

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
 Data File : VN076667.D
 Acq On : 14 Feb 2023 17:48
 Operator : JC\MD
 Sample : 01549-14
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1930

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\82N021323W.M
 Title : SW846 8260

Signal : TIC: VN076667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.096	23	27	38	rVB4	18536	30162	1.39%	0.117%
2	2.490	88	94	100	rBV2	34331	60835	2.80%	0.235%
3	2.831	144	152	159	rVB5	20152	46534	2.14%	0.180%
4	4.442	417	426	434	rBV	53828	152056	7.01%	0.588%
5	5.537	602	612	623	rBV4	18072	63639	2.93%	0.246%
6	7.236	888	901	915	rBV	303092	850340	39.18%	3.289%
7	7.495	940	945	953	rVB2	9418	22792	1.05%	0.088%
8	8.172	1050	1060	1065	rBV	267161	648192	29.86%	2.507%
9	8.230	1065	1070	1083	rVB2	501910	1093665	50.39%	4.230%
10	8.589	1116	1131	1143	rBV2	315574	880745	40.58%	3.407%
11	9.107	1209	1219	1228	rBV	730024	1489913	68.64%	5.763%
12	9.277	1240	1248	1253	rBV4	17264	39877	1.84%	0.154%
13	10.571	1457	1468	1475	rBV	1121827	2065798	95.17%	7.991%
14	10.630	1475	1478	1488	rVB2	89628	162717	7.50%	0.629%
15	11.301	1585	1592	1597	rBV5	18078	35286	1.63%	0.136%
16	11.866	1678	1688	1698	rBV	974023	1770958	81.59%	6.850%
17	11.966	1698	1705	1714	rVB	68515	130032	5.99%	0.503%
18	12.065	1716	1722	1731	rBV	234161	461614	21.27%	1.786%
19	12.401	1772	1779	1788	rBV	204440	380423	17.53%	1.472%
20	12.695	1822	1829	1835	rVB3	19507	36822	1.70%	0.142%
21	12.854	1848	1856	1865	rBV	743789	1313860	60.53%	5.082%
22	13.036	1882	1887	1892	rBV	62965	104532	4.82%	0.404%
23	13.101	1892	1898	1902	rBV	299273	530444	24.44%	2.052%
24	13.177	1907	1911	1918	rVB	160537	254433	11.72%	0.984%
25	13.336	1931	1938	1949	rVB	226831	406857	18.74%	1.574%
26	13.483	1957	1963	1969	rBV	742807	1212459	55.86%	4.690%
27	13.618	1981	1986	1991	rBV5	20101	38737	1.78%	0.150%
28	13.683	1991	1997	2001	rVV3	49691	93597	4.31%	0.362%
29	13.795	2009	2016	2025	rBV2	945001	2170577	100.00%	8.396%
30	13.877	2025	2030	2038	rVV	407769	686967	31.65%	2.657%
31	13.954	2038	2043	2045	rVV2	77083	125914	5.80%	0.487%
32	13.995	2045	2050	2066	rVB3	422860	1154587	53.19%	4.466%
33	14.118	2066	2071	2077	rVB9	27102	49275	2.27%	0.191%
34	14.183	2077	2082	2087	rVB	72663	115598	5.33%	0.447%
35	14.248	2087	2093	2095	rBV3	136655	206532	9.52%	0.799%
36	14.277	2095	2098	2103	rVV2	107414	162559	7.49%	0.629%

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37	14.330	2103	2107	2113	rVV	166216	264478	12.18%	1.023%
38	14.401	2113	2119	2122	rVV	64132	111453	5.13%	0.431%
39	14.448	2122	2127	2135	rVB2	217595	371545	17.12%	1.437%
40	14.577	2144	2149	2154	rBV2	76415	124731	5.75%	0.482%
41	14.659	2157	2163	2166	rVV	100625	168628	7.77%	0.652%
42	14.695	2166	2169	2174	rVV2	163837	246968	11.38%	0.955%
43	14.736	2174	2176	2180	rVV4	31280	36772	1.69%	0.142%
44	14.877	2193	2200	2204	rBV6	36081	72086	3.32%	0.279%
45	14.930	2204	2209	2214	rBV	244658	403007	18.57%	1.559%
46	15.054	2221	2230	2236	rBV2	475123	1019153	46.95%	3.942%
47	15.118	2237	2241	2249	rVV6	53338	129886	5.98%	0.502%
48	15.212	2250	2257	2264	rVV	433002	796502	36.70%	3.081%
49	15.324	2264	2276	2288	rVV5	106514	450474	20.75%	1.742%
50	15.442	2289	2296	2306	rVB5	104375	302034	13.91%	1.168%
51	15.583	2315	2320	2325	rBV2	102393	190619	8.78%	0.737%
52	15.659	2325	2333	2337	rVV2	139041	395628	18.23%	1.530%
53	15.701	2337	2340	2345	rVV3	82369	151038	6.96%	0.584%
54	15.783	2345	2354	2375	rVB9	74837	370556	17.07%	1.433%
55	15.948	2375	2382	2388	rVB2	58195	119116	5.49%	0.461%
56	16.130	2402	2413	2414	rBV6	52081	129614	5.97%	0.501%
57	16.171	2414	2420	2430	rVV5	164541	406059	18.71%	1.571%
58	16.259	2431	2435	2439	rVV6	22265	43793	2.02%	0.169%
59	16.342	2442	2449	2465	rVB8	43700	161725	7.45%	0.626%
60	16.506	2468	2477	2485	rBV3	108135	255748	11.78%	0.989%
61	16.718	2502	2513	2518	rBV9	30512	81343	3.75%	0.315%

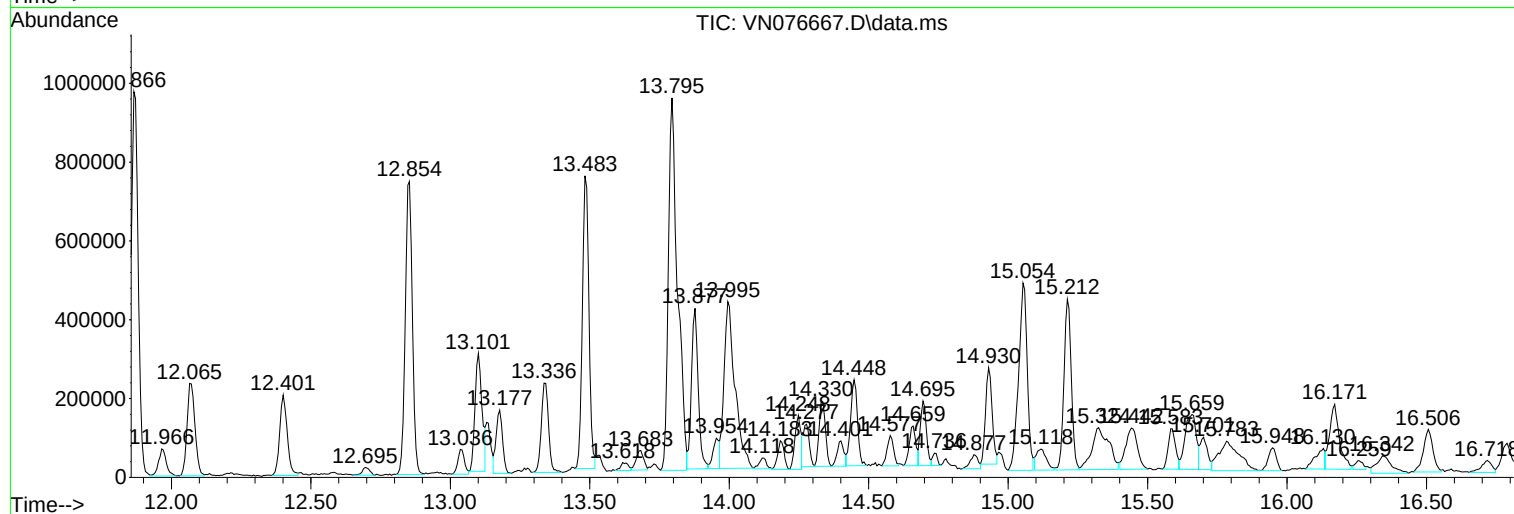
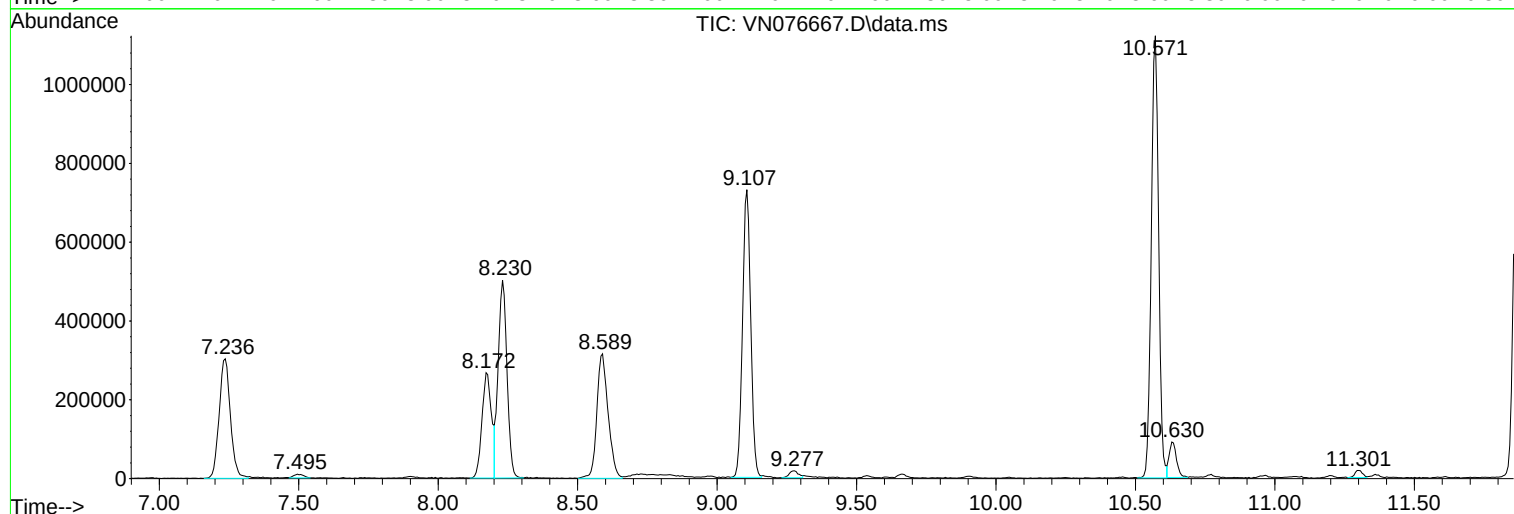
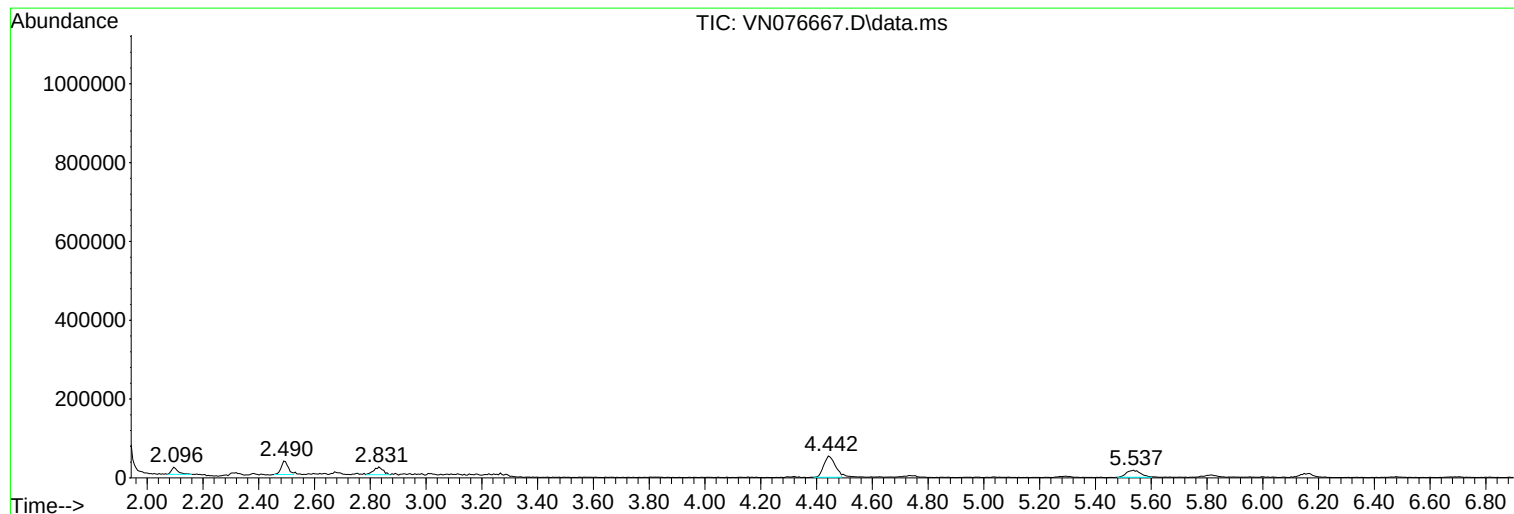
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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



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MSVOA_N
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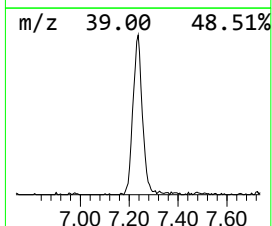
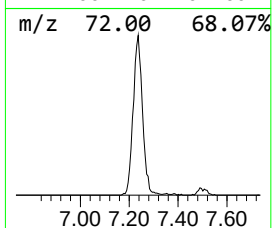
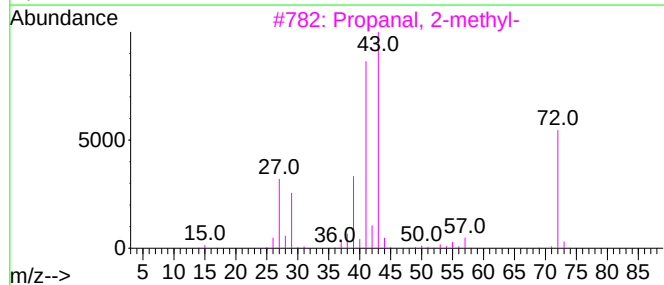
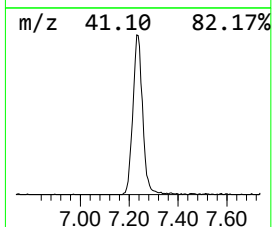
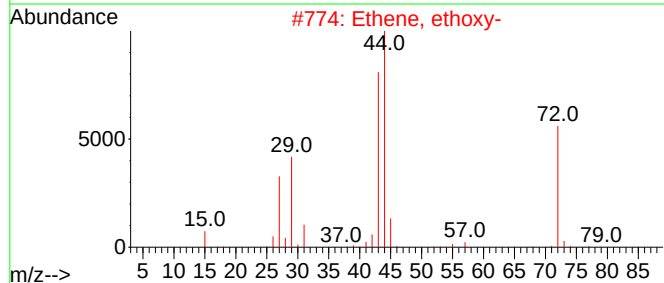
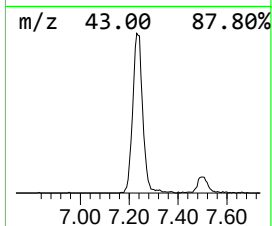
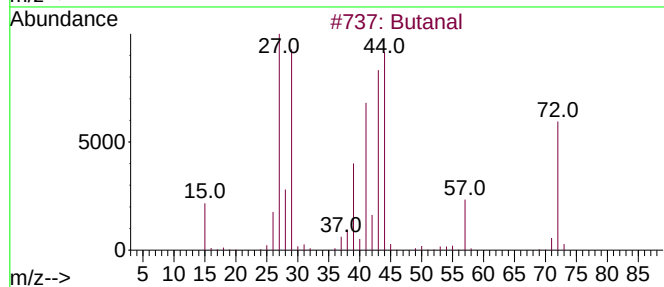
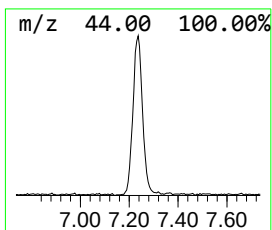
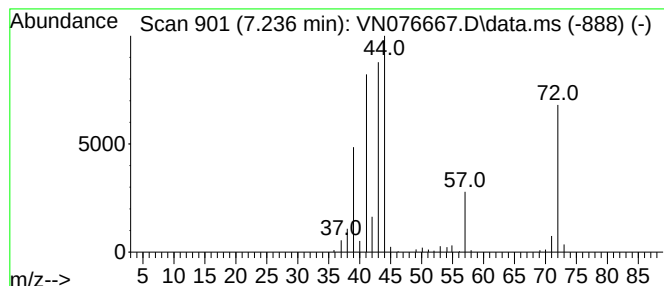
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.236	38.88 ug/l	850340	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23
5			2-Butenal, (E)-	70	C4H6O	000123-73-9	22



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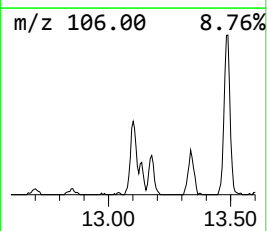
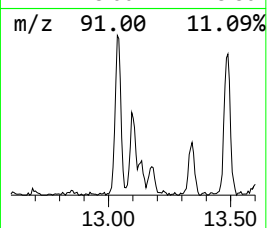
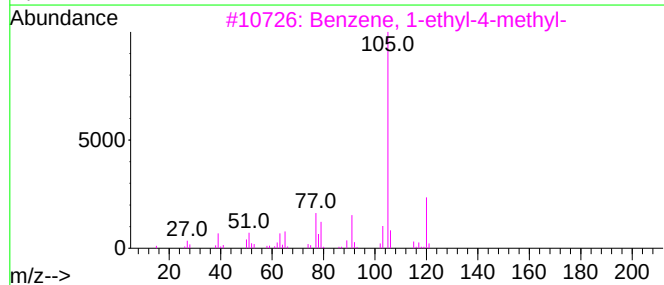
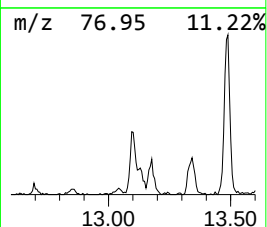
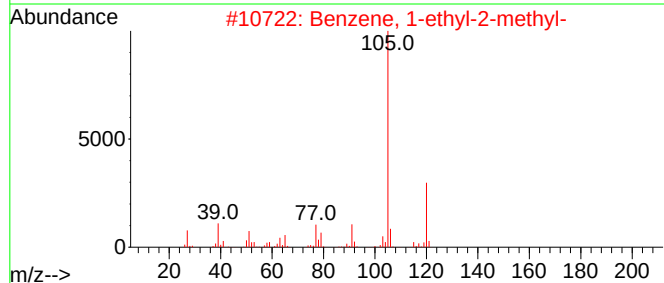
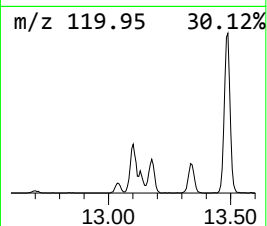
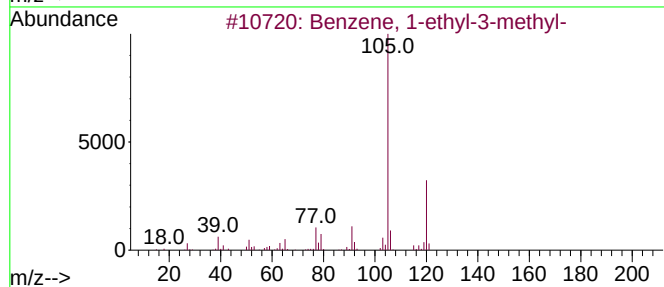
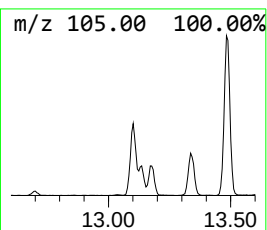
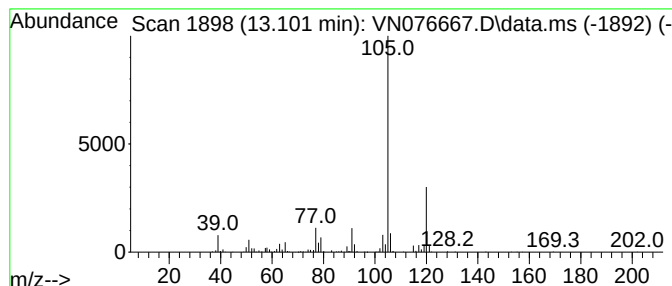
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.101	12.22 ug/l	530444	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



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ALS Vial : 17 Sample Multiplier: 1

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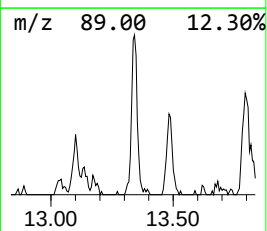
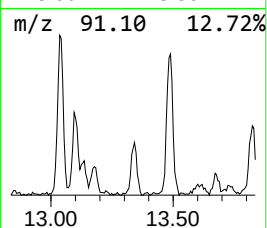
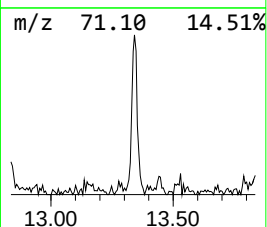
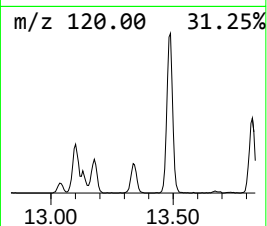
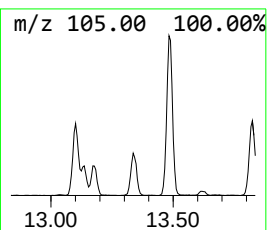
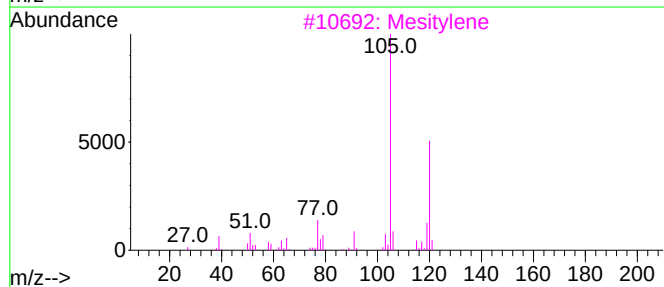
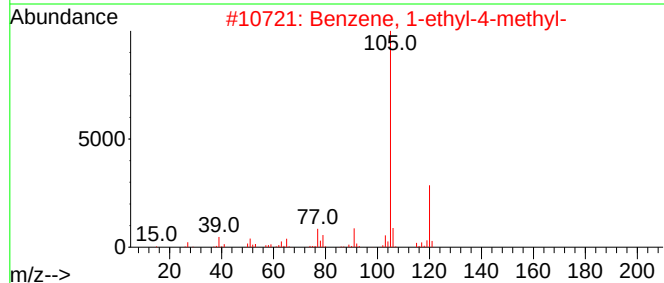
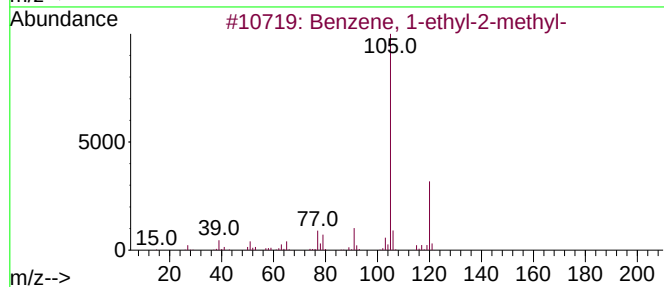
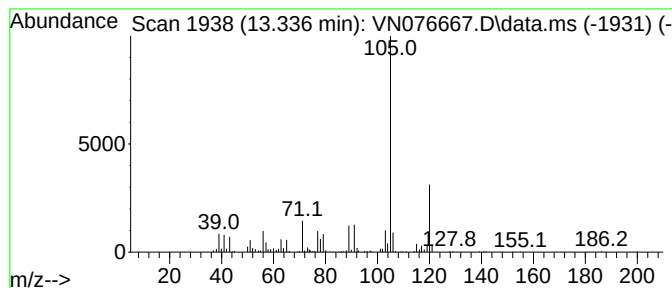
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.336	9.37 ug/l	406857	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	76
3			Mesitylene	120	C9H12	000108-67-8	76
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	76
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	70



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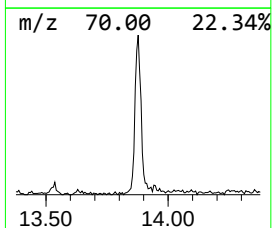
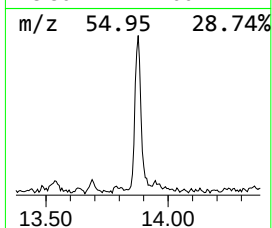
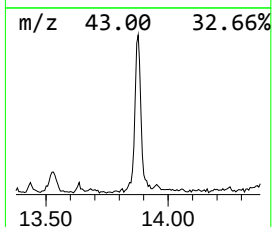
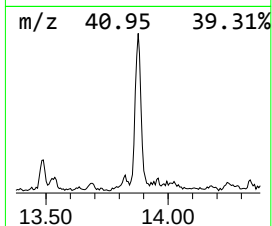
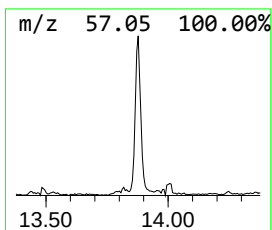
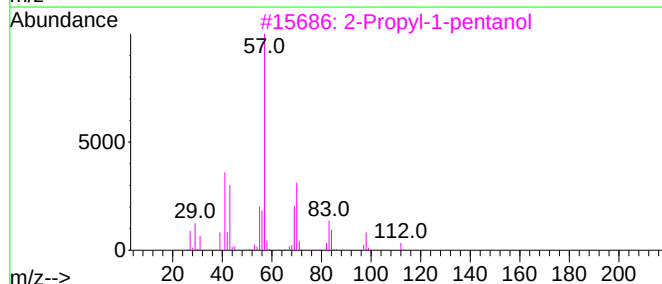
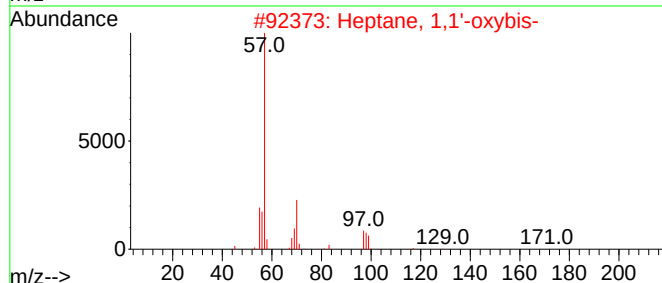
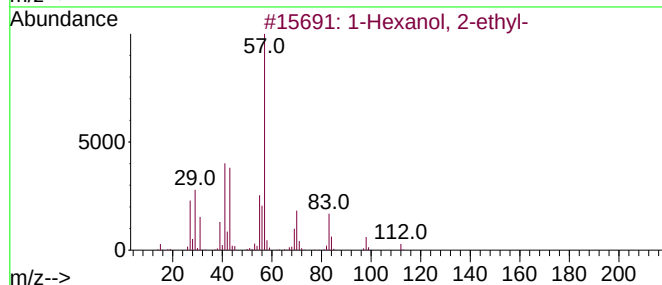
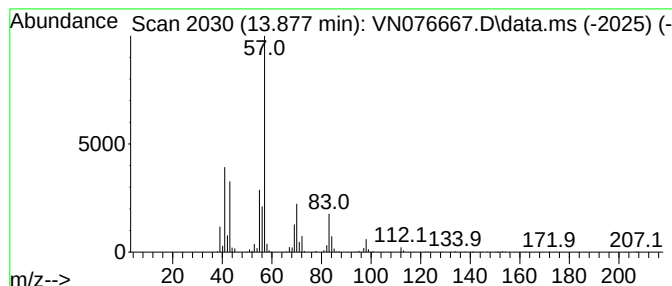
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.877	15.82 ug/l	686967	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50



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ClientSampleId :
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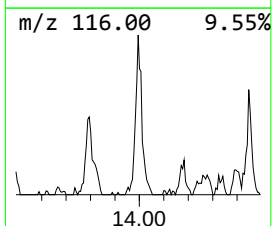
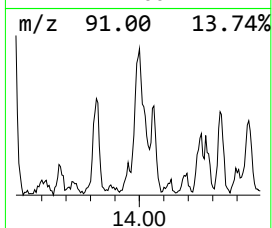
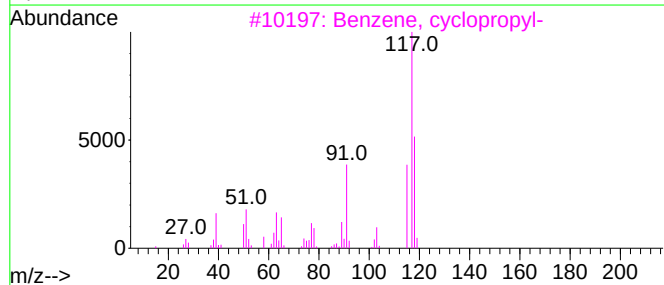
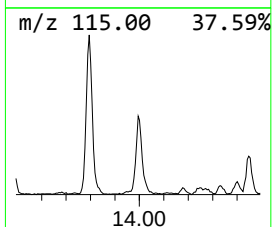
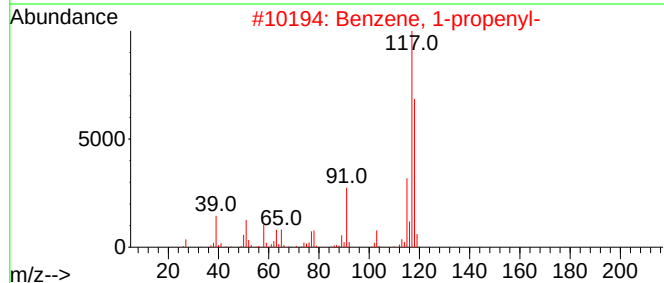
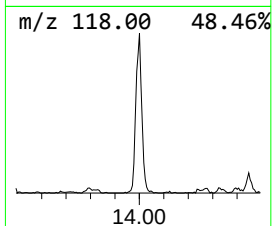
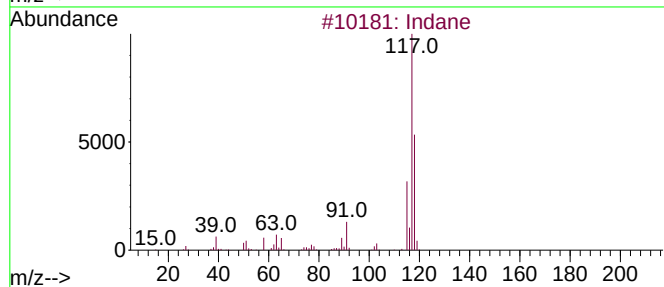
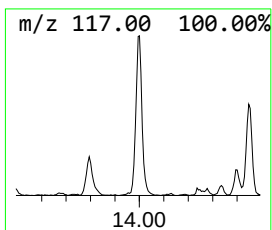
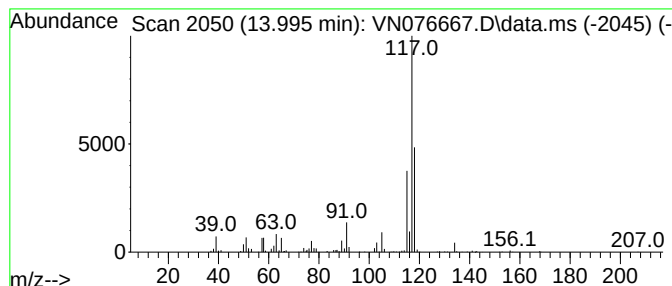
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.995	26.60 ug/l	1154590	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	76
5			Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076667.D
Acq On : 14 Feb 2023 17:48
Operator : JC\MD
Sample : 01549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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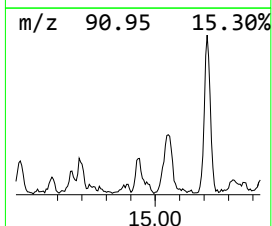
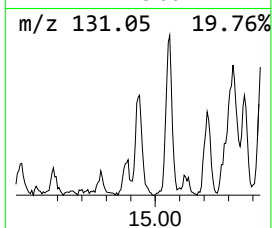
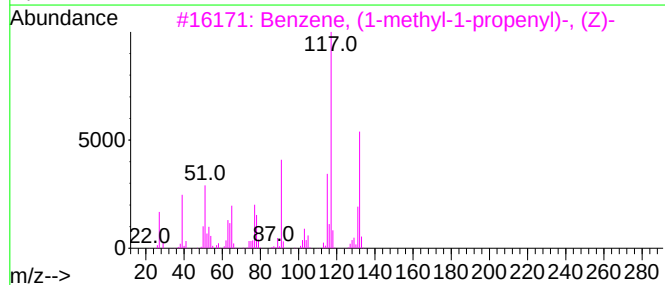
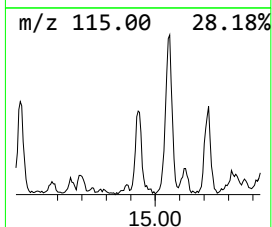
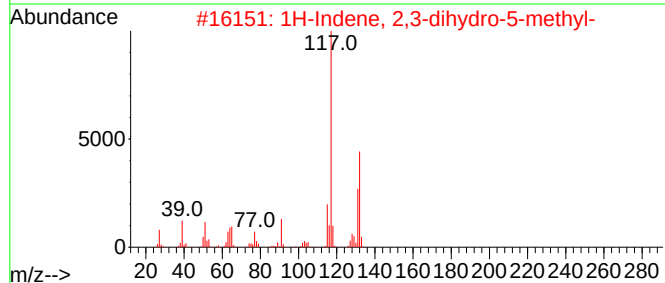
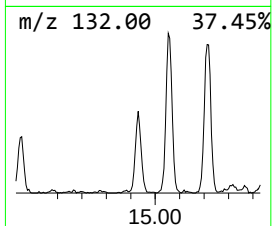
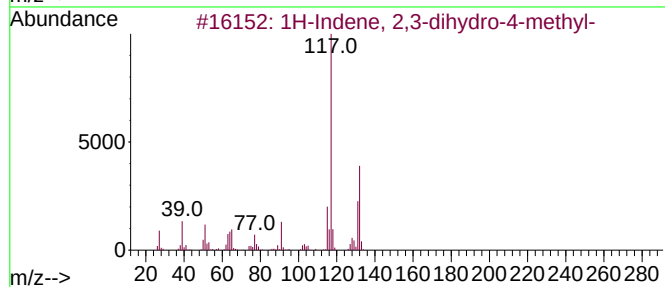
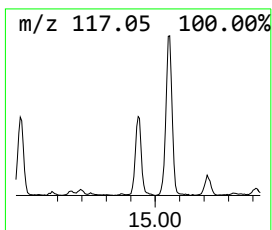
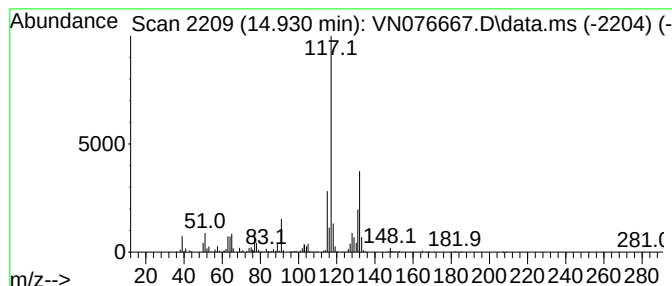
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	9.28 ug/l	403007	1,4-Dichlorobenzene-d4	13.795

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	87
4		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076667.D
Acq On : 14 Feb 2023 17:48
Operator : JC\MD
Sample : 01549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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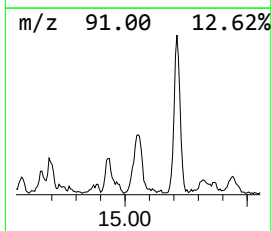
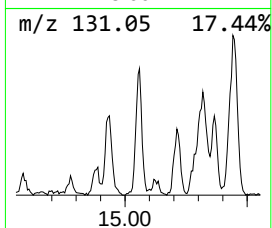
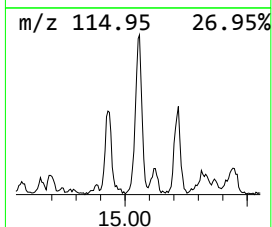
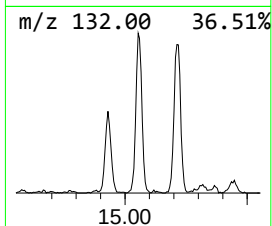
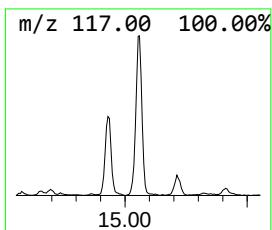
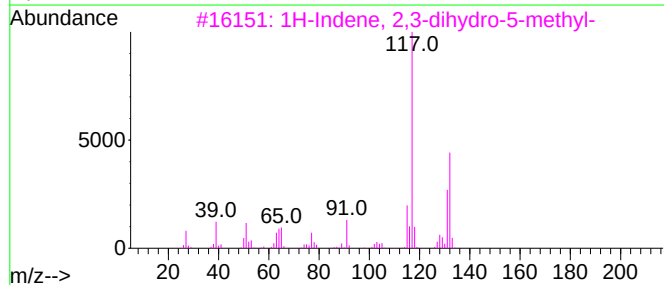
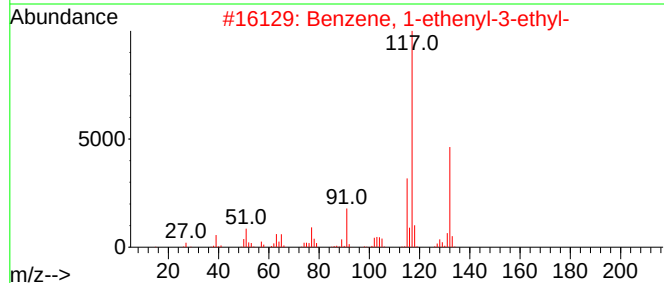
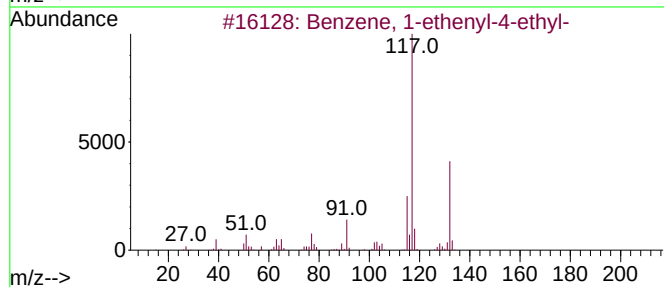
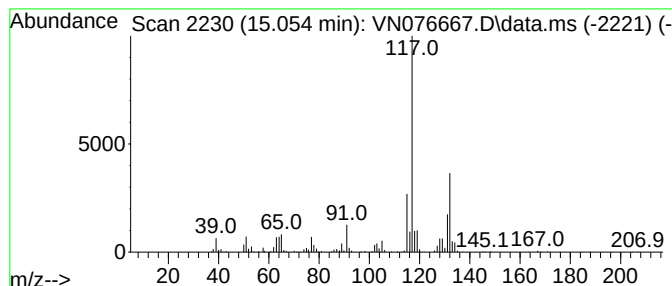
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.054	23.48 ug/l	1019150	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076667.D
Acq On : 14 Feb 2023 17:48
Operator : JC\MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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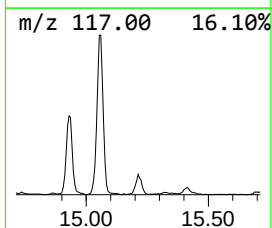
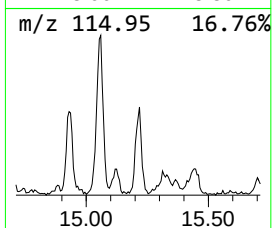
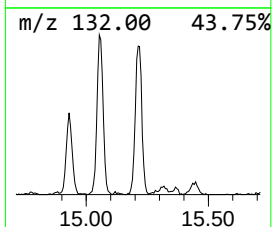
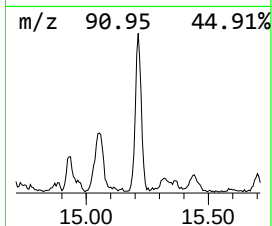
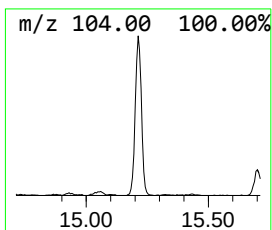
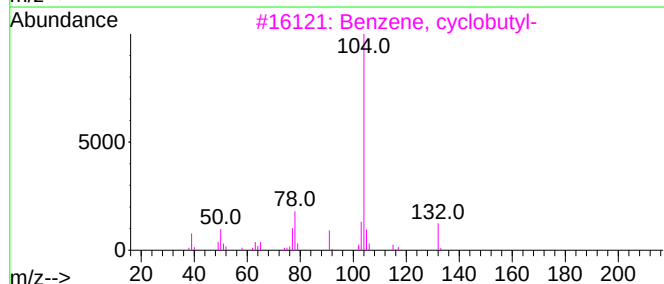
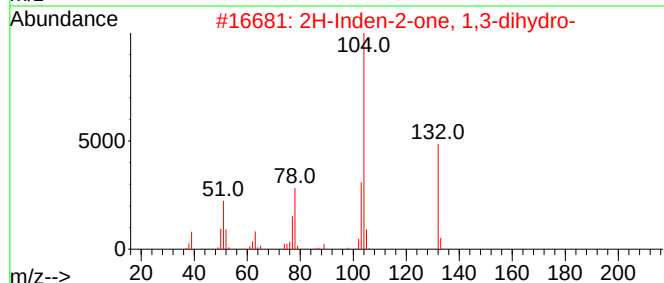
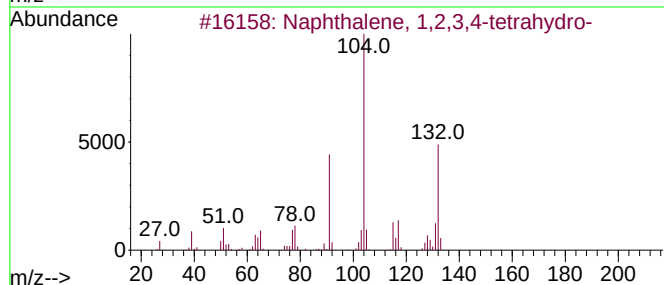
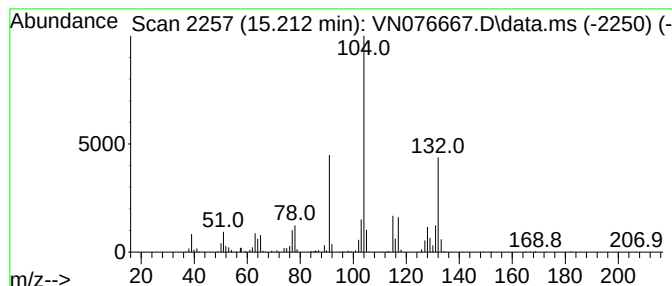
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	18.35 ug/l	796502	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	97
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	58
3			Benzene, cyclobutyl-	132	C10H12	004392-30-7	53
4			Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	47
5			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076667.D
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Operator : JC\MD
Sample : 01549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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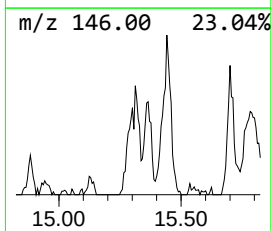
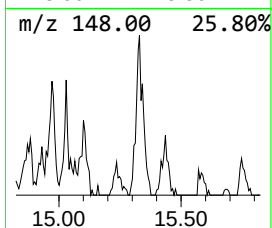
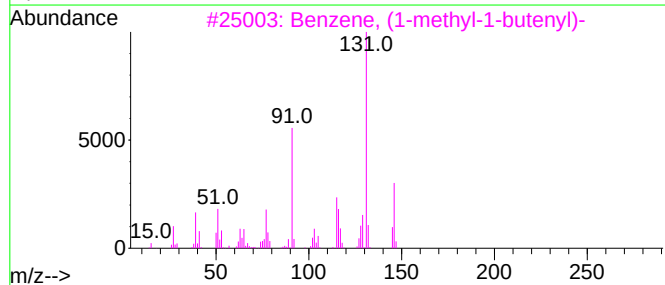
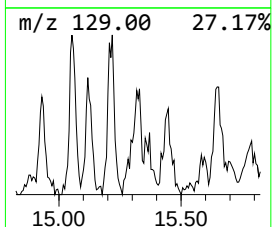
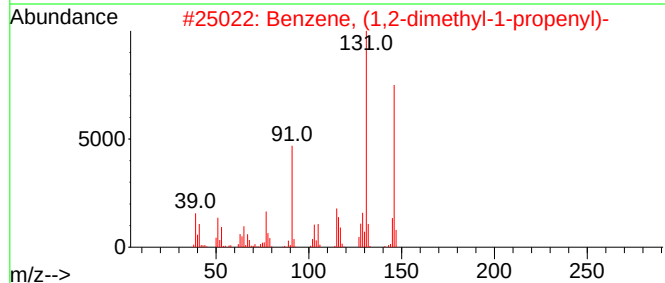
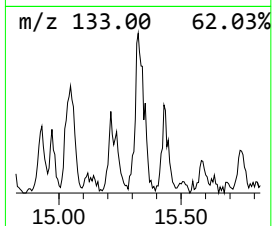
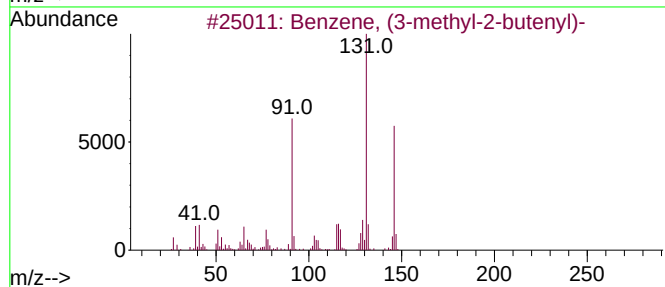
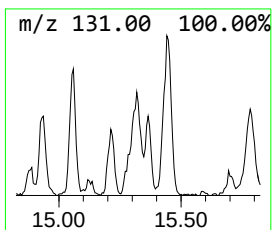
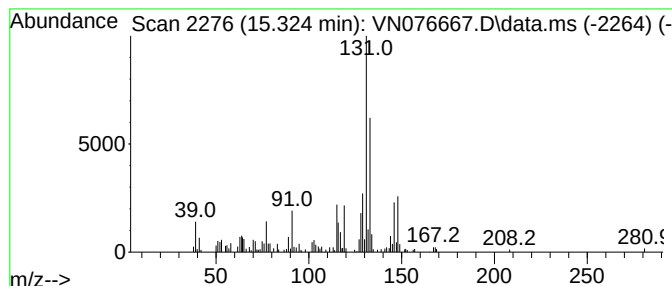
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, (3-methyl-2-butenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.324	10.38 ug/l	450474	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	90
2			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60
3			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	60
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	60
5			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076667.D
Acq On : 14 Feb 2023 17:48
Operator : JC\MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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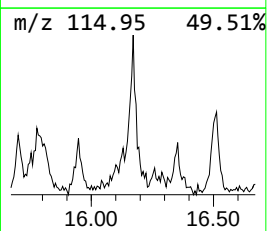
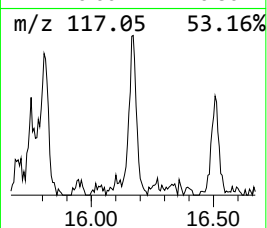
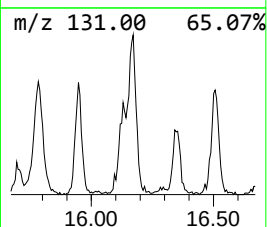
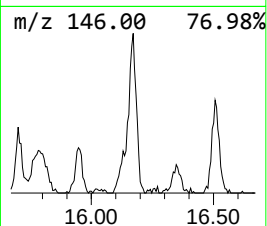
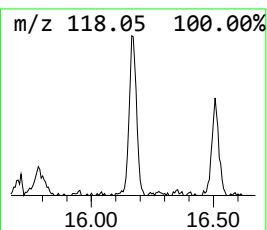
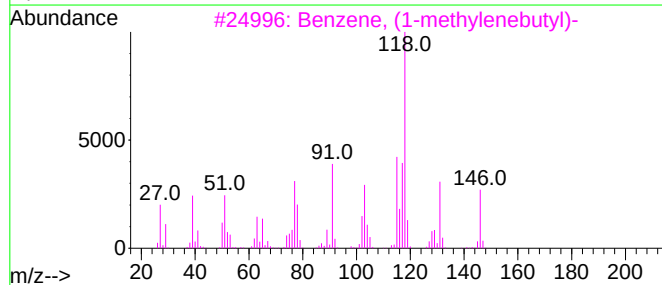
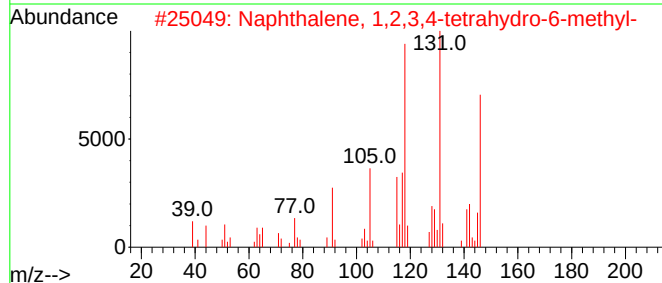
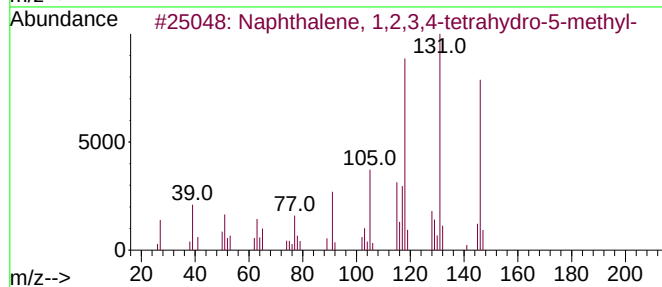
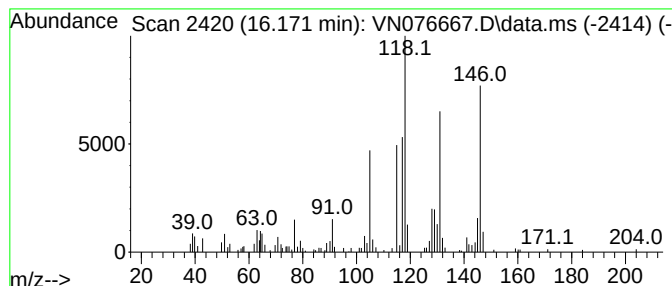
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.171	9.35 ug/l	406059	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	76
3			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	72
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	55
5			1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076667.D
Acq On : 14 Feb 2023 17:48
Operator : JC\MD
Sample : 01549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.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-ethy...	13.101	12.2	ug/l	530444	4	13.795	2170580	50.0
Benzene, 1-ethy...	13.336	9.4	ug/l	406857	4	13.795	2170580	50.0
1-Hexanol, 2-et...	13.877	15.8	ug/l	686967	4	13.795	2170580	50.0
Indane	13.995	26.6	ug/l	1154590	4	13.795	2170580	50.0
1H-Indene, 2,3-...	14.930	9.3	ug/l	403007	4	13.795	2170580	50.0
Benzene, 1-ethe...	15.054	23.5	ug/l	1019150	4	13.795	2170580	50.0
Naphthalene, 1,...	15.212	18.4	ug/l	796502	4	13.795	2170580	50.0
Benzene, (3-met...	15.324	10.4	ug/l	450474	4	13.795	2170580	50.0
Naphthalene, 1,...	16.171	9.3	ug/l	406059	4	13.795	2170580	50.0