

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011023\
 Data File : VN076180.D
 Acq On : 10 Jan 2023 14:01
 Operator : JC\MD
 Sample : 01067-01
 Misc : 1.05gr/10mL/100uL/5.0mL/MSVOA_N/MeOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31920

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN076180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.324	37	46	60	rVB3	15057	31385	2.05%	0.349%
2	3.077	173	174	180	rVB4	22395	30366	1.98%	0.338%
3	8.171	1030	1040	1044	rBV	206781	504044	32.91%	5.611%
4	8.224	1044	1049	1061	rVB	432995	931557	60.82%	10.370%
5	8.577	1101	1109	1122	rBV	208413	482809	31.52%	5.375%
6	9.100	1189	1198	1213	rBV	570971	1148718	75.00%	12.788%
7	10.565	1439	1447	1460	rBV	816607	1531550	100.00%	17.050%
8	11.865	1659	1668	1677	rBV	691032	1276552	83.35%	14.211%
9	12.853	1828	1836	1845	rBV	554142	942897	61.56%	10.497%
10	13.076	1865	1874	1877	rBV9	7471	18732	1.22%	0.209%
11	13.541	1937	1953	1969	rBV8	50880	233178	15.22%	2.596%
12	13.794	1989	1996	2012	rVB	692459	1209632	78.98%	13.466%
13	14.253	2065	2074	2089	rVB	29244	116184	7.59%	1.293%
14	14.417	2091	2102	2116	rVB5	65976	248932	16.25%	2.771%
15	14.570	2119	2128	2138	rBV5	19082	71551	4.67%	0.797%
16	14.694	2138	2149	2161	rVV9	25916	86131	5.62%	0.959%
17	14.941	2184	2191	2192	rBV6	11722	22278	1.45%	0.248%
18	16.076	2376	2384	2385	rBV8	8689	18912	1.23%	0.211%
19	16.258	2410	2415	2420	rVB6	10022	19491	1.27%	0.217%
20	16.388	2426	2437	2439	rBV9	20161	57992	3.79%	0.646%

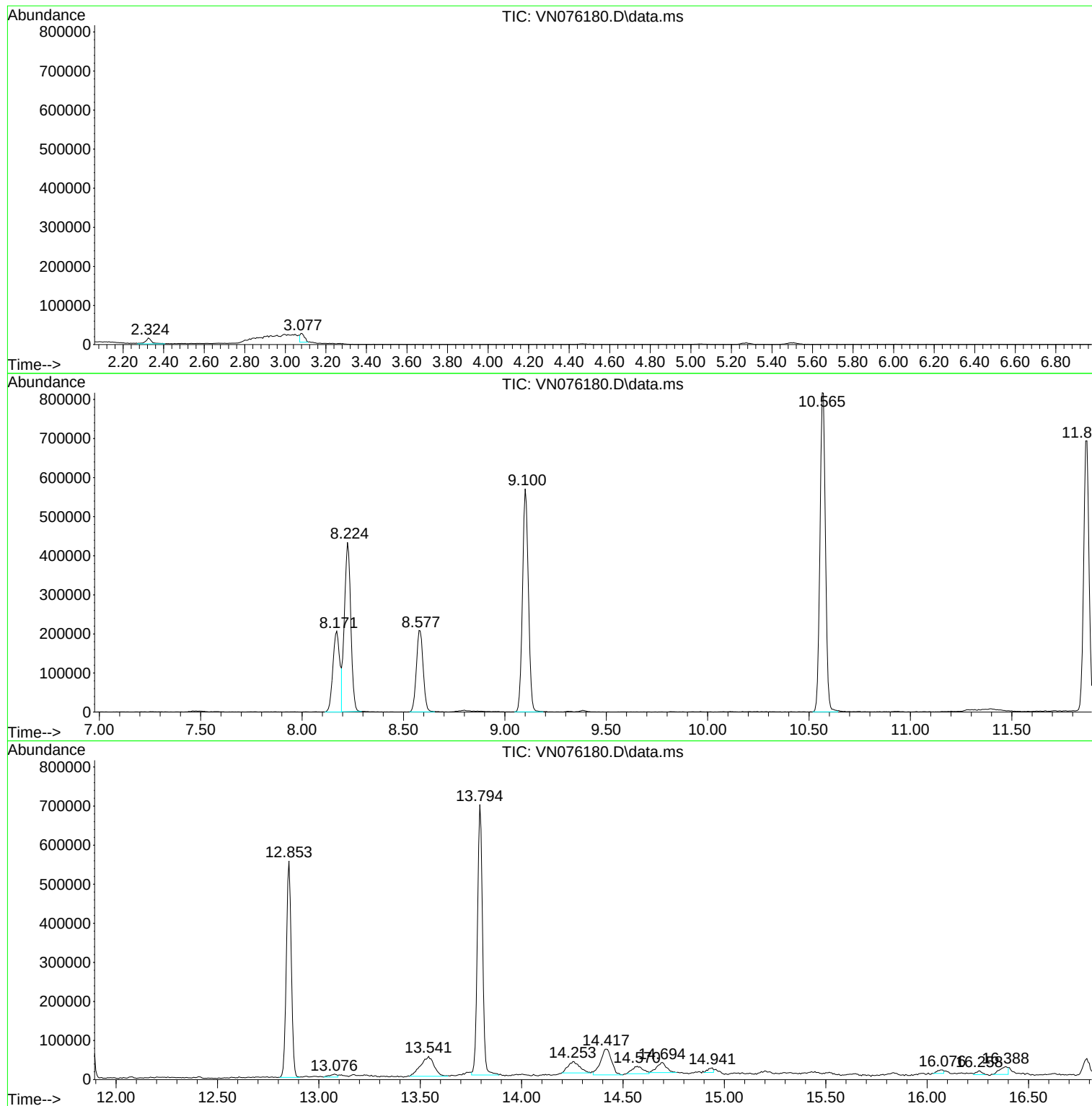
Sum of corrected areas: 8982891

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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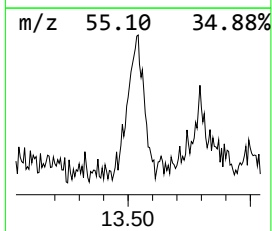
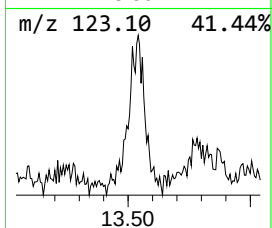
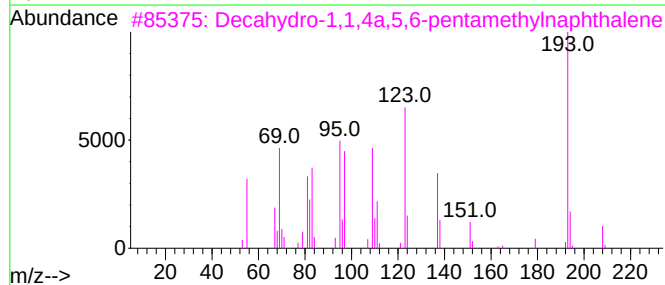
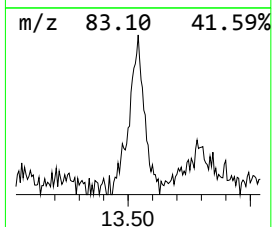
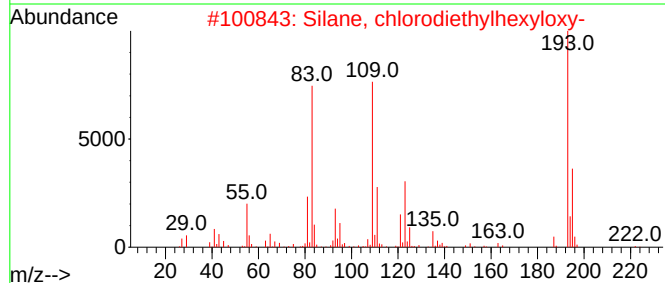
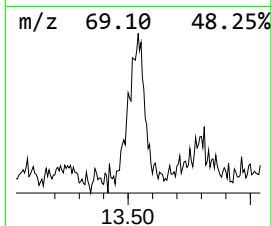
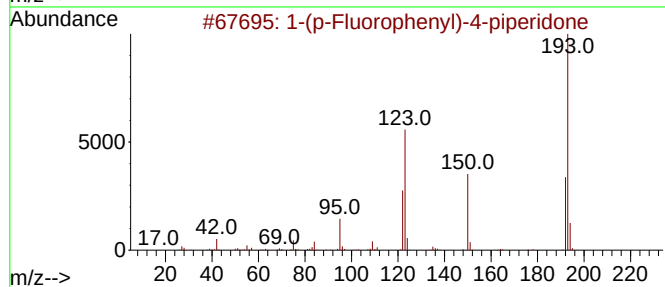
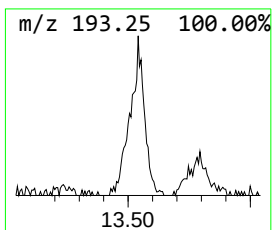
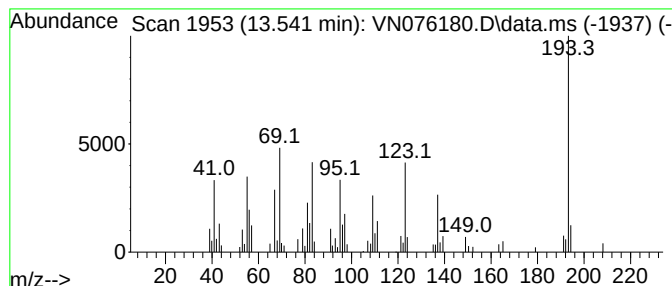
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown13.541 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.541	9.64 ug/l	233178	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	47
2	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	35
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
4	3-pyridinamine, 2-(1H-1,2,4-tria...	193	C7H7N5S	1000400-27-7	27
5	3-((2R,5S)-7-(Cyclohexylsulfonyl...	340	C17H28N2O3S	1000483-82-6	27



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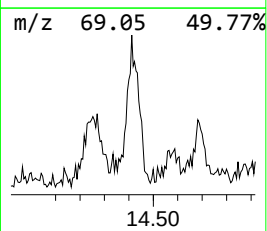
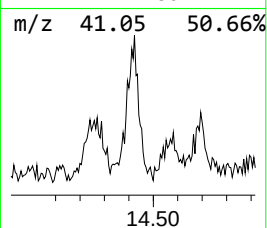
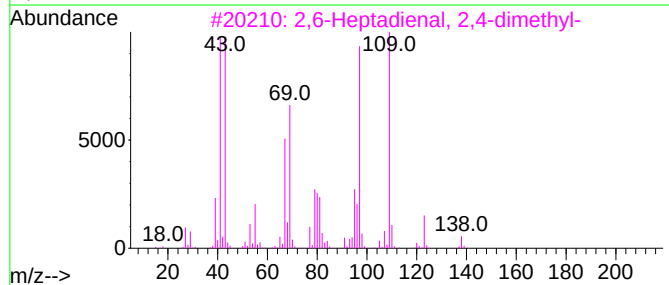
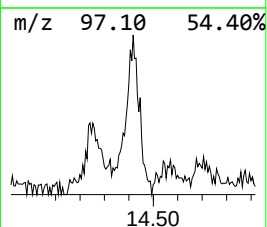
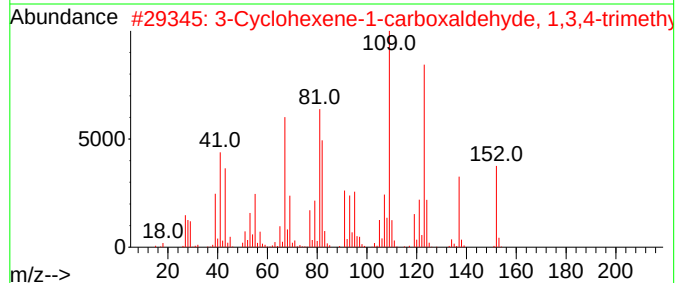
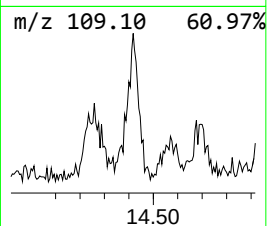
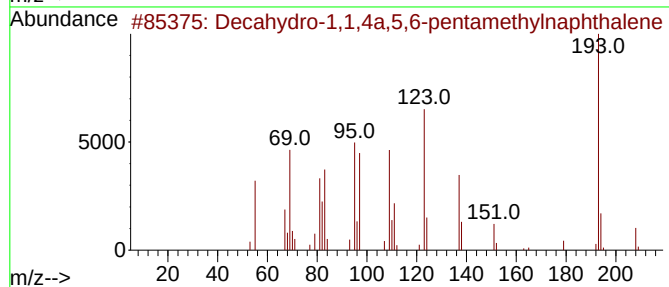
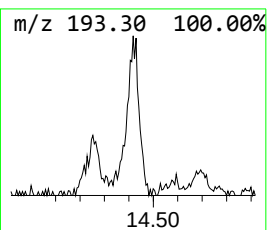
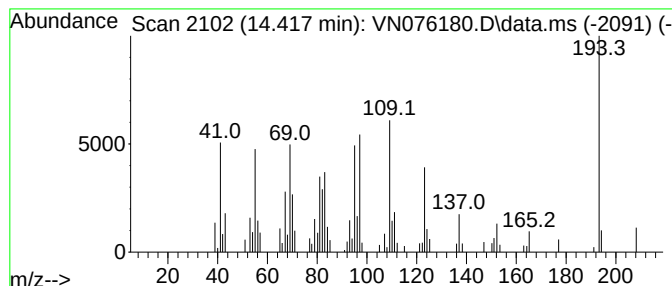
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Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.417	10.29 ug/l	248932	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	76
2			3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	38
3			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
4			Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	35
5			(4-tert-Butylphenoxy)acetic acid	208	C12H16O3	001798-04-5	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown13.541	13.541	9.6	ug/l	233178	4	13.794	1209630	50.0
Decahydro-1,1,4...	14.417	10.3	ug/l	248932	4	13.794	1209630	50.0