

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
 Data File : VN073685.D
 Acq On : 02 Aug 2022 14:22
 Operator : JC\MD
 Sample : N3971-11
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-16SR

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\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073685.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	79	87	94	rBV	59223	99201	2.46%	0.433%
2	3.087	196	204	213	rBV	75224	168541	4.18%	0.735%
3	3.934	338	348	359	rVB3	33685	91126	2.26%	0.397%
4	4.234	389	399	410	rBV	20268	61749	1.53%	0.269%
5	4.510	436	446	465	rBV	82692	269852	6.70%	1.177%
6	4.881	500	509	519	rVB	14733	42498	1.05%	0.185%
7	5.110	537	548	558	rBV3	30284	104082	2.58%	0.454%
8	7.069	871	881	890	rBV4	30616	92797	2.30%	0.405%
9	7.339	919	927	943	rVB2	30007	77709	1.93%	0.339%
10	7.951	1020	1031	1036	rBV	279699	646469	16.04%	2.819%
11	8.016	1036	1042	1053	rVB	491710	1131398	28.07%	4.934%
12	8.392	1092	1106	1117	rBV3	1115349	2952106	73.24%	12.874%
13	8.522	1123	1128	1135	rVB4	22731	51364	1.27%	0.224%
14	8.904	1184	1193	1205	rBV	668355	1371466	34.03%	5.981%
15	10.380	1437	1444	1451	rBV	979900	1749625	43.41%	7.630%
16	10.445	1451	1455	1461	rVB	44145	76465	1.90%	0.333%
17	10.586	1471	1479	1485	rBV	130453	232132	5.76%	1.012%
18	10.657	1485	1491	1498	rVB	141485	241982	6.00%	1.055%
19	11.074	1557	1562	1568	rVB	41975	70998	1.76%	0.310%
20	11.233	1582	1589	1602	rVB2	32143	65888	1.63%	0.287%
21	11.686	1657	1666	1676	rBV	964169	1715617	42.57%	7.482%
22	11.786	1676	1683	1693	rVV	297171	512173	12.71%	2.234%
23	11.898	1693	1702	1713	rVB	67398	138267	3.43%	0.603%
24	12.221	1751	1757	1764	rVB2	35927	64739	1.61%	0.282%
25	12.521	1799	1808	1813	rBV	209598	365815	9.08%	1.595%
26	12.674	1826	1834	1845	rVB	846204	1408968	34.96%	6.144%
27	12.863	1860	1866	1876	rVB	222160	366913	9.10%	1.600%
28	13.163	1906	1917	1926	rBV	171302	284081	7.05%	1.239%
29	13.310	1935	1942	1948	rBV	113233	195442	4.85%	0.852%
30	13.615	1986	1994	1998	rBV	1035027	1972108	48.93%	8.600%
31	13.710	2006	2010	2017	rVB	47838	81144	2.01%	0.354%
32	13.815	2017	2028	2044	rVB	2400136	4030505	100.00%	17.577%
33	14.157	2080	2086	2092	rVB	87775	137352	3.41%	0.599%
34	14.221	2092	2097	2100	rBV	31114	50022	1.24%	0.218%
35	14.268	2100	2105	2113	rVB	127412	205801	5.11%	0.897%
36	14.480	2134	2141	2146	rBV	42135	79216	1.97%	0.345%

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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

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37	14.751	2181	2187	2193	rBV	65364	108415	2.69%	0.473%
38	14.868	2200	2207	2214	rBV2	107014	213298	5.29%	0.930%
39	15.015	2226	2232	2239	rBV2	32105	58004	1.44%	0.253%
40	15.433	2293	2303	2315	rBV	707430	1345421	33.38%	5.867%

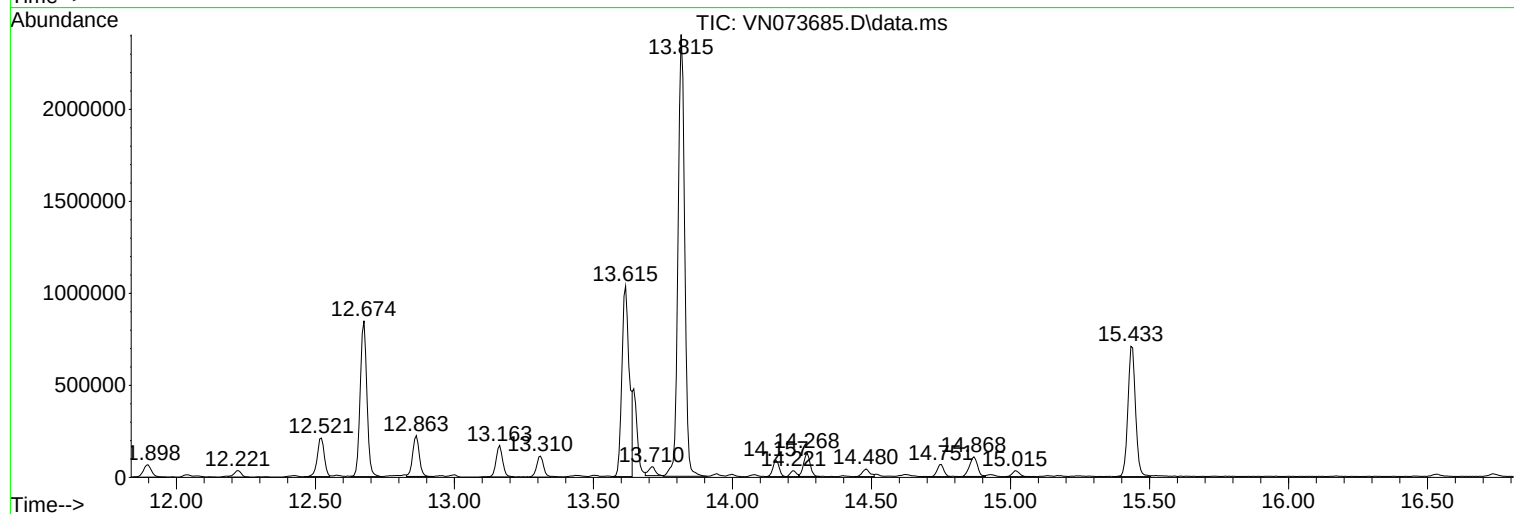
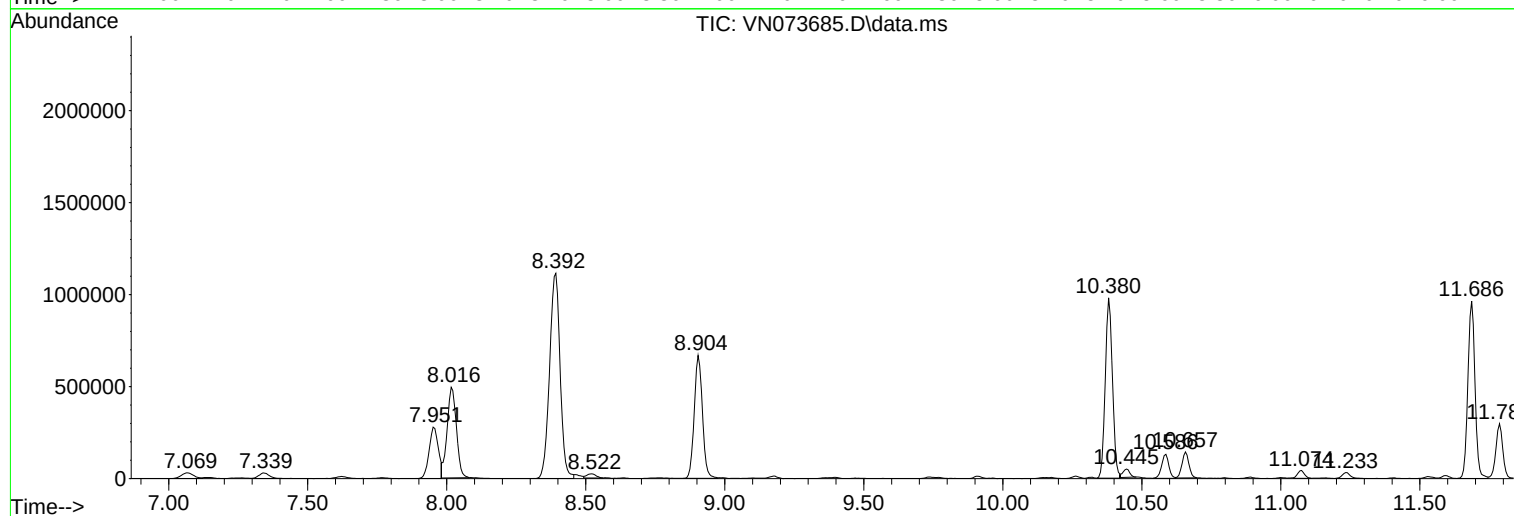
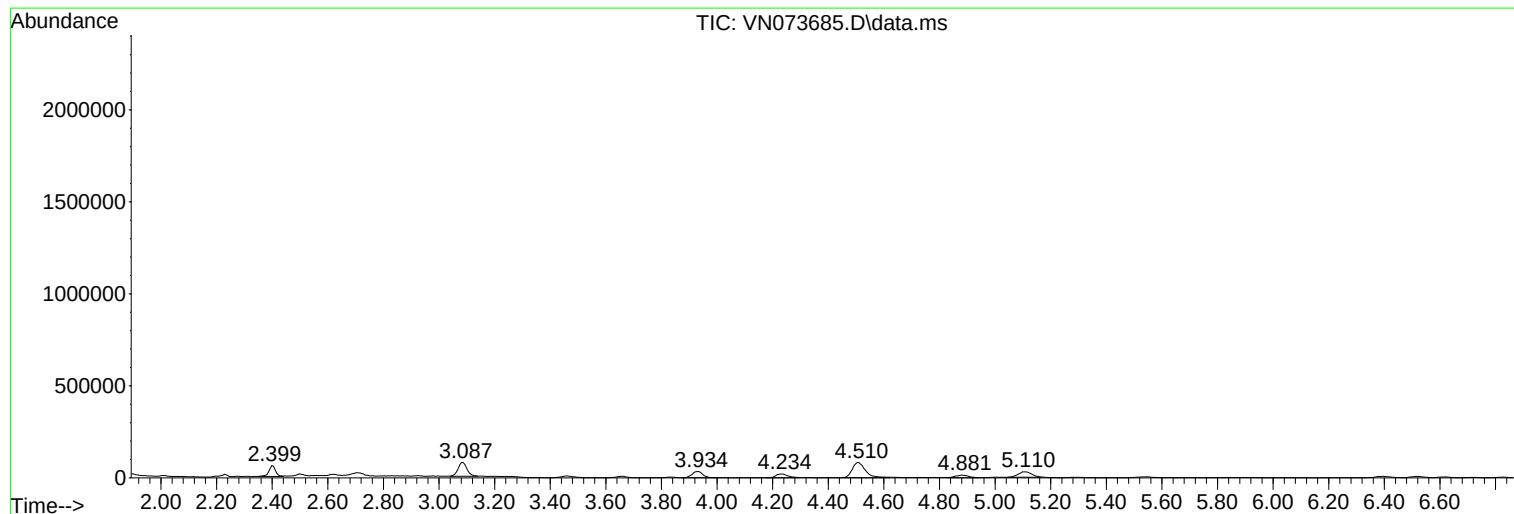
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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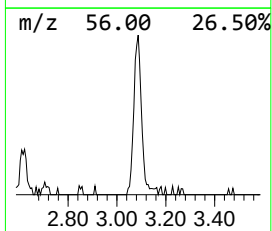
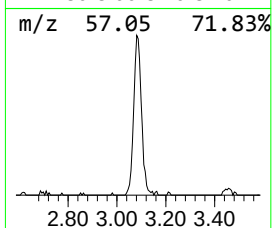
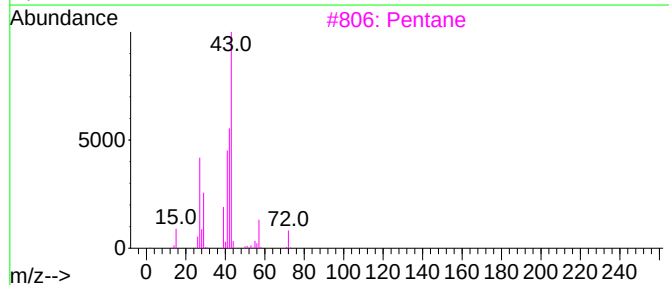
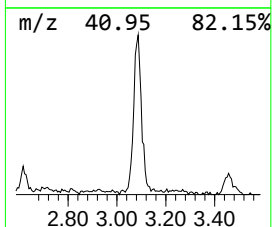
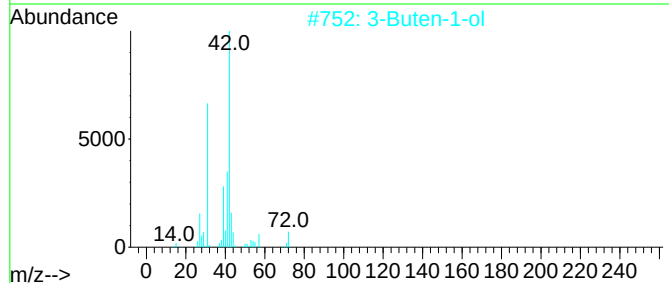
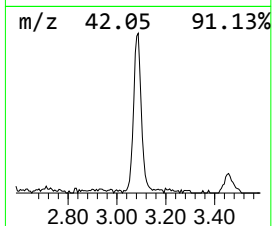
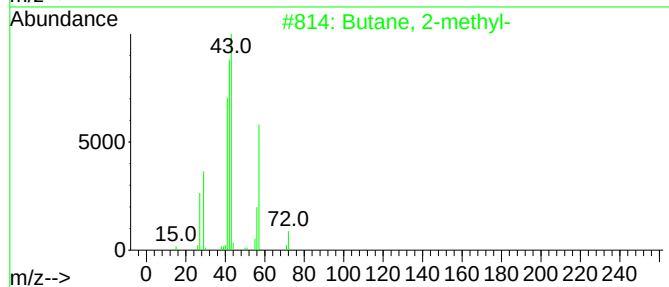
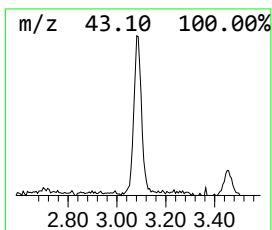
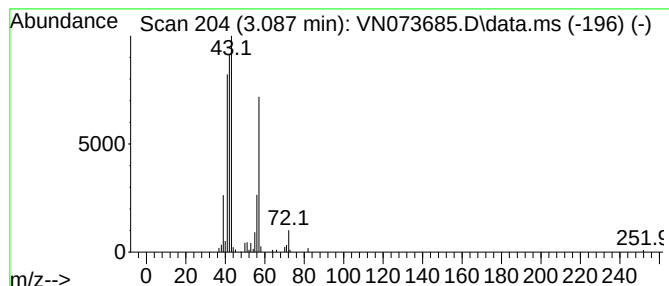
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	7.45 ug/l	168541	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Pentane	72	C5H12	000109-66-0	36
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	22



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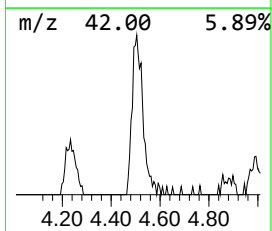
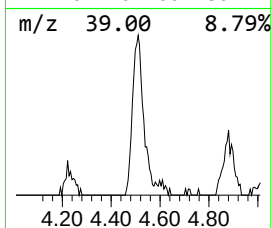
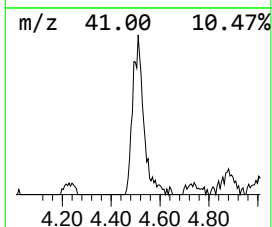
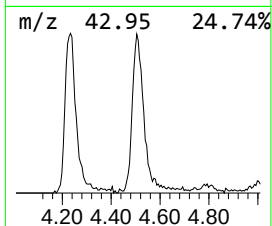
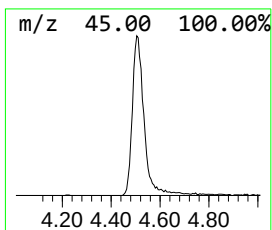
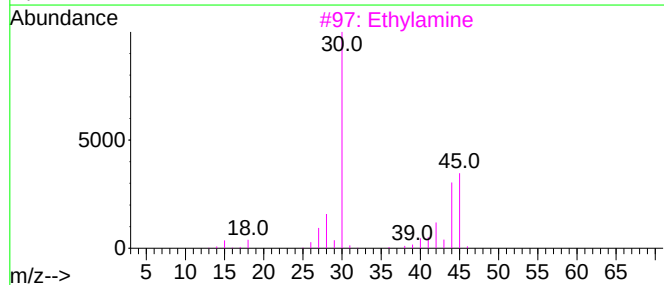
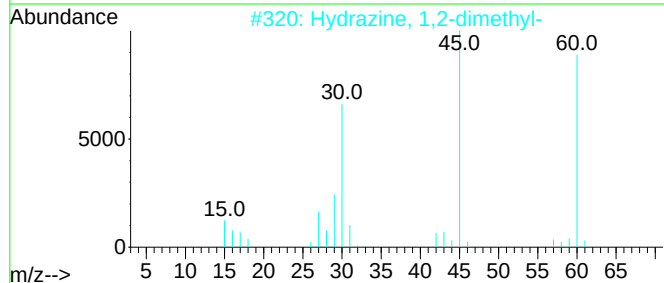
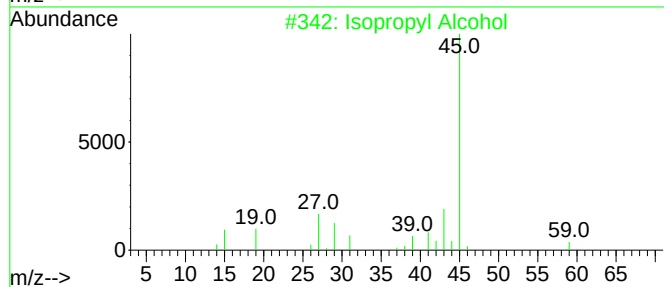
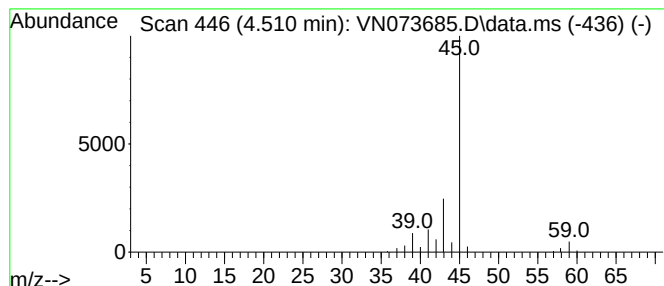
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	11.93 ug/l	269852	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Ethylamine	45	C2H7N	000075-04-7	5
4		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4
5		4-Penten-2-ol	86	C5H10O	000625-31-0	4



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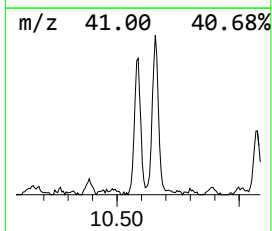
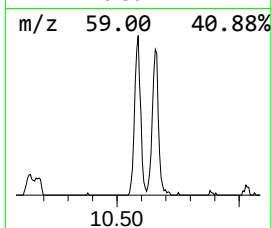
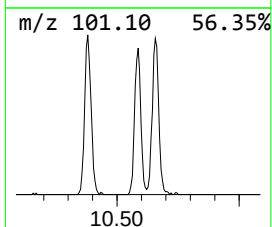
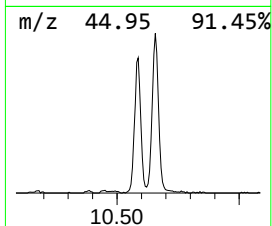
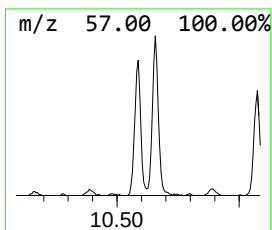
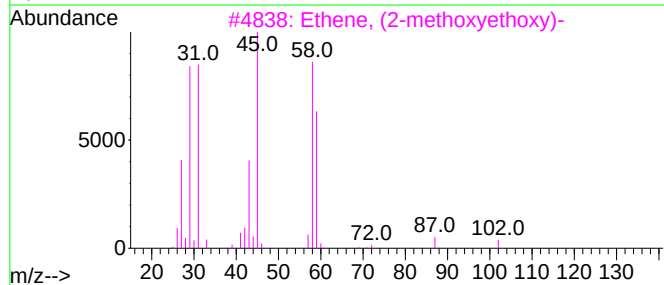
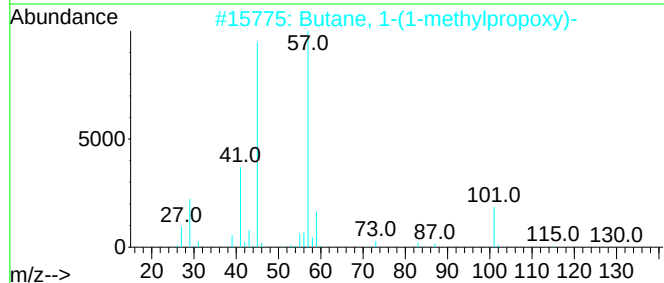
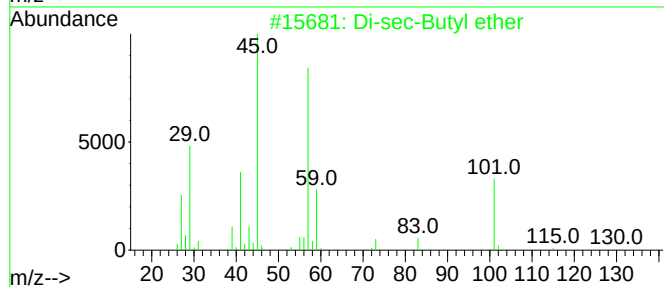
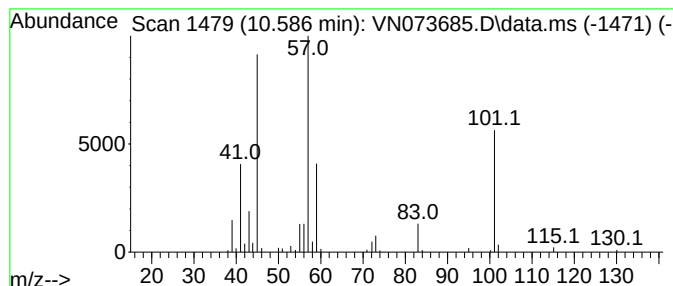
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 3 Di-sec-Butyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	6.77 ug/l	232132	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3			Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	43
4			2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	42
5			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	42



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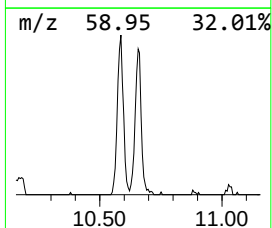
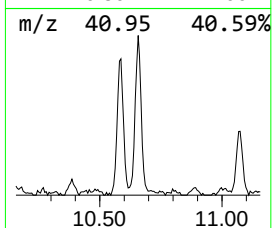
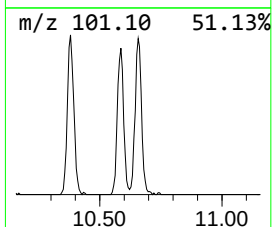
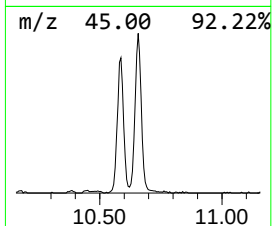
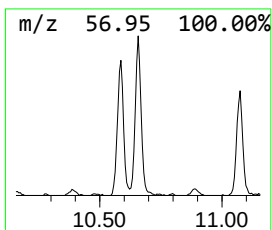
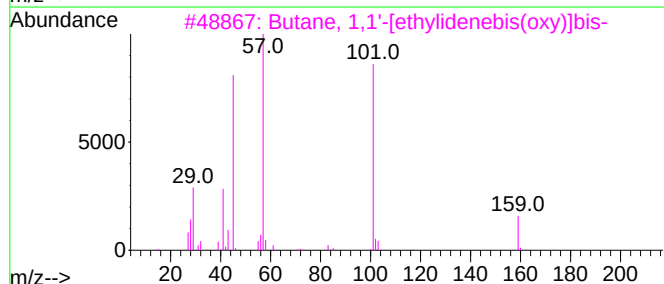
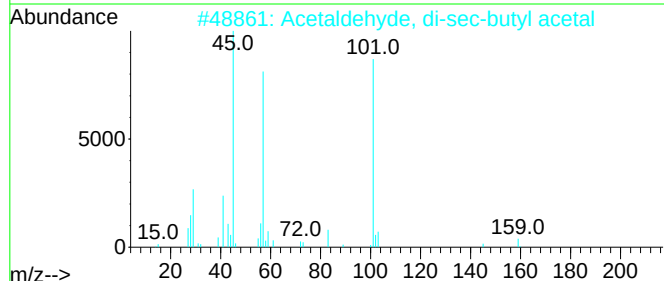
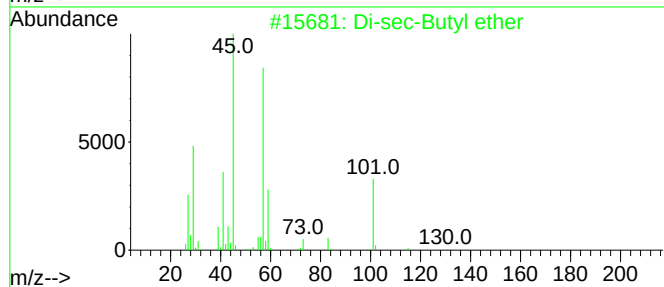
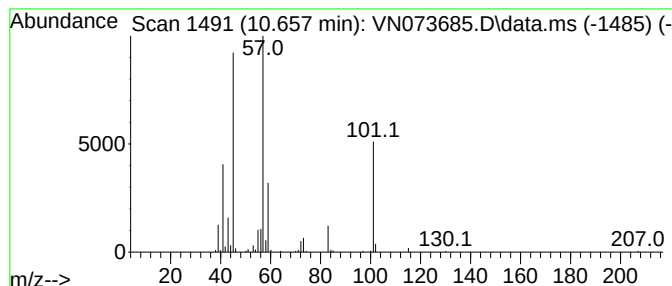
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Acetaldehyde, di-sec-butyl ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	7.05 ug/l	241982	Chlorobenzene-d5	11.686

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2		Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	78
3		Butane, 1,1'-[ethylidenebis(oxy)]...	174	C10H22O2	000871-22-7	64
4		Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	56
5		DL-Lactamide, N,O-dibutyl-	201	C11H23NO2	1000452-56-2	50



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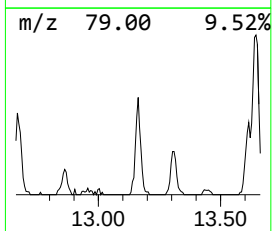
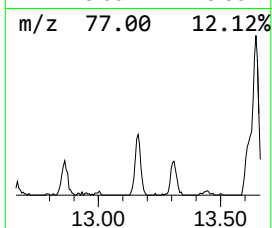
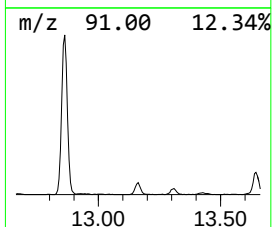
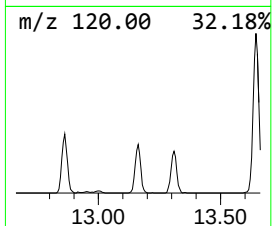
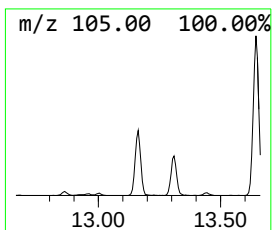
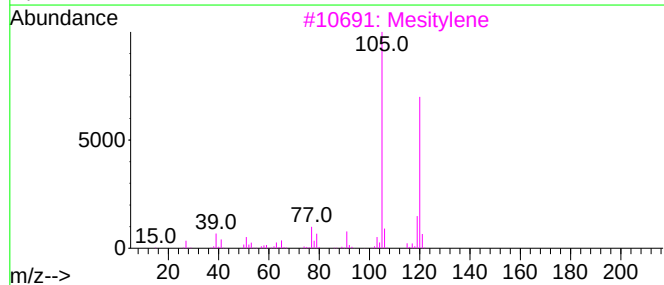
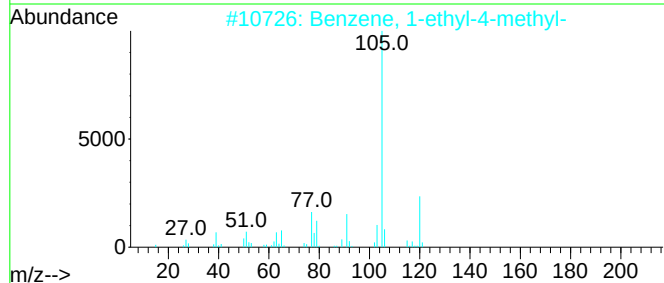
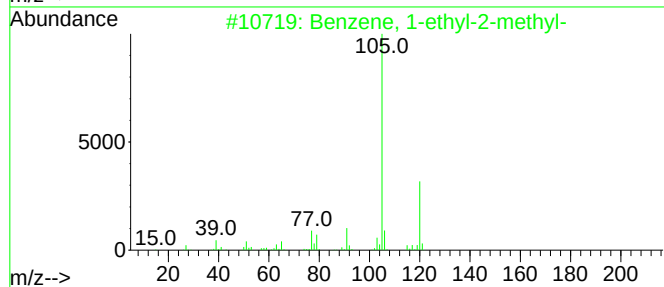
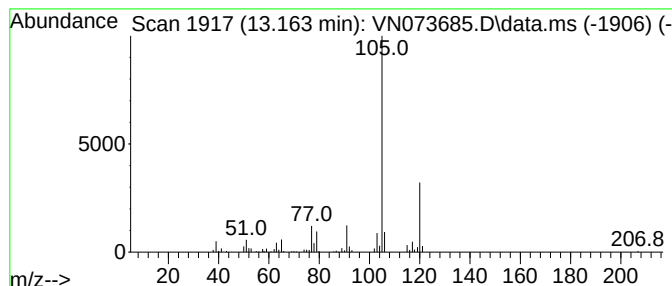
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	7.20 ug/l	284081	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073685.D
Acq On : 02 Aug 2022 14:22
Operator : JC\MD
Sample : N3971-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16SR

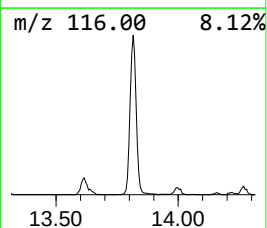
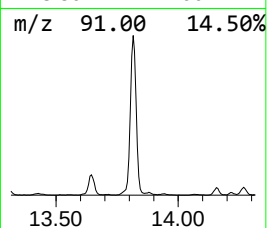
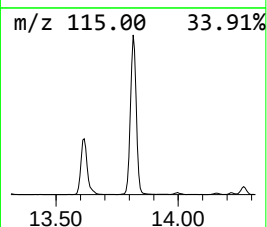
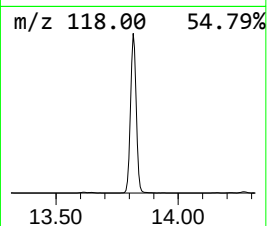
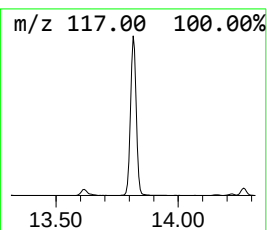
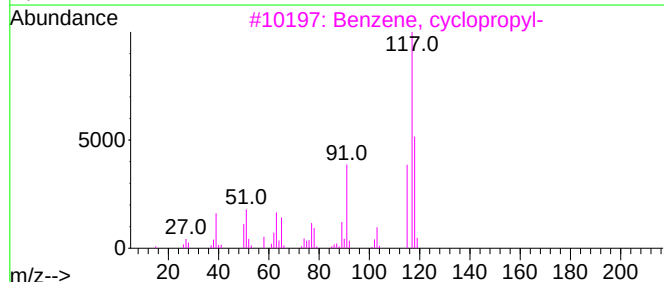
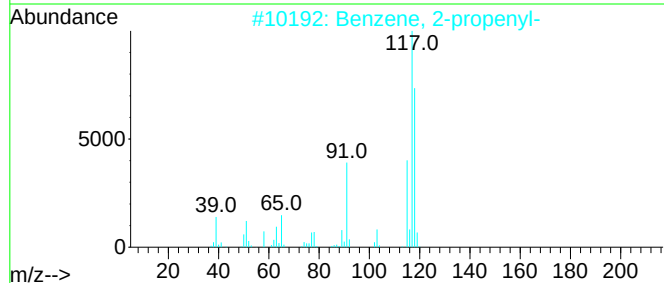
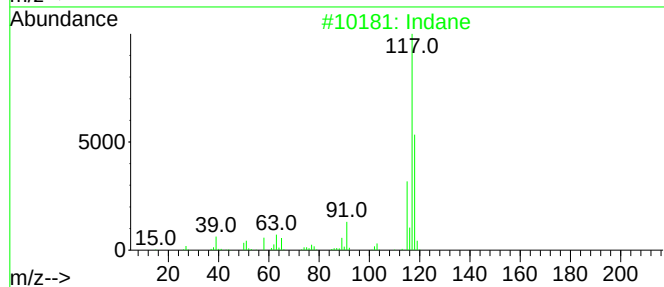
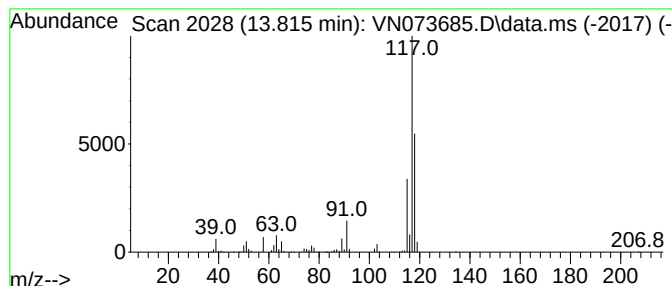
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	102.19 ug/l	4030510	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4			Deltacyclene	118	C9H10	007785-10-6	72
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073685.D
Acq On : 02 Aug 2022 14:22
Operator : JC\MD
Sample : N3971-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16SR

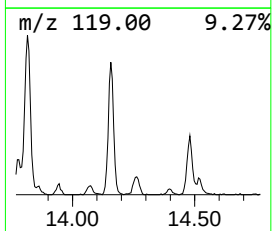
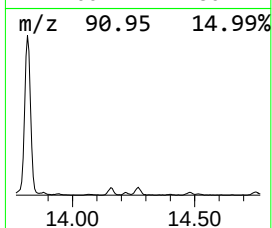
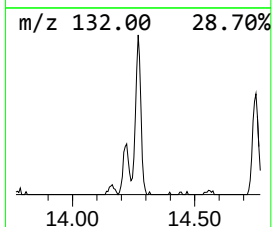
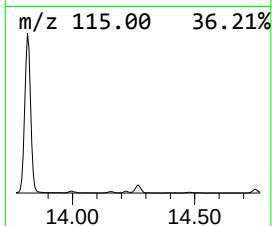
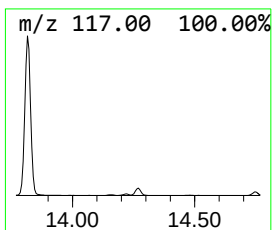
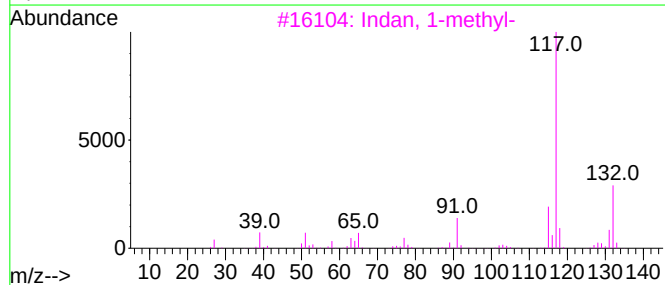
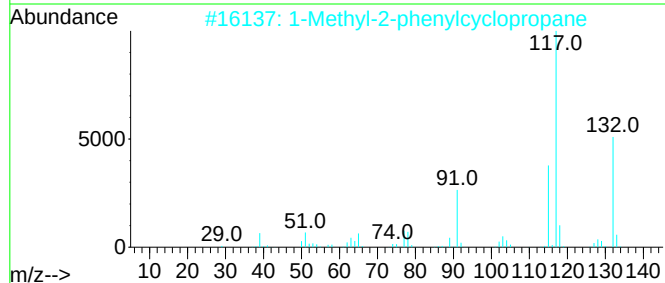
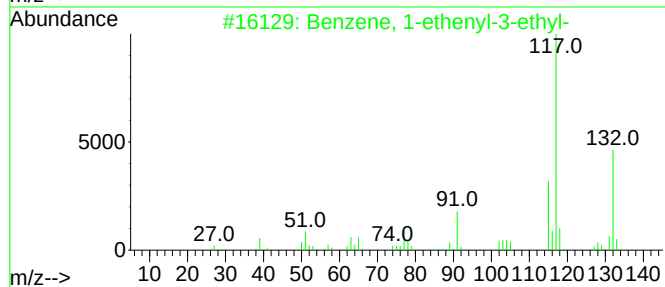
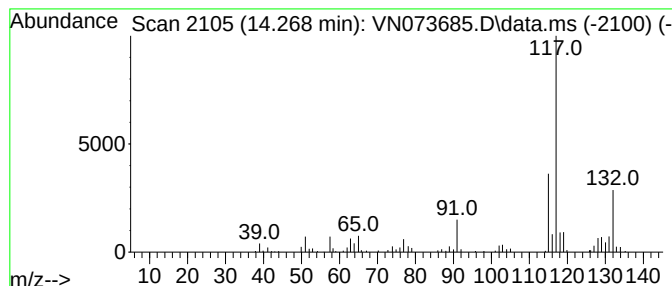
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	5.22 ug/l	205801	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
2			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
3			Indan, 1-methyl-	132	C10H12	000767-58-8	81
4			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	72
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073685.D
Acq On : 02 Aug 2022 14:22
Operator : JC\MD
Sample : N3971-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16SR

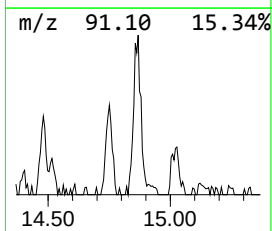
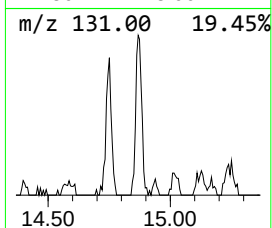
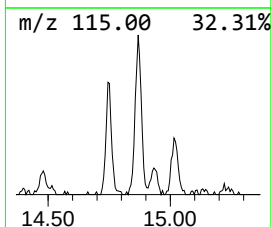
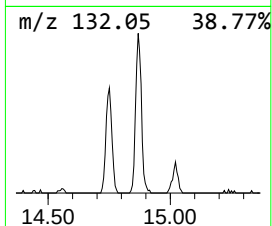
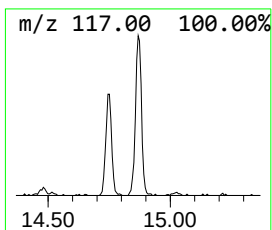
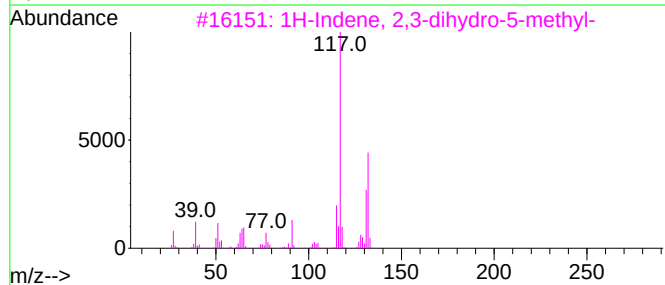
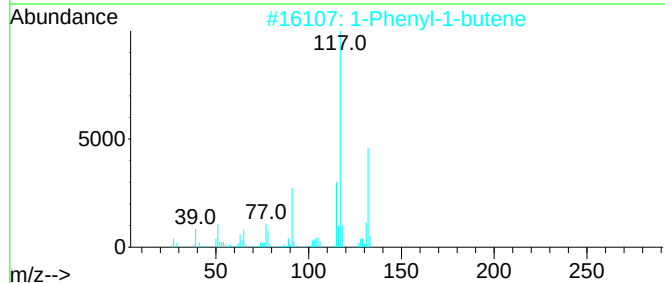
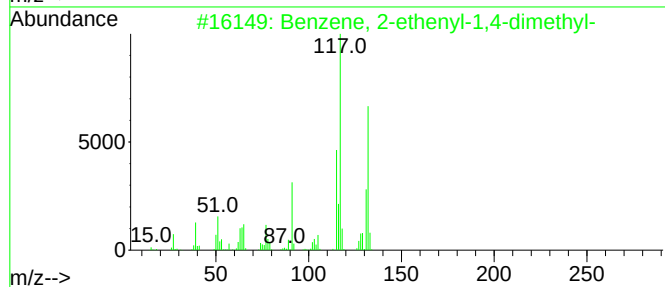
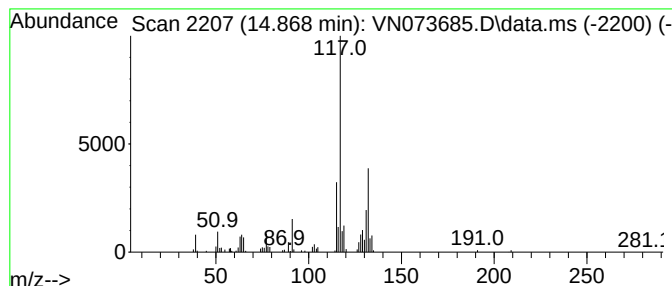
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	5.41 ug/l	213298	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	90
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073685.D
Acq On : 02 Aug 2022 14:22
Operator : JC\MD
Sample : N3971-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16SR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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
Butane, 2-methyl-	3.087	7.5	ug/l	168541	1	8.016	1131400	50.0
Isopropyl Alcohol	4.510	11.9	ug/l	269852	1	8.016	1131400	50.0
Di-sec-Butyl ether	10.586	6.8	ug/l	232132	3	11.686	1715620	50.0
Acetaldehyde, d...	10.657	7.0	ug/l	241982	3	11.686	1715620	50.0
Benzene, 1-ethy...	13.163	7.2	ug/l	284081	4	13.615	1972110	50.0
Indane	13.815	102.2	ug/l	4030510	4	13.615	1972110	50.0
Benzene, 1-ethe...	14.268	5.2	ug/l	205801	4	13.615	1972110	50.0
Benzene, 2-ethe...	14.868	5.4	ug/l	213298	4	13.615	1972110	50.0