

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
 Data File : VN080246.D
 Acq On : 22 Nov 2023 14:30
 Operator : JC\MD
 Sample : 05518-04 20X
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1109

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\82N111623W.M
 Title : SW846 8260

Signal : TIC: VN080246.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	51	57	64	rBV	10266	20844	2.00%	0.268%
2	2.836	142	150	156	rVB6	9638	20473	1.96%	0.264%
3	7.230	886	897	908	rBV5	23809	67099	6.43%	0.864%
4	7.435	924	932	942	rBV2	7337	18620	1.78%	0.240%
5	8.171	1046	1057	1061	rBV	158832	375719	36.01%	4.836%
6	8.229	1061	1067	1077	rVB	229228	525603	50.38%	6.765%
7	8.582	1112	1127	1138	rBV	158525	373503	35.80%	4.807%
8	9.106	1207	1216	1231	rBV	341882	707811	67.85%	9.110%
9	9.271	1236	1244	1253	rBV2	55190	116079	11.13%	1.494%
10	9.606	1294	1301	1306	rBV3	8541	17457	1.67%	0.225%
11	10.570	1456	1465	1472	rBV	566863	1043262	100.00%	13.428%
12	10.635	1472	1476	1482	rVB	14205	25846	2.48%	0.333%
13	10.747	1489	1495	1501	rVB3	15220	26385	2.53%	0.340%
14	11.276	1580	1585	1589	rBV2	7406	11384	1.09%	0.147%
15	11.647	1639	1648	1658	rVB7	13206	29230	2.80%	0.376%
16	11.753	1658	1666	1672	rBV2	10240	16052	1.54%	0.207%
17	11.870	1675	1686	1696	rBV	553833	995020	95.38%	12.807%
18	11.965	1697	1702	1707	rVB2	8410	14681	1.41%	0.189%
19	12.070	1713	1720	1730	rBV2	73004	135538	12.99%	1.745%
20	12.400	1766	1776	1783	rBV3	20464	50041	4.80%	0.644%
21	12.488	1786	1791	1797	rVB5	7020	11108	1.06%	0.143%
22	12.770	1831	1839	1841	rBV6	7389	15266	1.46%	0.196%
23	12.853	1846	1853	1863	rVB	476043	829945	79.55%	10.682%
24	13.100	1888	1895	1900	rBV3	12567	25173	2.41%	0.324%
25	13.164	1900	1906	1913	rVB3	52837	105734	10.13%	1.361%
26	13.341	1927	1936	1942	rBV6	12898	32288	3.09%	0.416%
27	13.482	1956	1960	1965	rVB2	19987	32402	3.11%	0.417%
28	13.729	1998	2002	2005	rVV4	13436	23862	2.29%	0.307%
29	13.794	2007	2013	2021	rVV	580656	991140	95.00%	12.757%
30	13.864	2021	2025	2031	rVB5	14397	31652	3.03%	0.407%
31	14.111	2061	2067	2074	rBV2	63638	110576	10.60%	1.423%
32	14.270	2091	2094	2098	rVV5	7096	12695	1.22%	0.163%
33	14.329	2100	2104	2109	rVB4	9171	15319	1.47%	0.197%
34	14.441	2117	2123	2127	rBV6	6343	13576	1.30%	0.175%
35	14.506	2127	2134	2140	rVV8	12410	29407	2.82%	0.378%
36	14.588	2140	2148	2151	rVV7	11694	26878	2.58%	0.346%

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37	14.629	2151	2155	2158	rVV5	31438	54085	5.18%	0.696%
38	14.664	2158	2161	2165	rVV2	34482	56967	5.46%	0.733%
39	14.741	2169	2174	2176	rVV5	12840	21690	2.08%	0.279%
40	14.776	2176	2180	2187	rVV5	22220	53193	5.10%	0.685%
41	14.835	2187	2190	2196	rVB5	10533	20398	1.96%	0.263%
42	14.964	2207	2212	2220	rVB	79609	117892	11.30%	1.517%
43	15.041	2220	2225	2229	rBV5	20214	41958	4.02%	0.540%
44	15.182	2244	2249	2253	rBV7	7205	13951	1.34%	0.180%
45	15.235	2253	2258	2259	rBV5	10913	15974	1.53%	0.206%
46	15.335	2268	2275	2279	rBV9	12898	34320	3.29%	0.442%
47	15.405	2282	2287	2288	rBV5	15795	22176	2.13%	0.285%
48	15.511	2301	2305	2308	rBV6	18138	32796	3.14%	0.422%
49	15.594	2315	2319	2325	rBV5	22560	46704	4.48%	0.601%
50	15.835	2355	2360	2371	rVB2	91661	168760	16.18%	2.172%
51	16.176	2413	2418	2426	rBV8	25400	61322	5.88%	0.789%
52	16.317	2436	2442	2445	rBV8	16384	29163	2.80%	0.375%
53	16.488	2463	2471	2472	rBV6	17097	37437	3.59%	0.482%
54	16.541	2478	2480	2488	rVB7	16349	28584	2.74%	0.368%
55	16.617	2490	2493	2498	rVB6	10030	14320	1.37%	0.184%

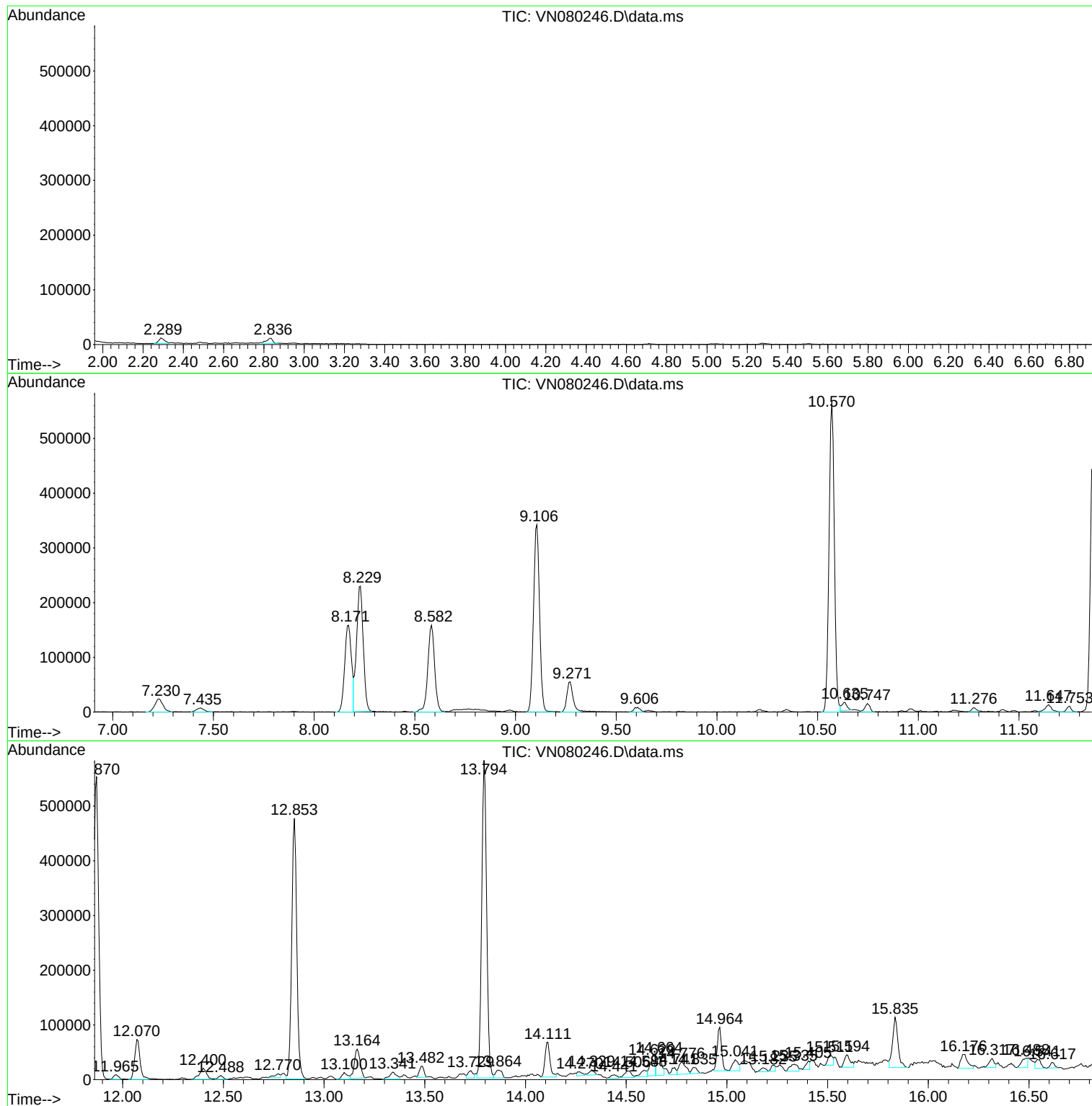
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Quant Title : SW846 8260

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



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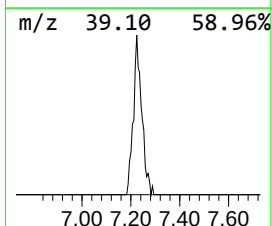
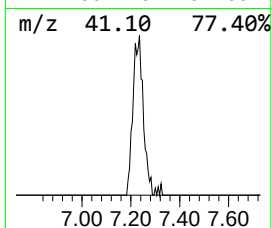
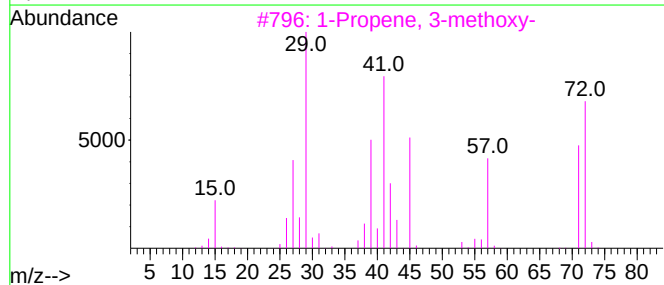
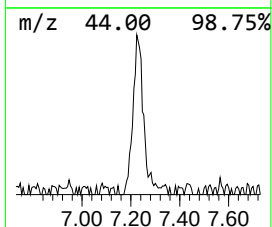
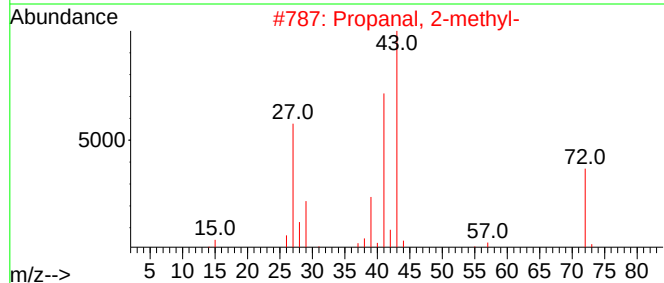
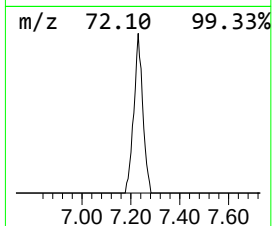
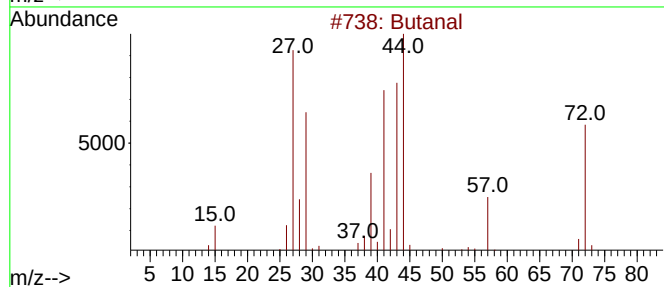
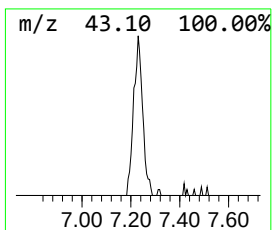
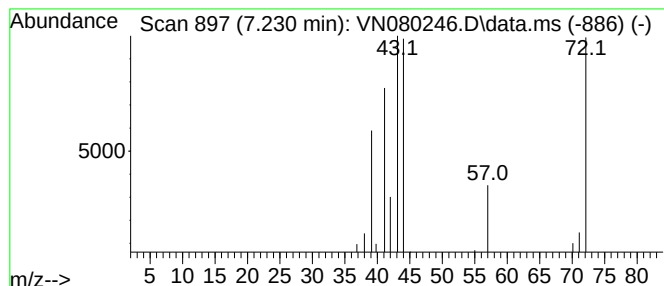
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	6.38 ug/l	67099	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	58
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
4			Propane	44	C3H8	000074-98-6	38
5			2-Hexynoic acid	112	C6H8O2	000764-33-0	23



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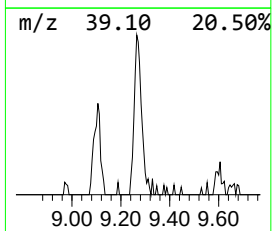
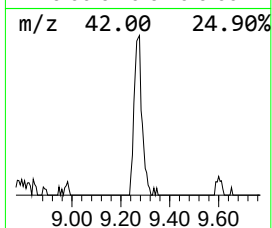
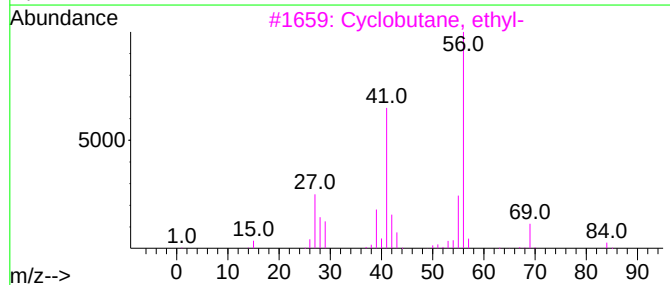
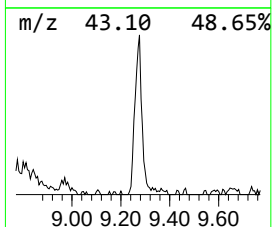
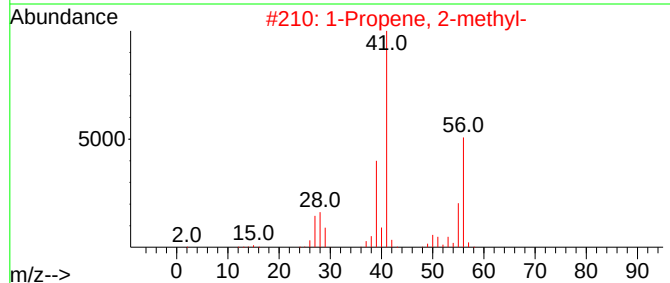
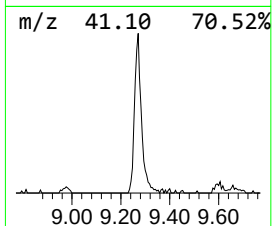
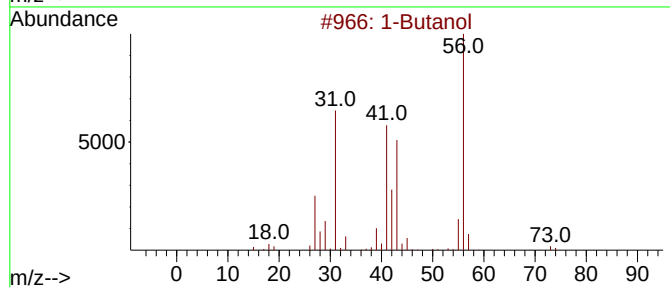
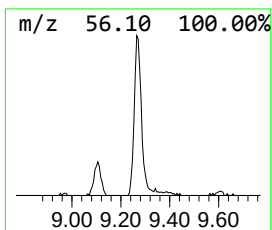
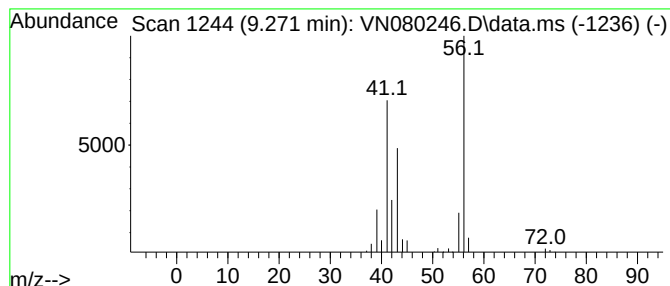
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	8.20 ug/l	116079	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			1-Propene, 2-methyl-	56	C4H8	000115-11-7	40
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	39
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	9



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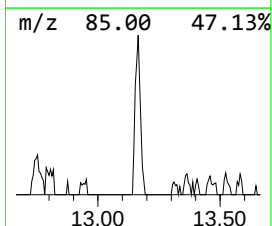
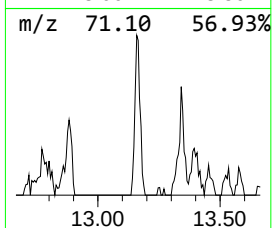
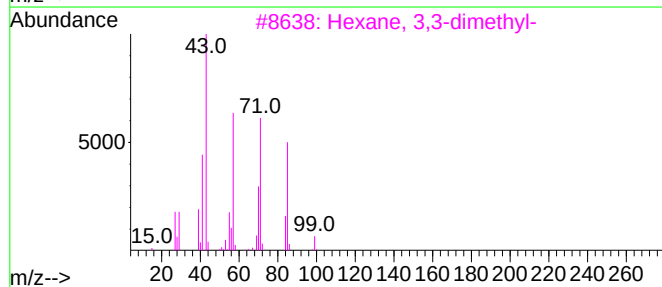
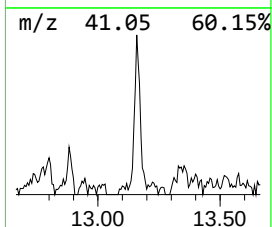
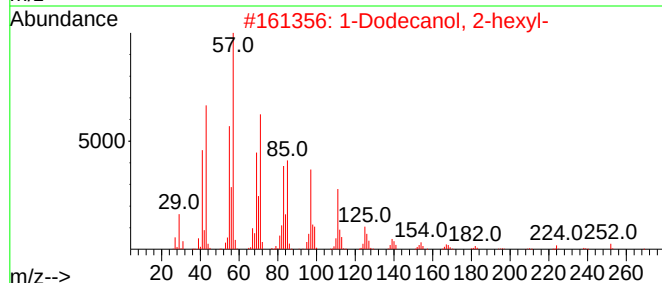
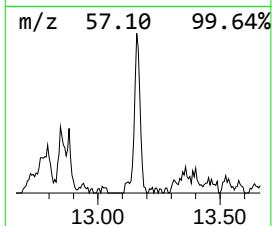
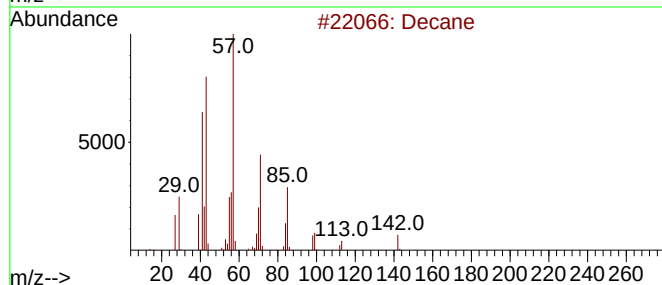
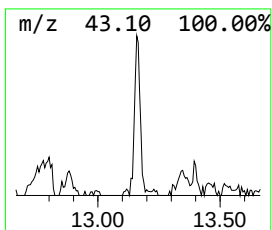
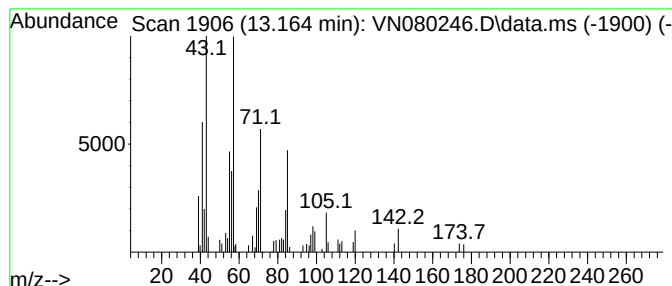
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Quant Title : SW846 8260

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

Peak Number 3 Decane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.164	5.33 ug/l	105734	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	93
2			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	78
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Pentadecane	212	C15H32	000629-62-9	53
5			Tetradecane	198	C14H30	000629-59-4	53



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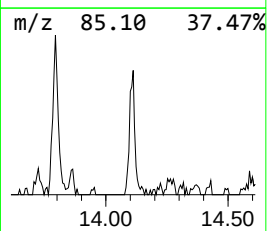
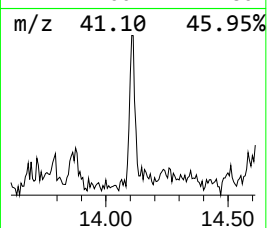
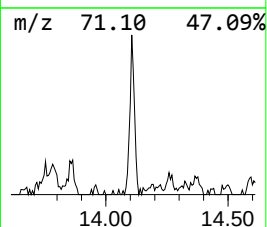
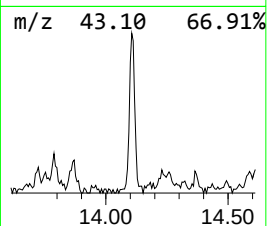
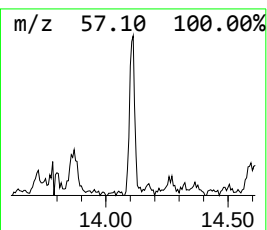
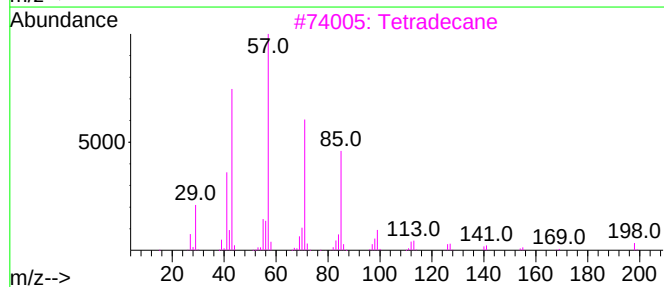
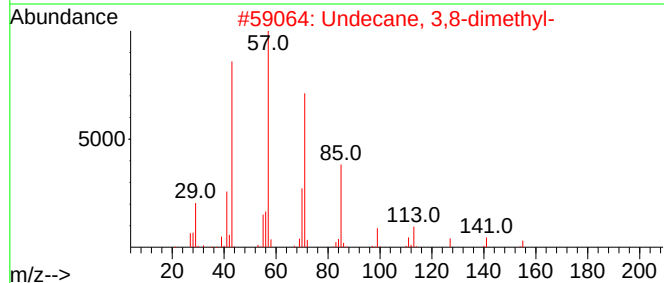
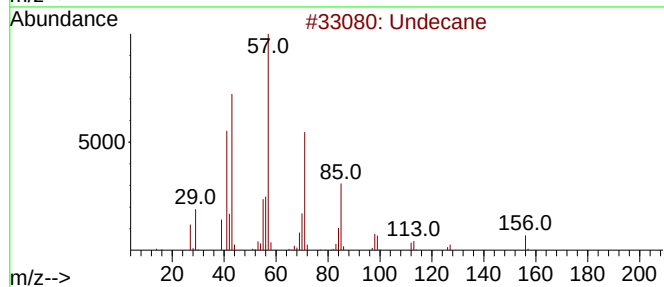
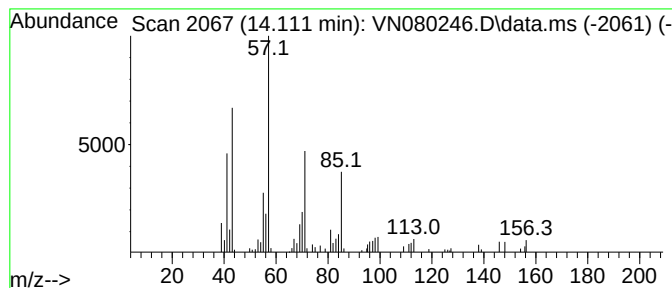
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.111	5.58 ug/l	110576	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	59
3	Tetradecane	198	C14H30	000629-59-4	58
4	Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	53
5	Pentadecane	212	C15H32	000629-62-9	53



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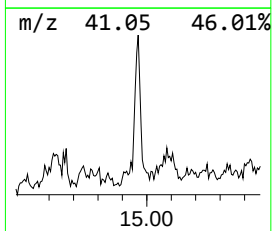
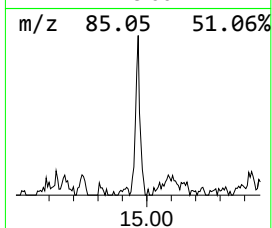
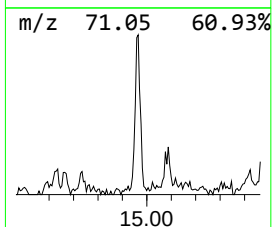
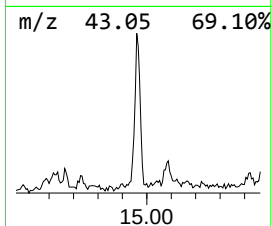
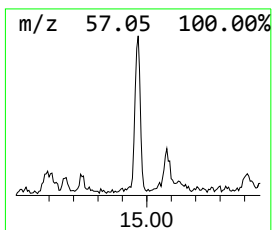
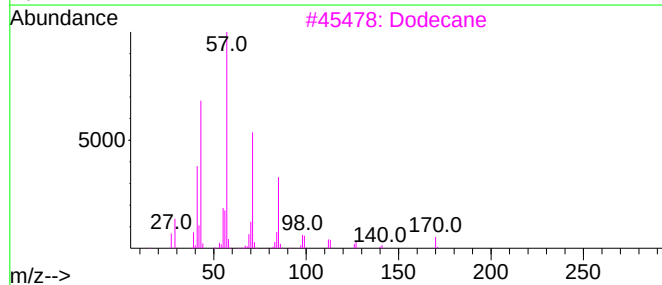
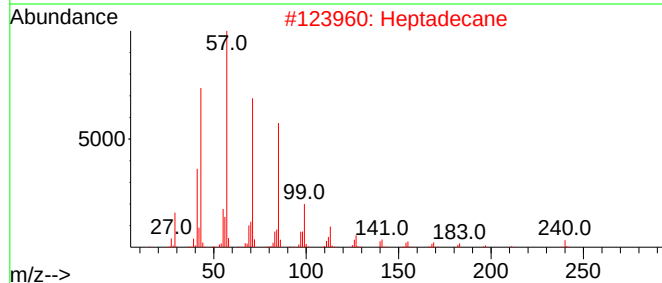
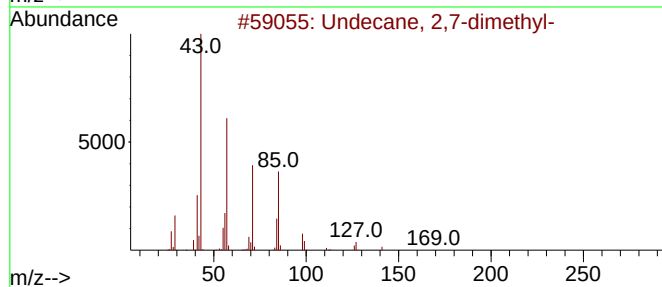
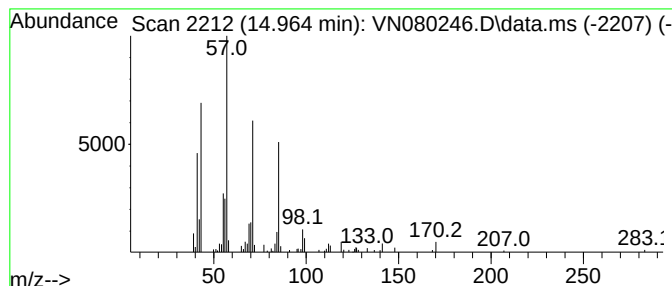
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Quant Title : SW846 8260

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

Peak Number 5 Undecane, 2,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	5.95 ug/l	117892	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	80
2			Heptadecane	240	C17H36	000629-78-7	80
3			Dodecane	170	C12H26	000112-40-3	76
4			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	72
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080246.D
Acq On : 22 Nov 2023 14:30
Operator : JC\MD
Sample : 05518-04 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

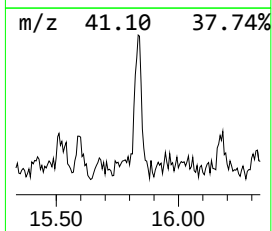
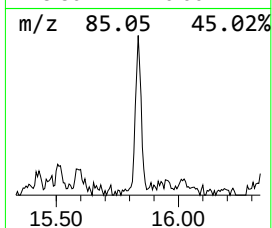
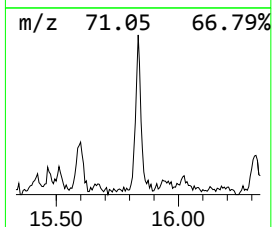
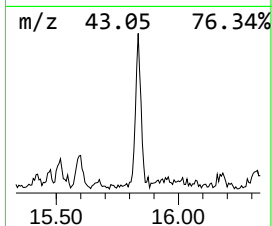
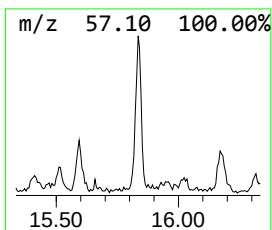
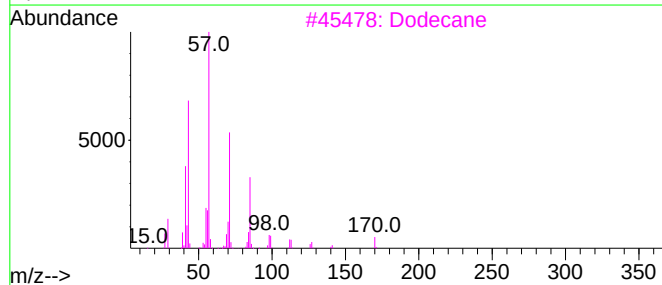
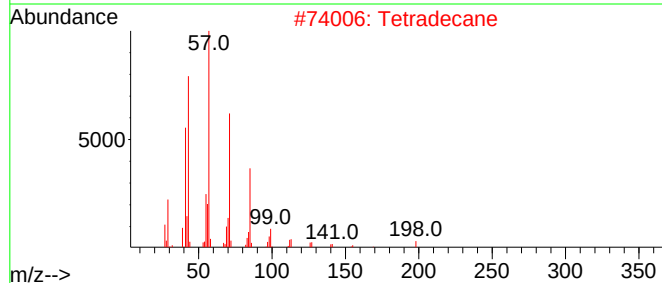
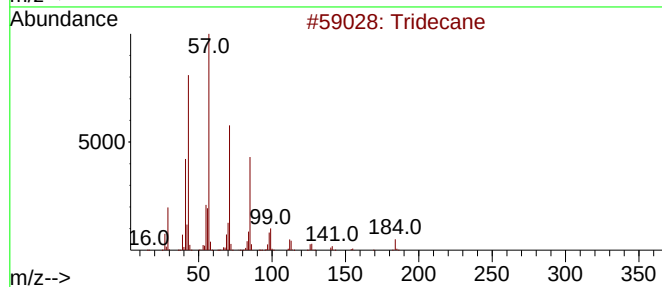
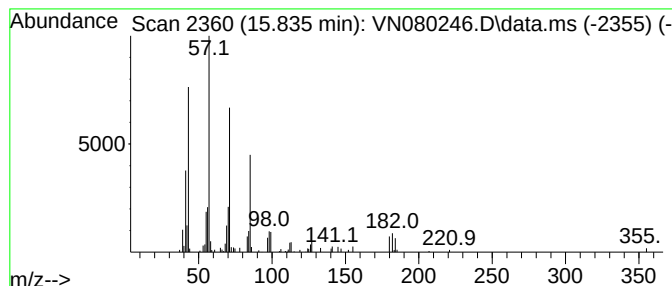
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Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	8.51 ug/l	168760	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	97
2		Tetradecane	198	C14H30	000629-59-4	86
3		Dodecane	170	C12H26	000112-40-3	86
4		Pentadecane	212	C15H32	000629-62-9	72
5		Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112223\
Data File : VN080246.D
Acq On : 22 Nov 2023 14:30
Operator : JC\MD
Sample : 05518-04 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.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
Butanal	7.230	6.4	ug/l	67099	1	8.224	525603	50.0
1-Butanol	9.271	8.2	ug/l	116079	2	9.106	707811	50.0
Decane	13.164	5.3	ug/l	105734	4	13.794	991140	50.0
Undecane	14.111	5.6	ug/l	110576	4	13.794	991140	50.0
Undecane, 2,7-d...	14.964	6.0	ug/l	117892	4	13.794	991140	50.0
Tridecane	15.835	8.5	ug/l	168760	4	13.794	991140	50.0