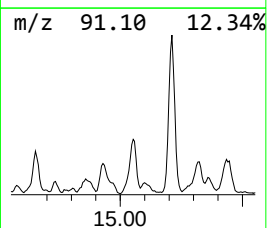
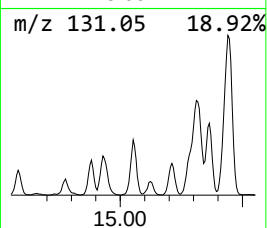
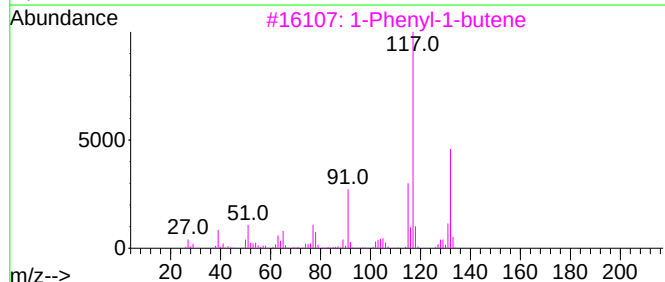
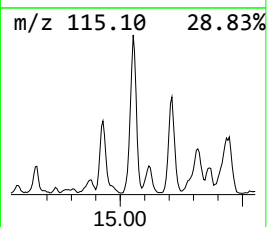
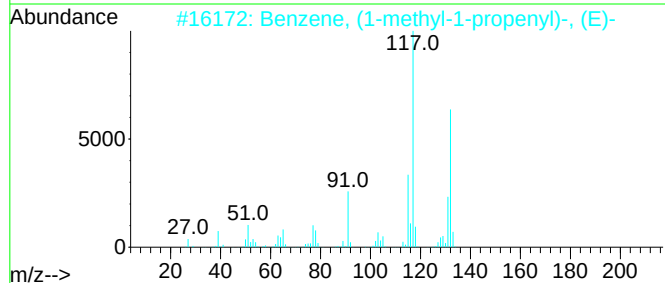
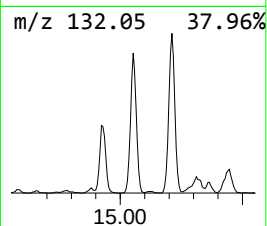
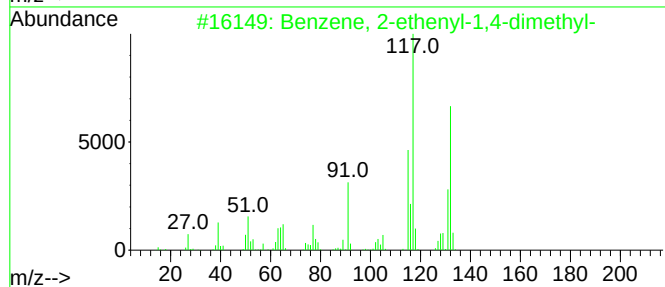
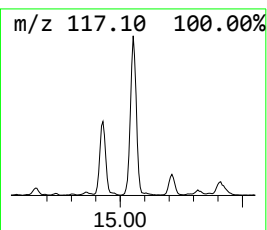
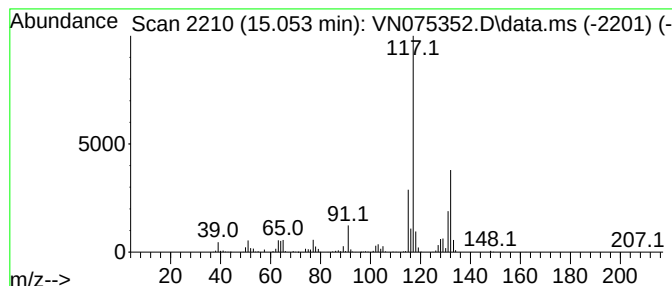
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	83.48 ug/l	1161770	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	92
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

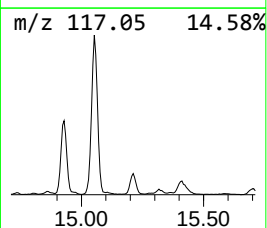
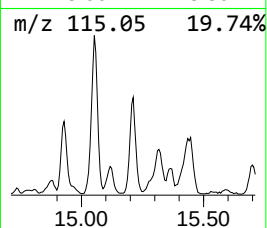
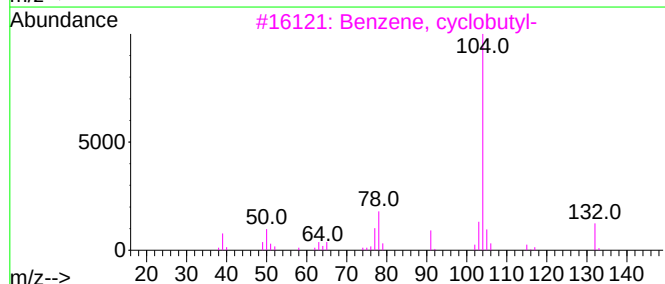
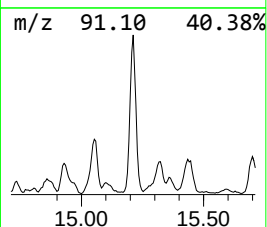
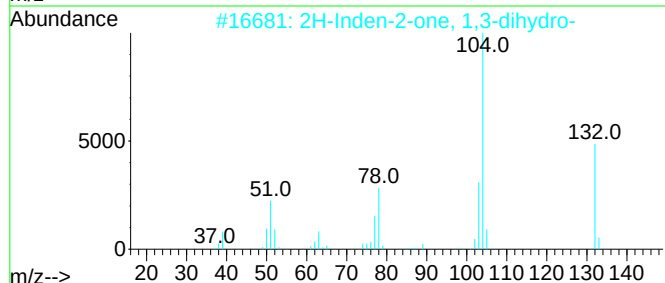
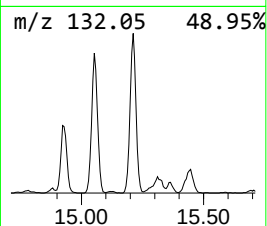
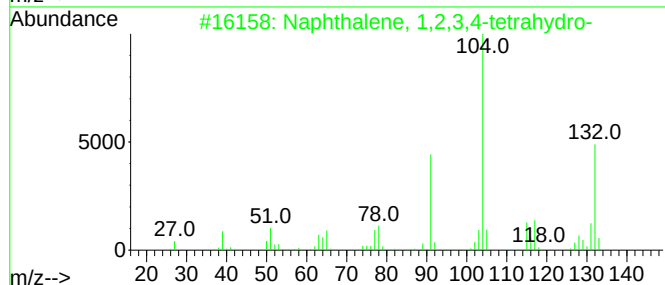
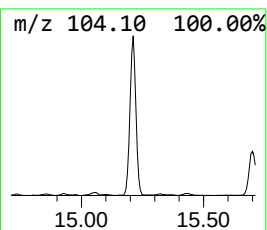
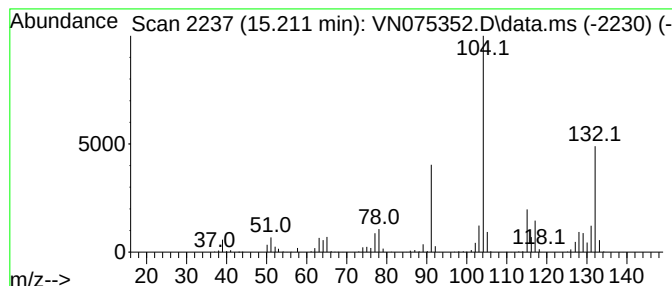
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	81.30 ug/l	1131450	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	52
3			Benzene, cyclobutyl-	132	C10H12	004392-30-7	38
4			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	35
5			3(2H)-Furanone, dihydro-2,2-dime...	190	C12H14O2	063678-00-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

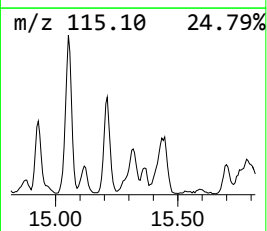
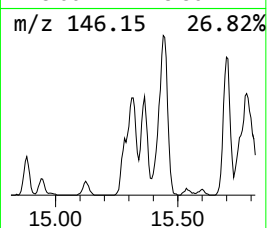
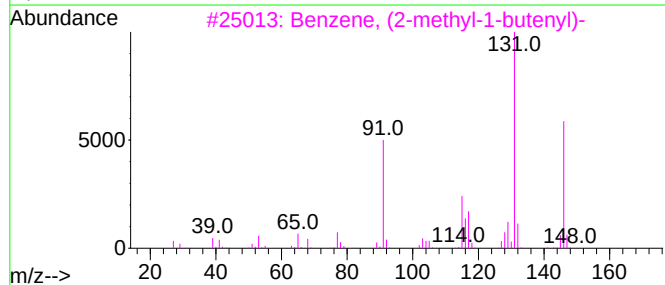
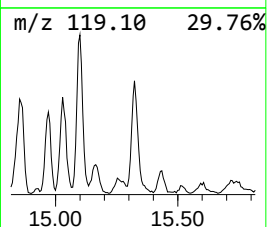
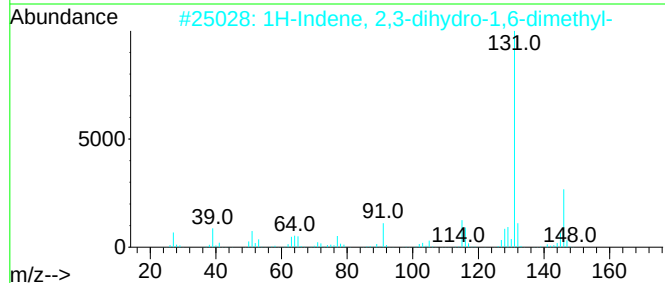
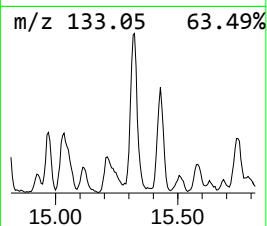
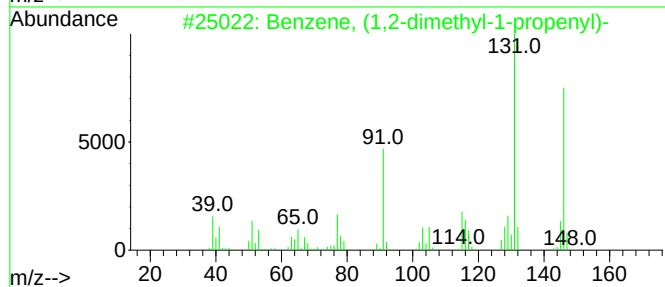
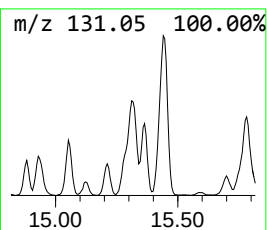
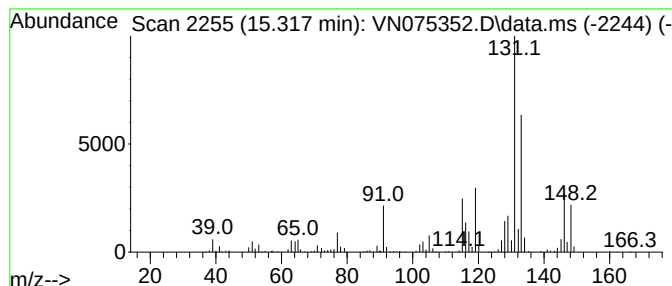
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, (1,2-dimethyl-1-propenyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	56.20 ug/l	782074	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	92
2			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	90
3			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	90
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	83
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

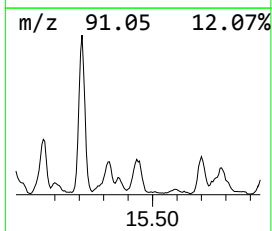
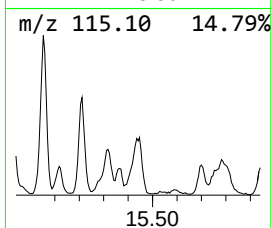
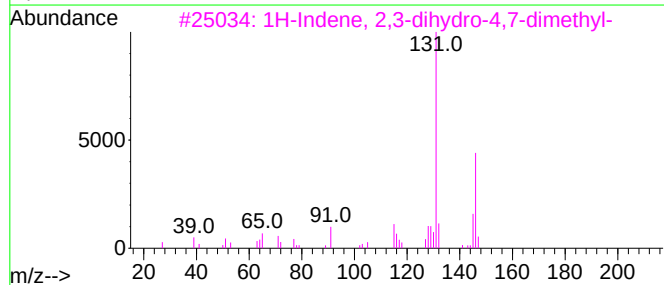
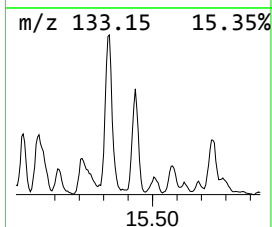
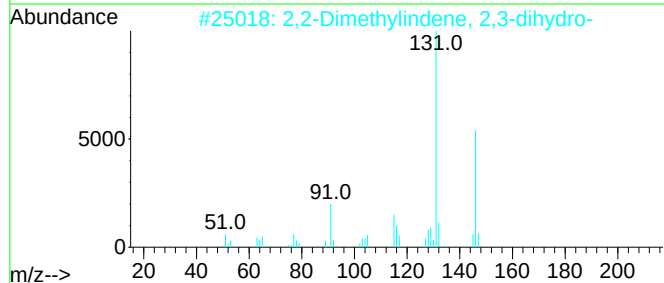
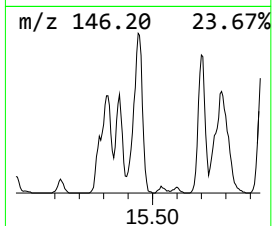
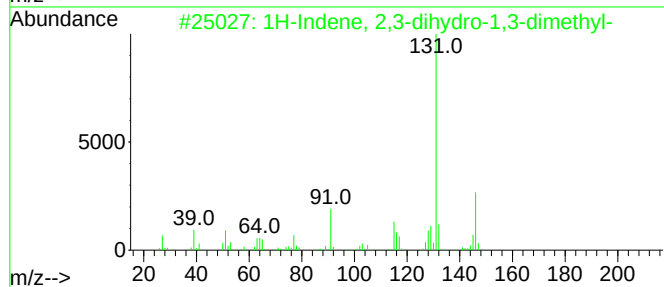
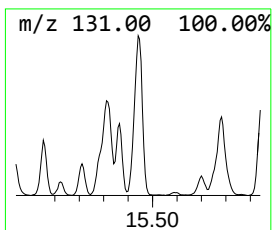
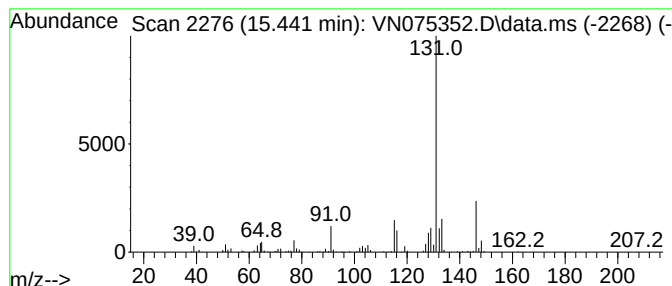
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-1,3-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.441	57.18 ug/l	795744	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	90
2		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	90
3		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
4		1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	90
5		1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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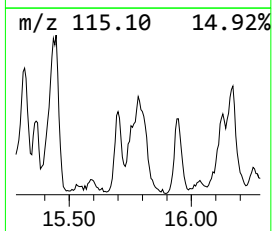
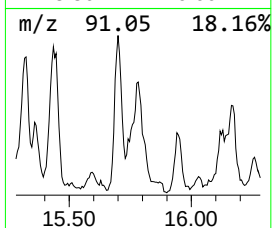
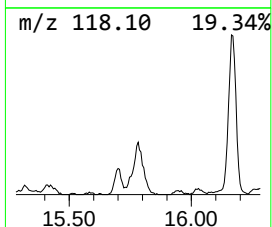
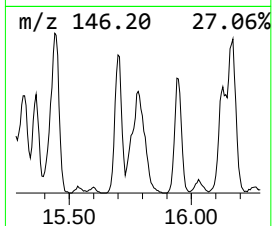
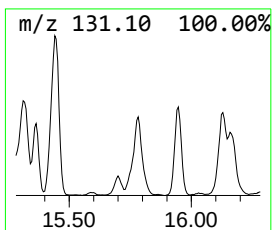
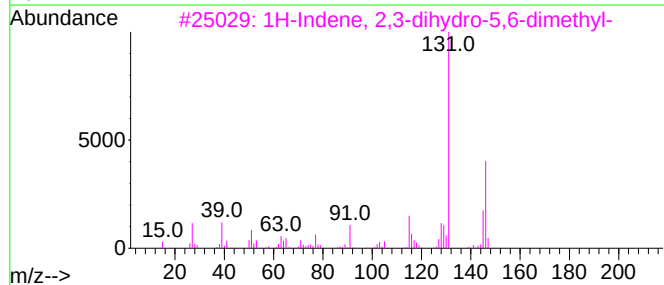
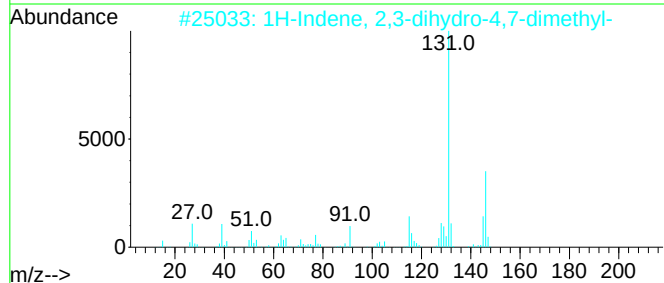
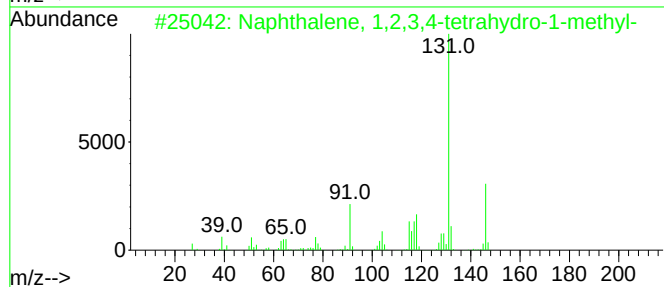
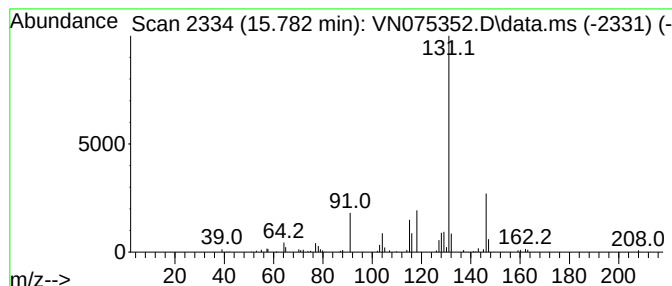
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.782	45.60 ug/l	634640	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	93
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
3			1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	87
4			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	83
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

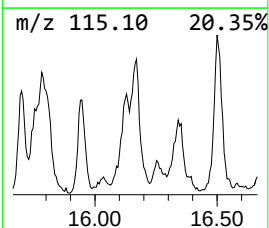
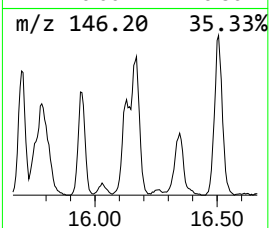
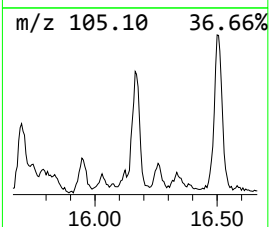
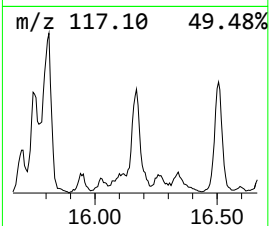
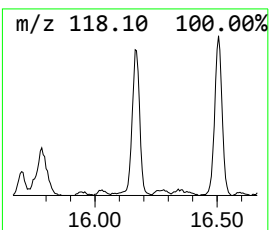
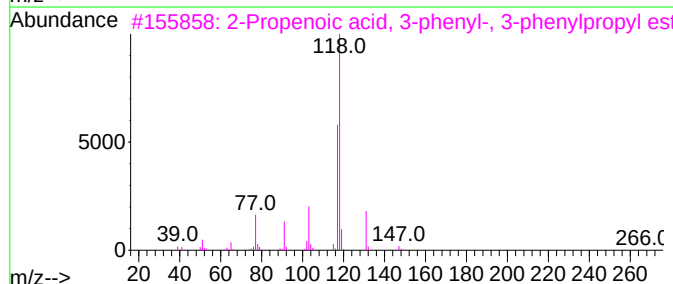
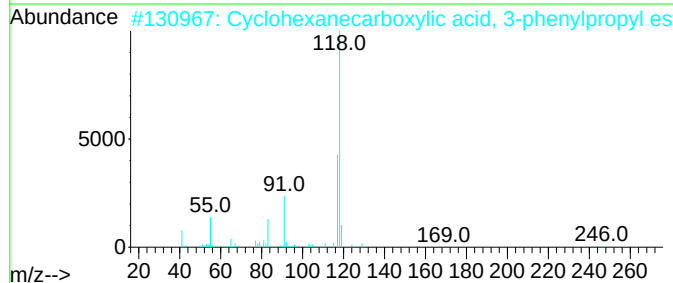
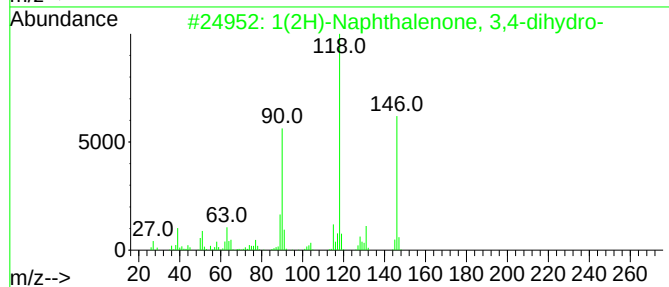
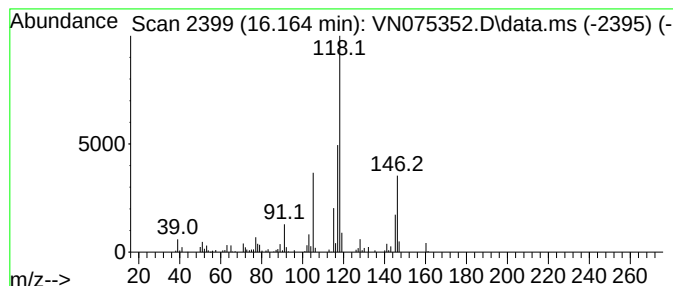
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.164 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.164	39.58 ug/l	550841	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	47
2			Cyclohexanecarboxylic acid, 3-phenyl-	246	C16H22O2	070275-61-5	47
3			2-Propenoic acid, 3-phenyl-, 3-phenylpropyl ester	266	C18H18O2	000122-68-9	38
4			Butanoic acid, 3-methyl-, 3-phenylpropyl ester	220	C14H20O2	005452-07-3	38
5			Benzylcyclobutane	146	C11H14	005244-88-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

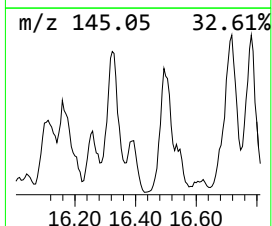
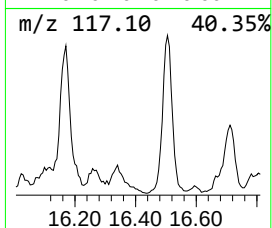
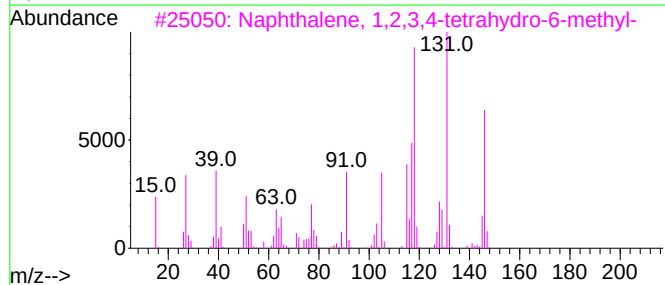
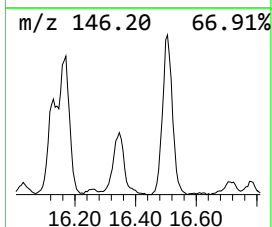
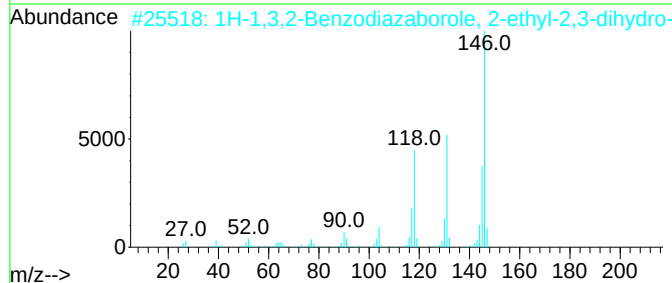
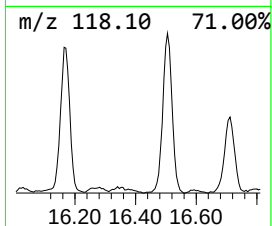
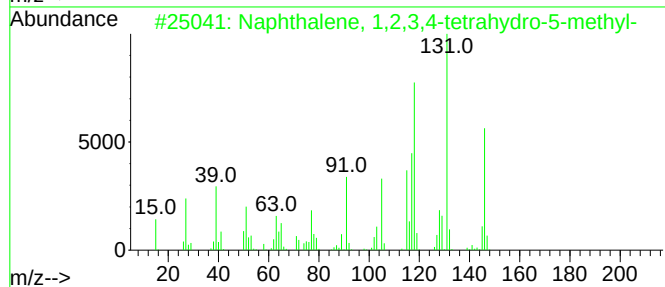
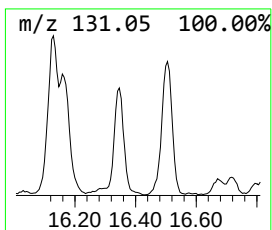
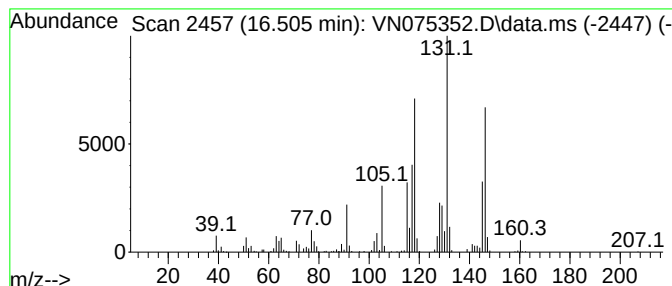
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	49.87 ug/l	694005	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	90
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	90
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075352.D
Acq On : 21 Nov 2022 19:30
Operator : JC\MD
Sample : N5557-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.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, 4-ethy...	14.329	51.2	ug/l	712185	4	13.794	695838	50.0
Benzene, 1-ethe...	14.447	65.2	ug/l	907351	4	13.794	695838	50.0
Benzene, 2-ethe...	15.053	83.5	ug/l	1161770	4	13.794	695838	50.0
Naphthalene, 1,...	15.211	81.3	ug/l	1131450	4	13.794	695838	50.0
Benzene, (1,2-d...	15.317	56.2	ug/l	782074	4	13.794	695838	50.0
1H-Indene, 2,3-...	15.441	57.2	ug/l	795744	4	13.794	695838	50.0
Naphthalene, 1,...	15.782	45.6	ug/l	634640	4	13.794	695838	50.0
unknown16.164	16.164	39.6	ug/l	550841	4	13.794	695838	50.0
Naphthalene, 1,...	16.506	49.9	ug/l	694005	4	13.794	695838	50.0