

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022421\
 Data File : VN066006.D
 Acq On : 24 Feb 2021 16:05
 Operator : JC/MD
 Sample : M1473-09
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 GW803-32-37-022321

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\82N021721W.M
 Title : SW846 8260

Signal : TIC: VN066006.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.814	17	23	34	rBV6	4926	7240	1.12%	0.195%
2	2.312	170	178	185	rBV2	4535	6695	1.03%	0.181%
3	3.714	602	614	627	rVB4	5721	14523	2.25%	0.392%
4	4.036	699	714	730	rBV2	4674	13005	2.01%	0.351%
5	6.785	1556	1569	1571	rBV4	6773	10400	1.61%	0.280%
6	7.335	1721	1740	1758	rBV2	29522	74641	11.54%	2.013%
7	7.553	1789	1808	1819	rBV	80480	200811	31.04%	5.415%
8	7.627	1819	1831	1851	rVB	156879	371422	57.42%	10.016%
9	7.991	1927	1944	1968	rBV2	90616	213795	33.05%	5.766%
10	8.550	2102	2118	2138	rBV	223857	469184	72.53%	12.653%
11	9.132	2287	2299	2310	rVB2	8541	16392	2.53%	0.442%
12	9.370	2361	2373	2388	rBV	14145	27113	4.19%	0.731%
13	10.058	2572	2587	2604	rBV	352814	646864	100.00%	17.445%
14	10.823	2814	2825	2849	rBV2	60857	116067	17.94%	3.130%
15	11.380	2984	2998	3022	rBV	315104	554412	85.71%	14.951%
16	12.106	3212	3224	3238	rBV2	39871	79129	12.23%	2.134%
17	12.373	3295	3307	3332	rVB	234746	410405	63.45%	11.068%
18	13.315	3587	3600	3621	rBV	270386	476018	73.59%	12.837%

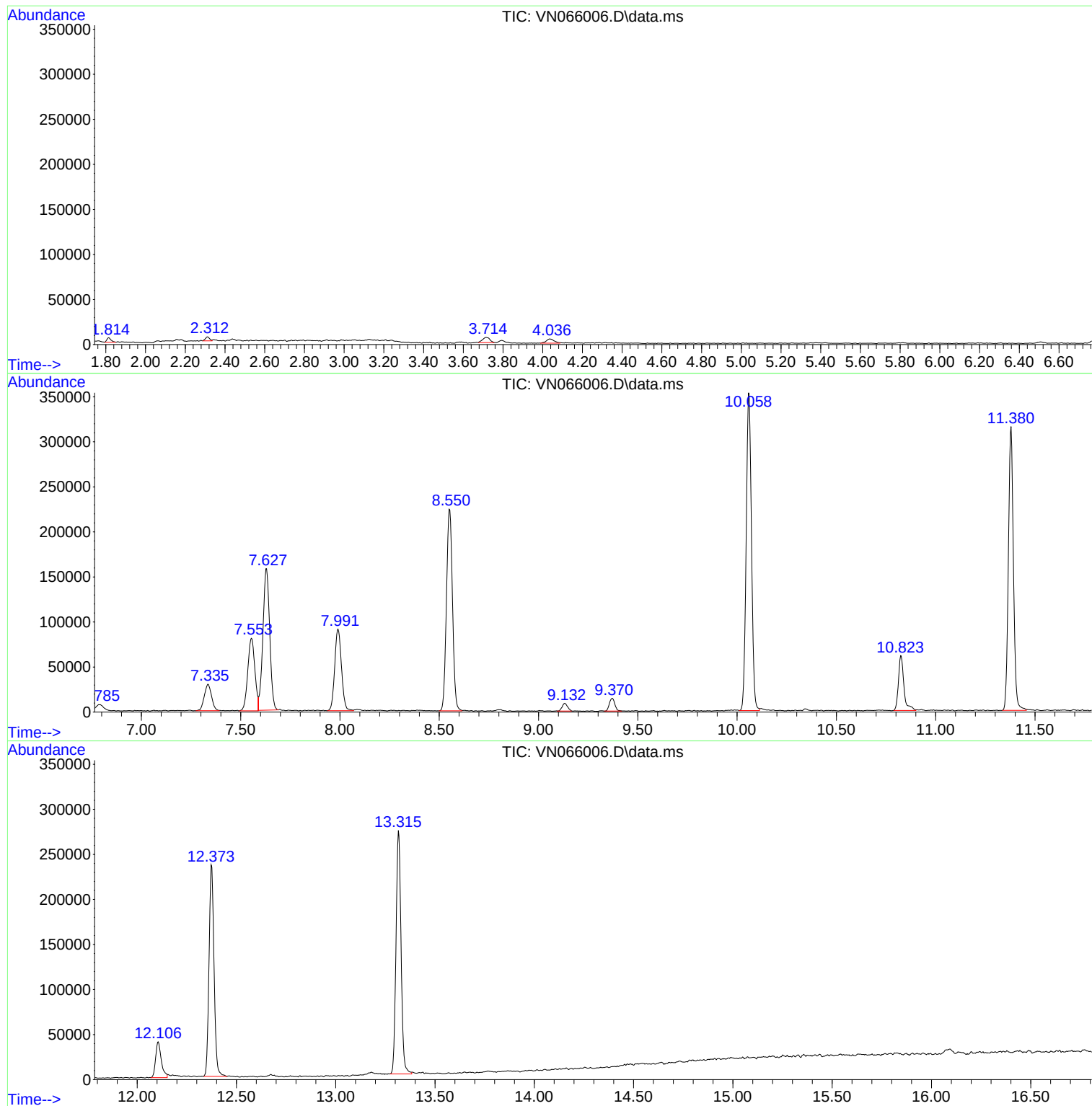
Sum of corrected areas: 3708116

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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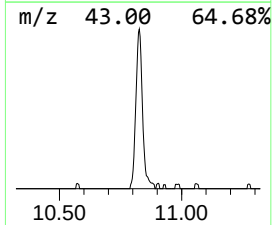
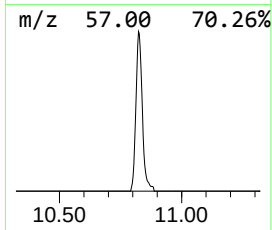
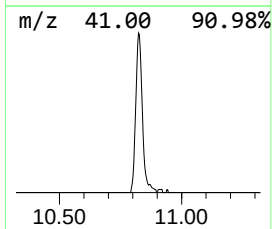
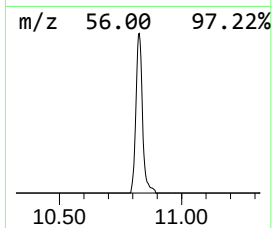
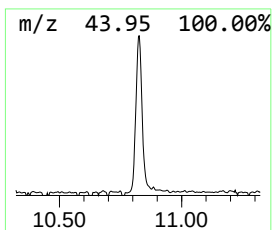
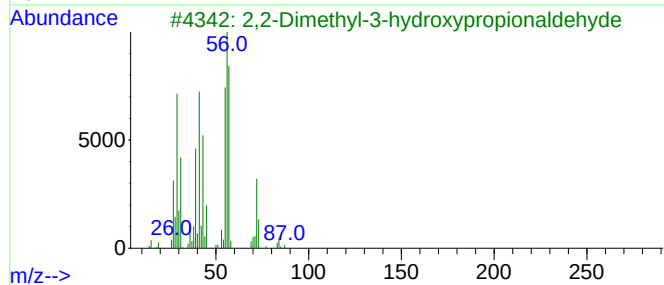
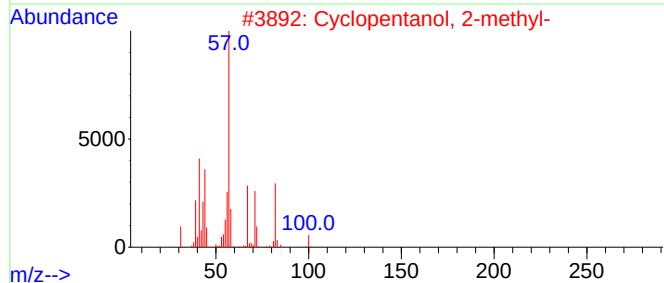
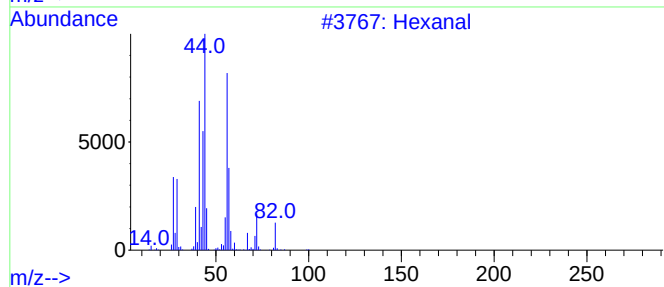
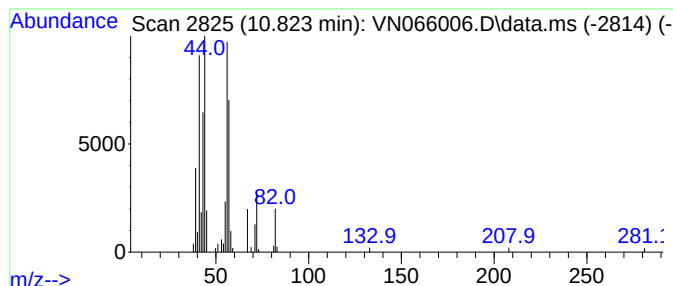
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Peak Number 1 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	10.47 ug/l	116067	Chlorobenzene-d5	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	64
2			Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	38
3			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	35
5			Glutaraldehyde	100	C5H8O2	000111-30-8	27



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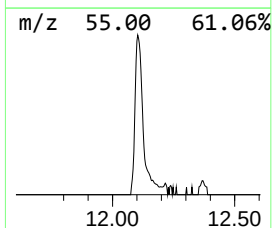
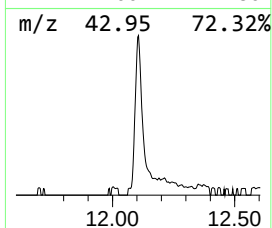
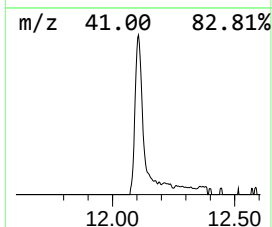
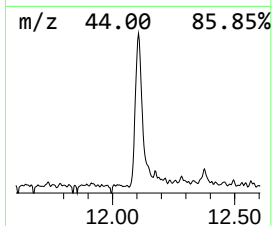
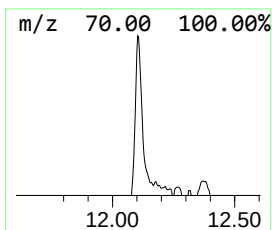
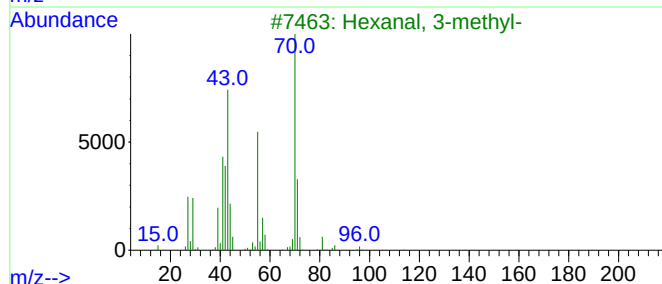
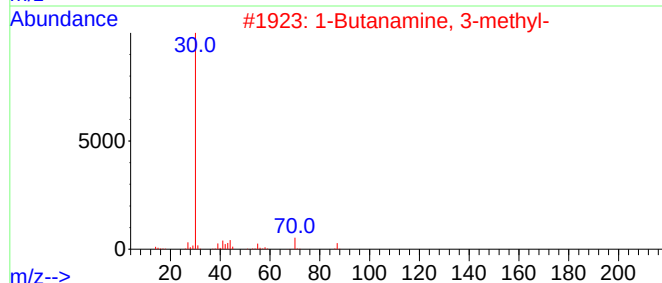
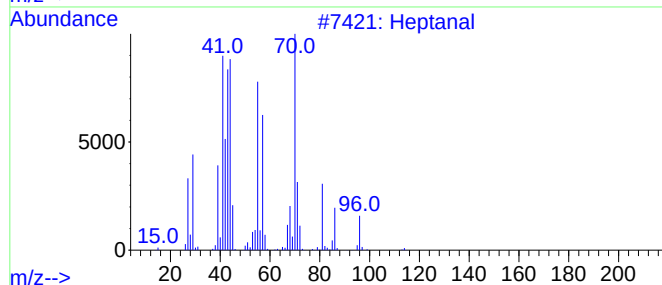
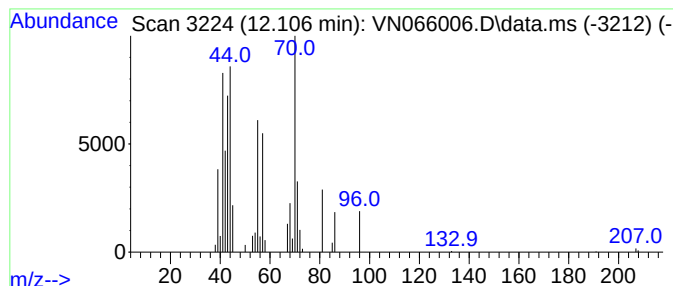
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Peak Number 2 Heptanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.106	7.14 ug/l	79129	Chlorobenzene-d5	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	91
2			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	59
3			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	38
4			N-Methylallylamine	71	C4H9N	000627-37-2	23
5			3-Hexene, 2,2,5,5-tetramethyl-, ...	140	C10H20	000692-47-7	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	10.823	10.5	ug/l	116067	3	11.380	554412	50.0
Heptanal	12.106	7.1	ug/l	79129	3	11.380	554412	50.0