

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070122\
 Data File : VN073298.D
 Acq On : 01 Jul 2022 15:36
 Operator : JC\MD
 Sample : N3569-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 152140-SPC-05-30

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.005	15	20	27	rVB2	32638	47675	3.15%	0.399%
2	7.951	1021	1031	1036	rBV	219001	526776	34.81%	4.409%
3	8.016	1036	1042	1054	rVB	414269	937322	61.95%	7.846%
4	8.369	1093	1102	1116	rBV	232555	526756	34.81%	4.409%
5	8.904	1184	1193	1205	rBV	589708	1206120	79.71%	10.096%
6	10.380	1435	1444	1460	rBV	805660	1513114	100.00%	12.666%
7	10.551	1467	1473	1482	rVB7	11589	29549	1.95%	0.247%
8	10.722	1496	1502	1508	rVB3	17251	31870	2.11%	0.267%
9	10.816	1511	1518	1524	rBV5	11734	22818	1.51%	0.191%
10	11.280	1593	1597	1604	rVB	14655	22635	1.50%	0.189%
11	11.686	1658	1666	1677	rBV	825816	1481630	97.92%	12.402%
12	12.192	1745	1752	1756	rBV5	13936	27919	1.85%	0.234%
13	12.245	1758	1761	1771	rVB5	7213	15306	1.01%	0.128%
14	12.398	1782	1787	1791	rBV4	13253	18502	1.22%	0.155%
15	12.669	1826	1833	1843	rBV	703921	1176946	77.78%	9.852%
16	12.745	1843	1846	1854	rVB6	10502	17378	1.15%	0.145%
17	12.839	1854	1862	1869	rBV8	15495	36104	2.39%	0.302%
18	12.992	1883	1888	1896	rVB7	14578	26824	1.77%	0.225%
19	13.157	1908	1916	1924	rVB4	9137	23994	1.59%	0.201%
20	13.233	1924	1929	1936	rVB9	12319	24624	1.63%	0.206%
21	13.310	1936	1942	1948	rBV7	7656	16734	1.11%	0.140%
22	13.439	1956	1964	1969	rBV3	38989	77358	5.11%	0.648%
23	13.492	1969	1973	1980	rVB10	11251	22839	1.51%	0.191%
24	13.610	1987	1993	2004	rBV	872306	1488388	98.37%	12.459%
25	13.774	2017	2021	2025	rBV2	15064	22882	1.51%	0.192%
26	13.857	2031	2035	2044	rBV2	23325	45596	3.01%	0.382%
27	13.933	2044	2048	2055	rVB4	27069	46897	3.10%	0.393%
28	14.004	2055	2060	2067	rBV5	18586	45563	3.01%	0.381%
29	14.098	2073	2076	2081	rVB3	19703	29230	1.93%	0.245%
30	14.151	2081	2085	2091	rVB3	19903	31482	2.08%	0.264%
31	14.268	2098	2105	2109	rVB6	36702	76250	5.04%	0.638%
32	14.339	2109	2117	2122	rBV4	34445	75969	5.02%	0.636%
33	14.398	2123	2127	2131	rVB2	14841	19836	1.31%	0.166%
34	14.445	2131	2135	2138	rBV4	16868	24093	1.59%	0.202%
35	14.480	2138	2141	2144	rVV5	13699	22268	1.47%	0.186%
36	14.516	2144	2147	2150	rVB	22052	28692	1.90%	0.240%

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37	14.557	2150	2154	2158	rVB2	37062	48780	3.22%	0.408%
38	14.698	2174	2178	2183	rVB	36252	55737	3.68%	0.467%
39	14.763	2183	2189	2192	rBV5	27653	57140	3.78%	0.478%
40	14.792	2192	2194	2199	rVB4	24383	33674	2.23%	0.282%
41	14.851	2199	2204	2205	rBV3	45079	61775	4.08%	0.517%
42	14.927	2212	2217	2222	rBV4	20787	40379	2.67%	0.338%
43	15.051	2231	2238	2239	rBV5	14931	24104	1.59%	0.202%
44	15.121	2246	2250	2254	rBV2	37821	62463	4.13%	0.523%
45	15.168	2254	2258	2263	rVV2	36250	56864	3.76%	0.476%
46	15.245	2265	2271	2280	rVB2	123820	286807	18.95%	2.401%
47	15.339	2282	2287	2291	rBV2	16258	22996	1.52%	0.192%
48	15.392	2291	2296	2301	rBV6	21148	46988	3.11%	0.393%
49	15.486	2307	2312	2316	rBV3	32381	59887	3.96%	0.501%
50	15.563	2323	2325	2346	rVB4	67188	261081	17.25%	2.185%
51	15.727	2346	2353	2361	rBV3	51044	111263	7.35%	0.931%
52	15.810	2361	2367	2370	rBV8	15903	33349	2.20%	0.279%
53	15.886	2372	2380	2392	rVV5	40021	134401	8.88%	1.125%
54	16.027	2400	2404	2410	rBV7	25585	48798	3.23%	0.408%
55	16.098	2411	2416	2421	rVV4	31493	74805	4.94%	0.626%
56	16.257	2435	2443	2449	rBV4	90787	208775	13.80%	1.748%
57	16.462	2467	2478	2484	rBV3	70420	175084	11.57%	1.466%
58	16.527	2484	2489	2494	rBV4	30752	74376	4.92%	0.623%
59	16.739	2515	2525	2530	rBV7	60747	179130	11.84%	1.499%

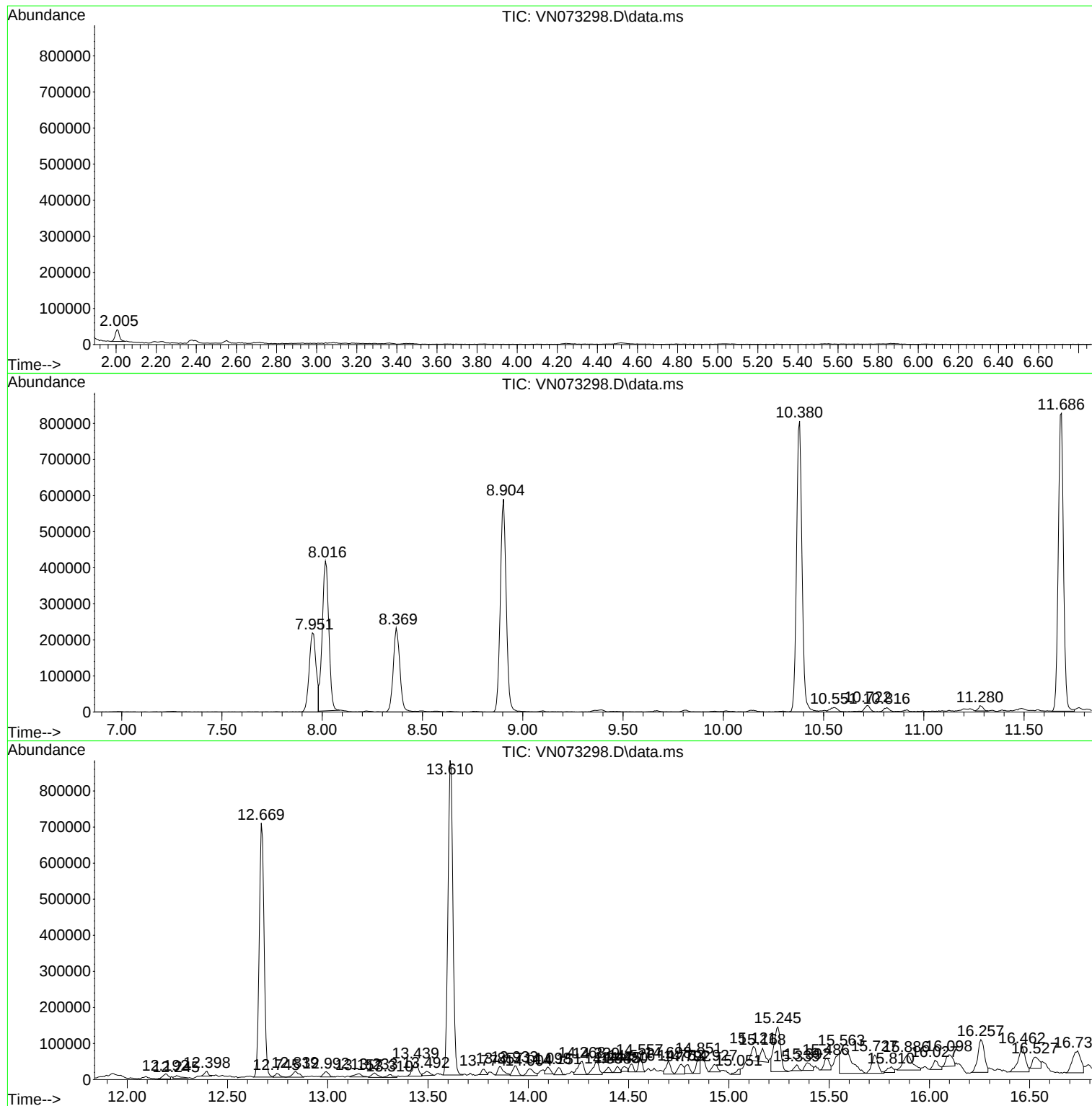
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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152140-SPC-05-30

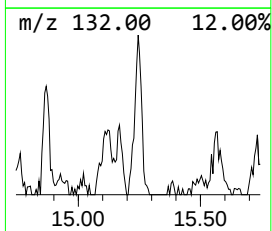
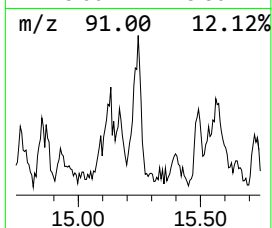
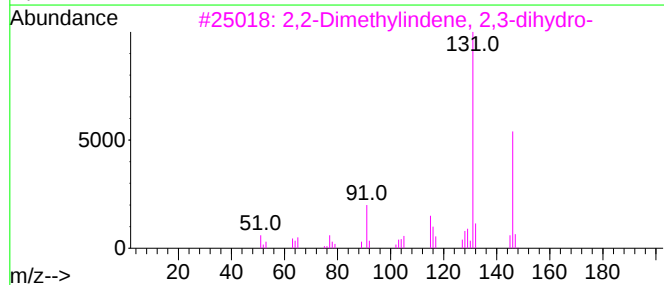
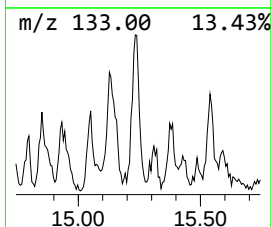
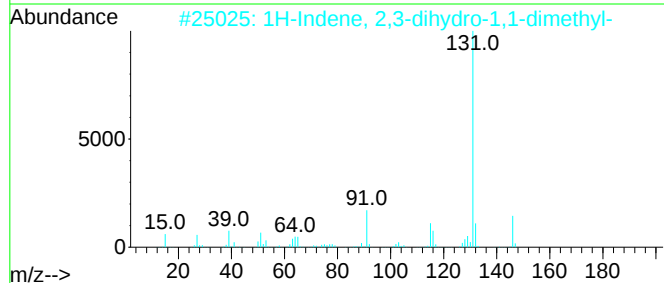
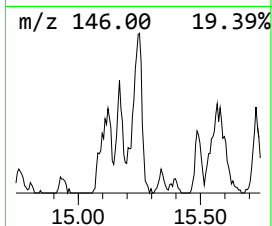
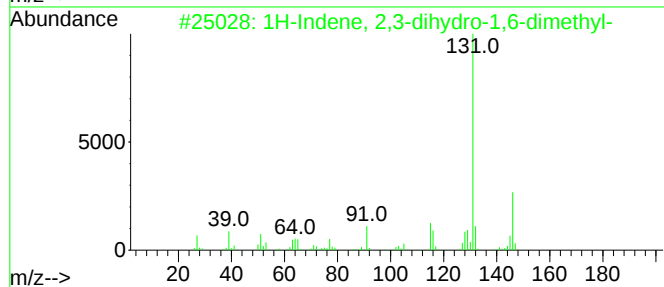
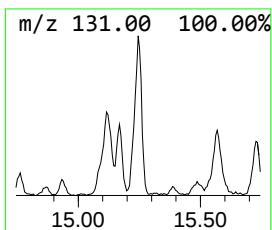
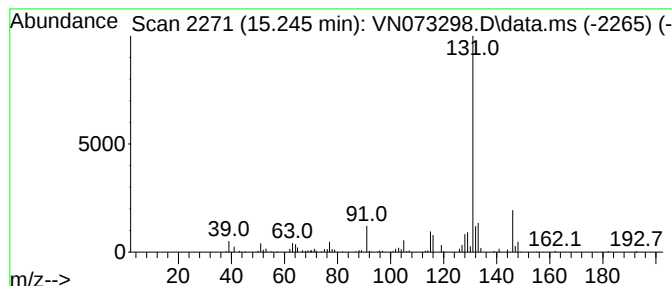
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	9.63 ug/l	286807	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	93		
2	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	90		
3	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	87		
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	83		
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	80		



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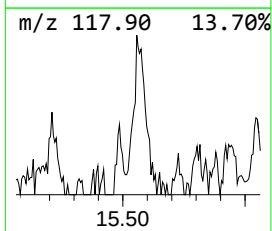
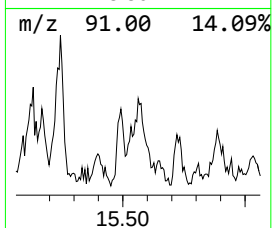
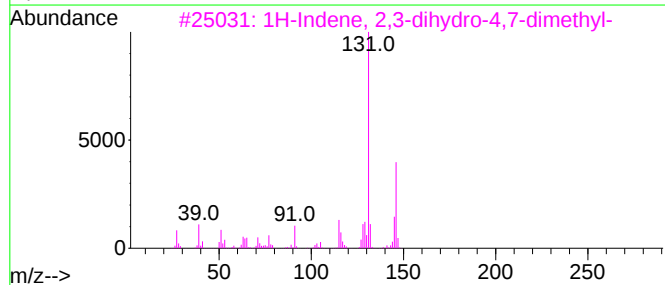
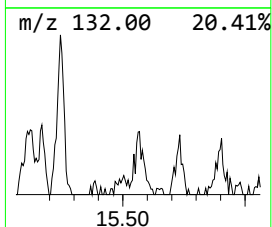
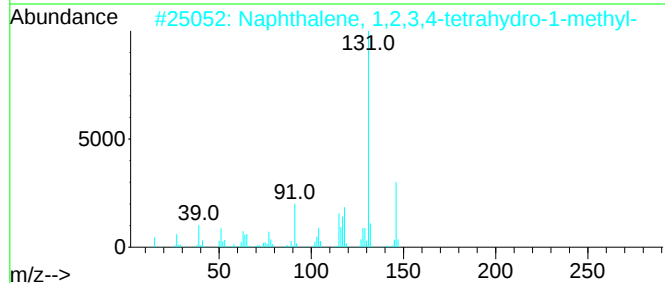
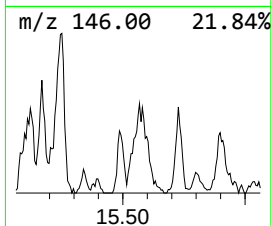
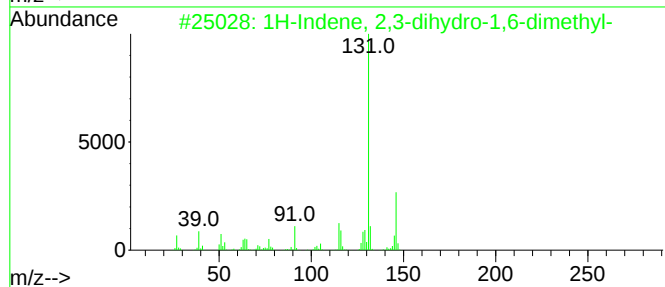
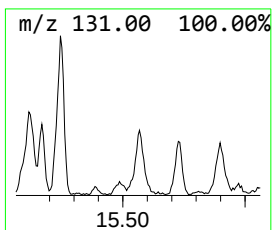
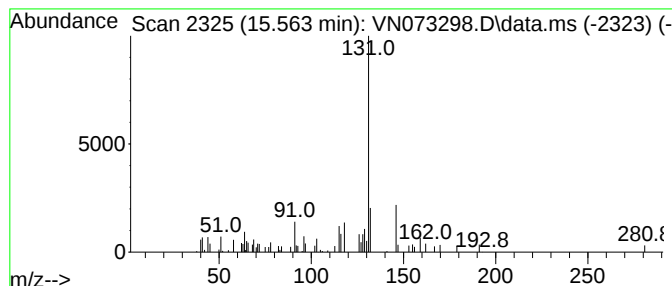
Instrument :
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ClientSampleId :
152140-SPC-05-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.563	8.77 ug/l	261081	1,4-Dichlorobenzene-d4		13.616	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...		146	C11H14	017059-48-2	76
2	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	001559-81-5	76
3	1H-Indene, 2,3-dihydro-4,7-dimet...		146	C11H14	006682-71-9	76
4	1H-Indene, 2,3-dihydro-1,1-dimet...		146	C11H14	004912-92-9	76
5	1H-Indene, 2,3-dihydro-1,3-dimet...		146	C11H14	004175-53-5	76



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
152140-SPC-05-30

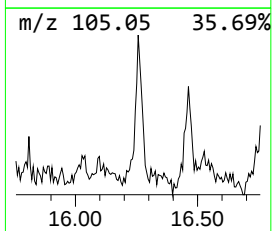
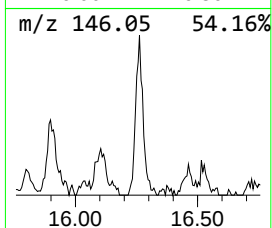
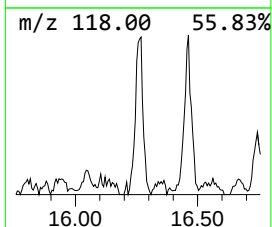
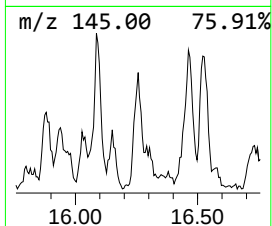
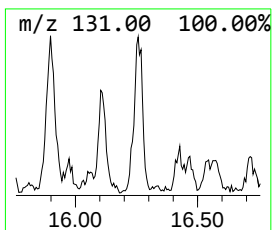
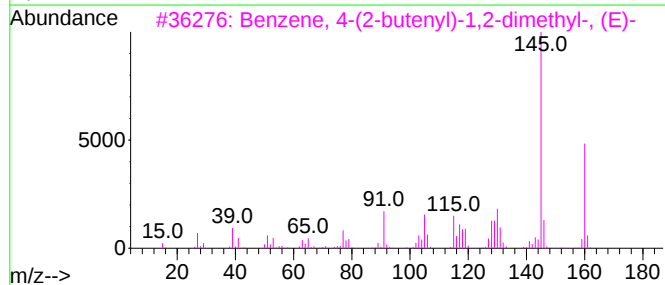
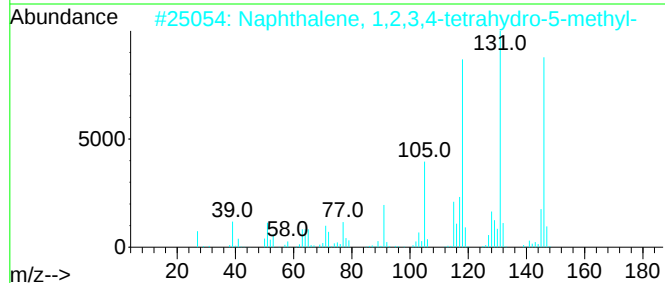
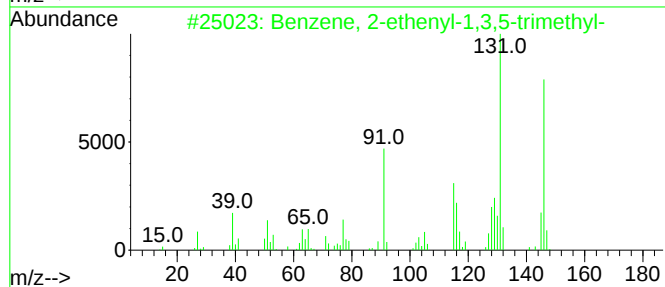
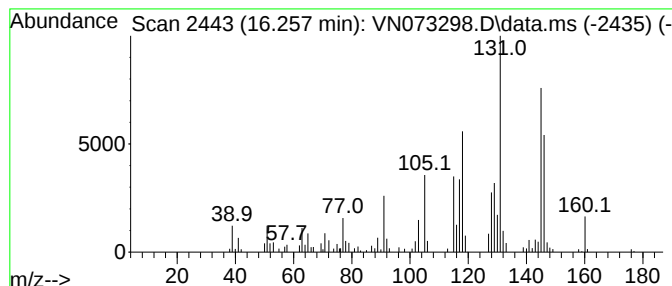
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	7.01 ug/l	208775	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	58
3			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	55
4			2,3-Dimethyl-1H-pyrrolo[2,3-b]py...	146	C9H10N2	010299-69-1	52
5			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	50



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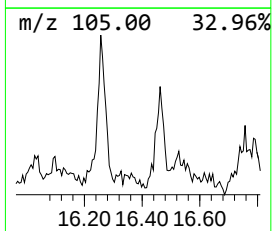
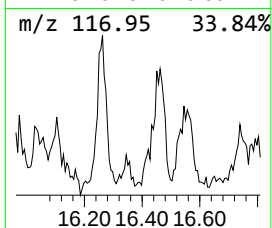
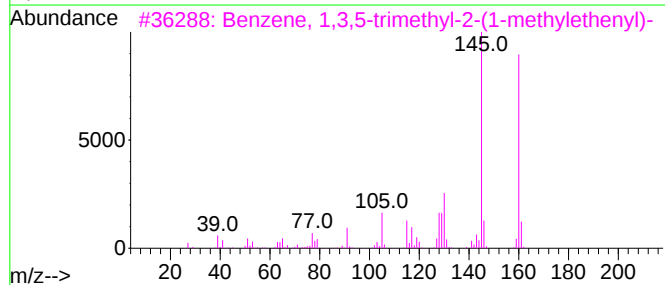
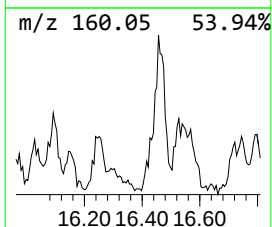
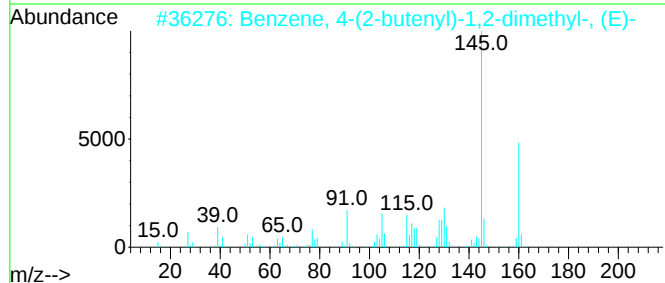
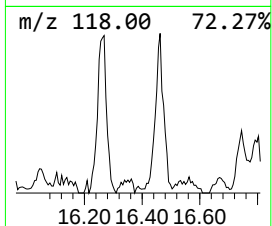
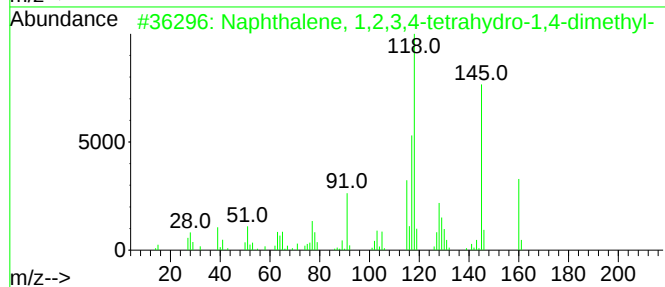
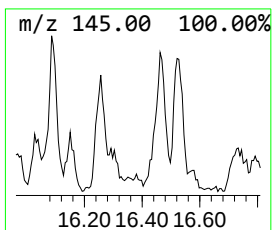
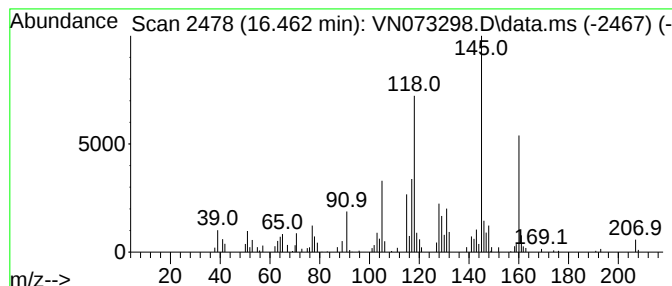
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	5.88 ug/l	175084	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	91
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	81
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	64
4			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	64
5			1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	58



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Operator : JC\MD
Sample : N3569-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-05-30

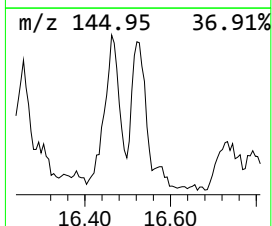
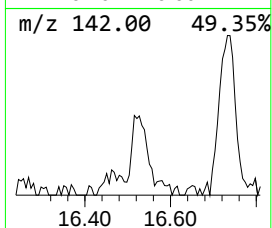
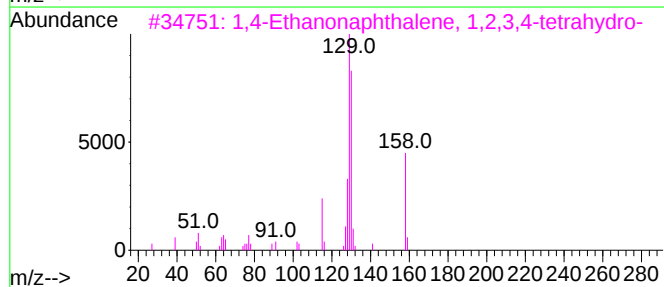
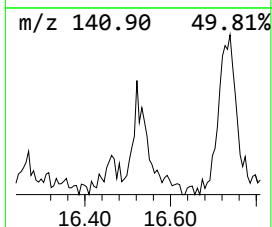
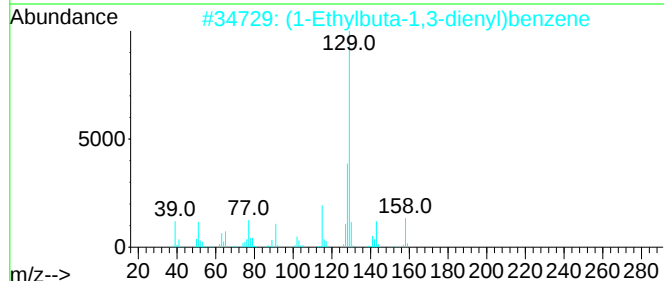
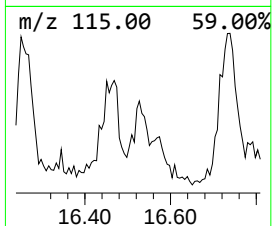
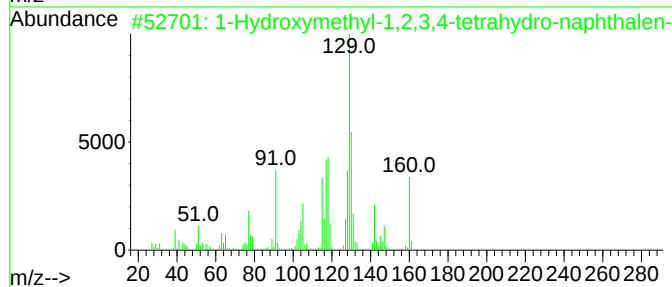
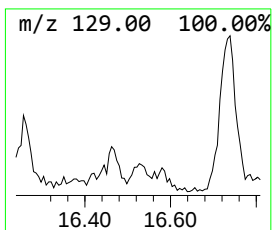
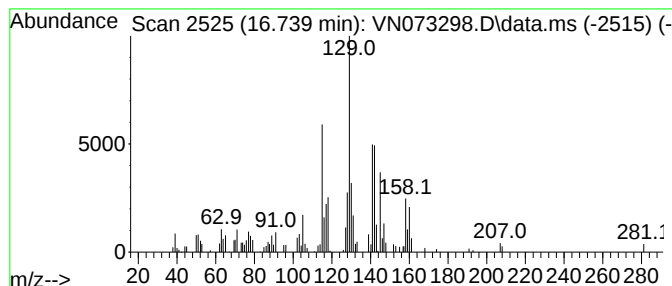
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Quant Title : SW846 8260

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

Peak Number 5 unknown16.739 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	6.02 ug/l	179130	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hydroxymethyl-1,2,3,4-tetrahyd...	178	C11H14O2	343332-31-0	38
2			(1-Ethylbuta-1,3-dienyl)benzene	158	C12H14	1000210-05-6	27
3			1,4-Ethanonaphthalene, 1,2,3,4-t...	158	C12H14	004175-52-4	27
4			Hydrazine, tripropyl-	158	C9H22N2	067398-42-9	22
5			2,7-Methanonaphth[2,3-b]oxirene,...	158	C11H10O	013137-34-3	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070122\
Data File : VN073298.D
Acq On : 01 Jul 2022 15:36
Operator : JC\MD
Sample : N3569-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
152140-SPC-05-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-Indene, 2,3-...	15.245	9.6	ug/l	286807	4	13.616	1488390	50.0
Naphthalene, 1,...	15.563	8.8	ug/l	261081	4	13.616	1488390	50.0
Benzene, 2-ethe...	16.257	7.0	ug/l	208775	4	13.616	1488390	50.0
Naphthalene, 1,...	16.462	5.9	ug/l	175084	4	13.616	1488390	50.0
unknown16.739	16.739	6.0	ug/l	179130	4	13.616	1488390	50.0