

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063022\
 Data File : VN073271.D
 Acq On : 30 Jun 2022 17:26
 Operator : JC\MD
 Sample : N3524-04
 Misc : 1.15g/10mL/100uL/5.0mL/MeOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31546

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.945	1020	1030	1035	rBV	201130	498132	7.90%	2.891%
2	8.004	1035	1040	1058	rVB	381064	867122	13.75%	5.033%
3	8.363	1092	1101	1111	rBV	213251	494384	7.84%	2.869%
4	8.892	1182	1191	1201	rBV	538147	1131525	17.95%	6.568%
5	9.498	1285	1294	1301	rBV2	34377	76632	1.22%	0.445%
6	10.374	1435	1443	1451	rBV	764919	1415572	22.45%	8.216%
7	11.686	1658	1666	1673	rBV	817467	1468199	23.29%	8.522%
8	12.521	1804	1808	1813	rBV3	47531	83943	1.33%	0.487%
9	12.668	1827	1833	1844	rVB	717712	1247522	19.79%	7.241%
10	13.010	1884	1891	1896	rBV3	62063	134059	2.13%	0.778%
11	13.527	1972	1979	1986	rVB	3919596	6304103	100.00%	36.590%
12	13.610	1988	1993	2003	rVB	936383	1565925	24.84%	9.089%
13	13.710	2007	2010	2017	rVB2	59661	94777	1.50%	0.550%
14	14.386	2120	2125	2131	rBV	254021	435148	6.90%	2.526%
15	14.786	2189	2193	2200	rBV2	130503	239724	3.80%	1.391%
16	14.904	2209	2213	2220	rVB4	228427	474155	7.52%	2.752%
17	15.033	2232	2235	2238	rBV5	92504	129249	2.05%	0.750%
18	15.398	2293	2297	2303	rBV3	316563	568799	9.02%	3.301%

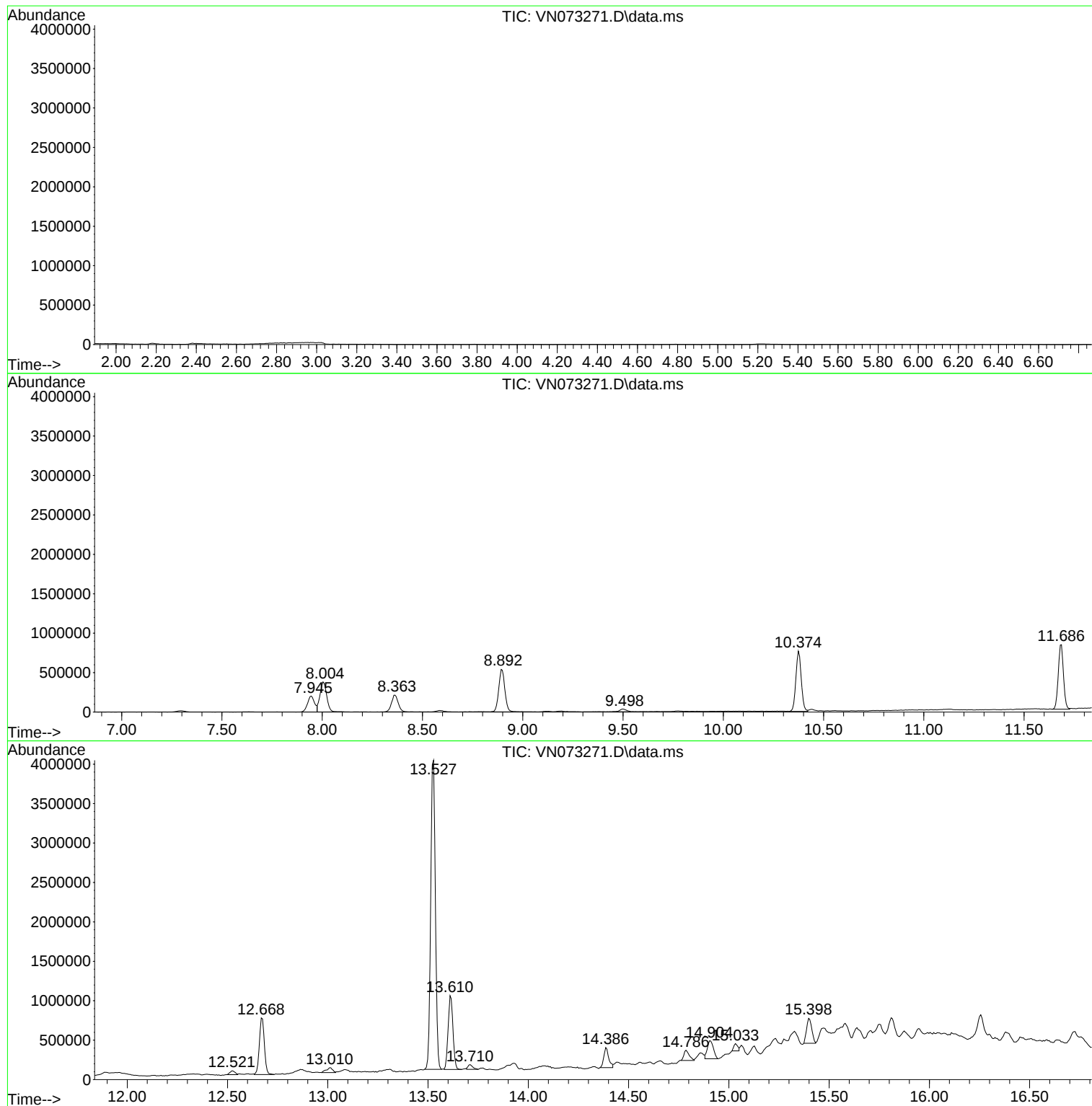
Sum of corrected areas: 17228970

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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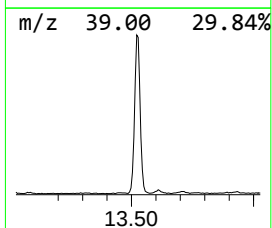
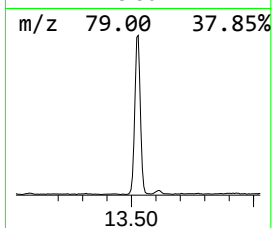
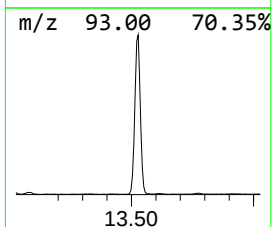
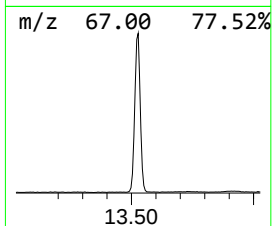
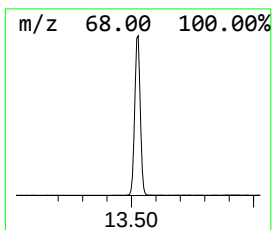
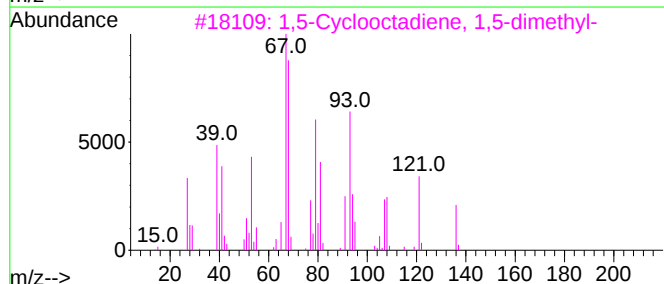
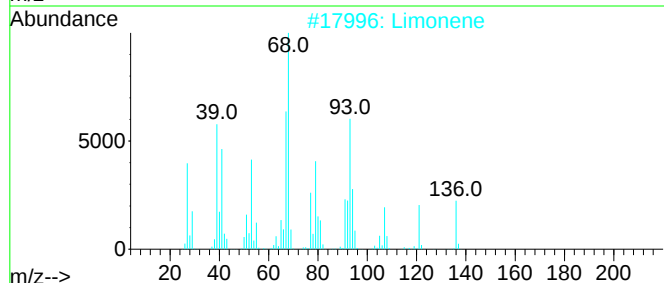
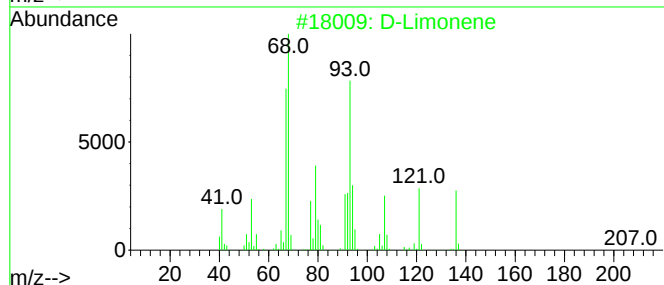
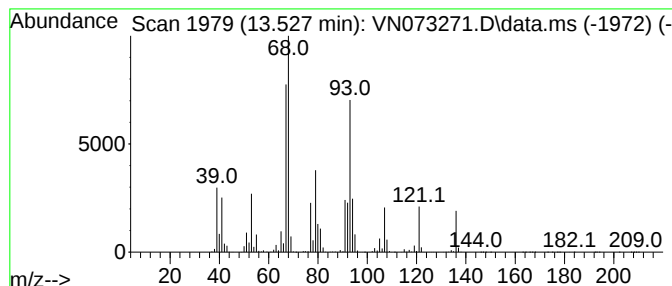
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Quant Title : SW846 8260

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

Peak Number 1 D-Limonene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.527	201.29 ug/l	6304100	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	97
2			Limonene	136	C10H16	000138-86-3	94
3			1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	76
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	74
5			Cyclohexanol, 1-methyl-4-(1-meth...	196	C12H20O2	010198-23-9	64



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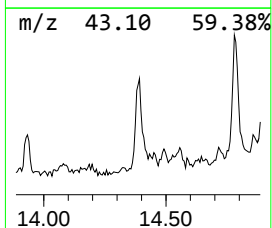
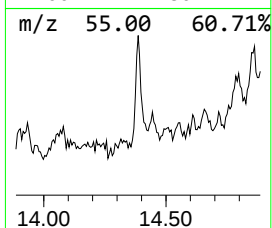
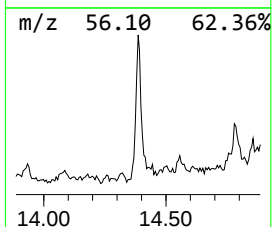
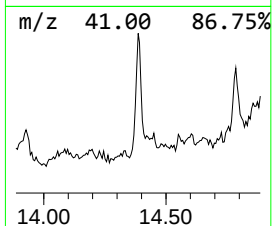
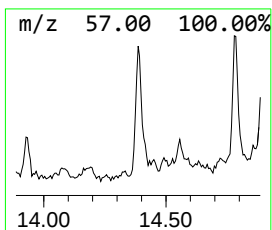
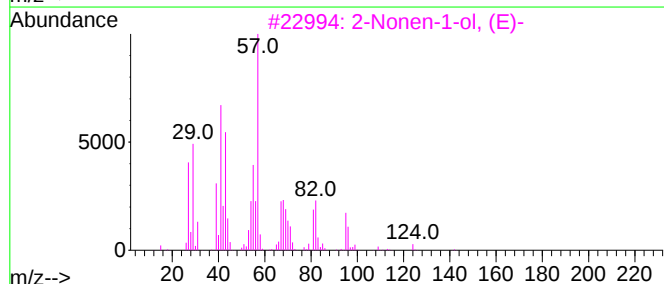
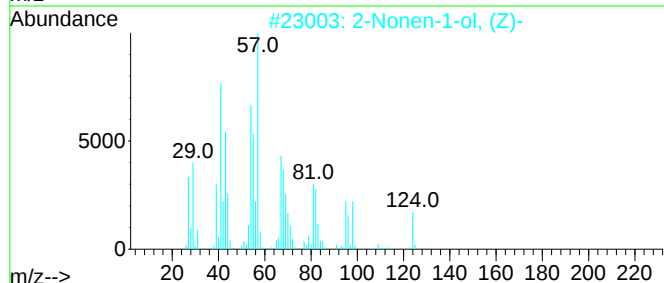
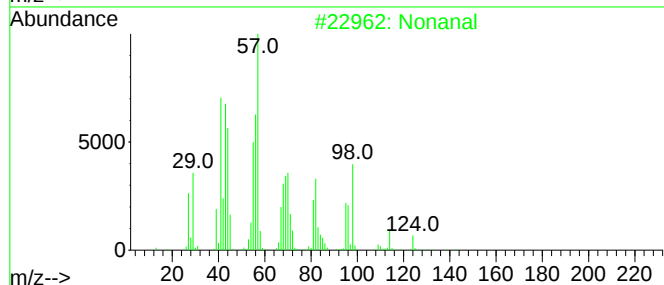
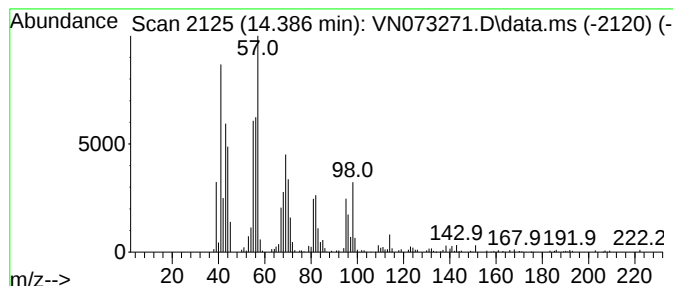
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.386	13.89 ug/l	435148	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	95
2			2-Nonen-1-ol, (Z)-	142	C9H18O	041453-56-9	43
3			2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	41
4			2-Nonen-1-ol	142	C9H18O	022104-79-6	38
5			trans-2-Undecen-1-ol	170	C11H22O	075039-84-8	38



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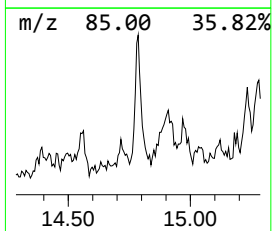
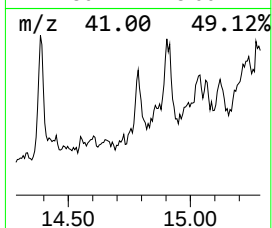
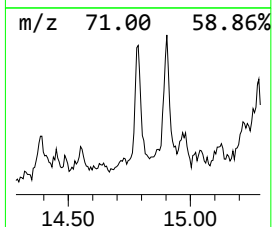
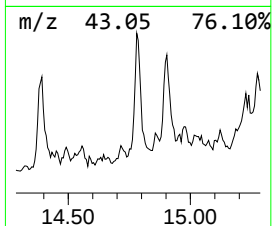
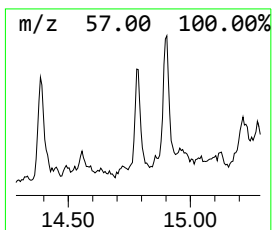
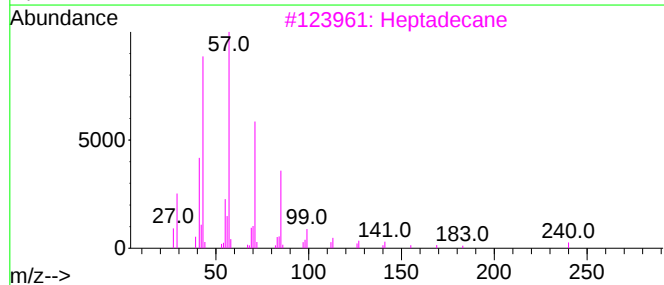
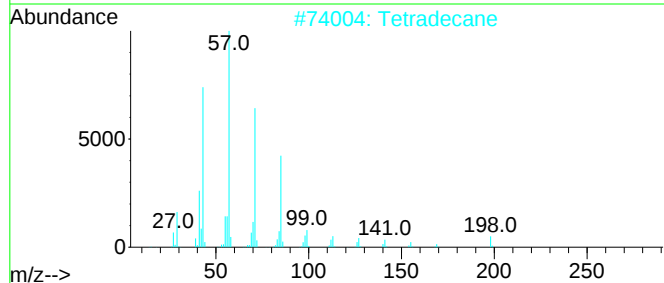
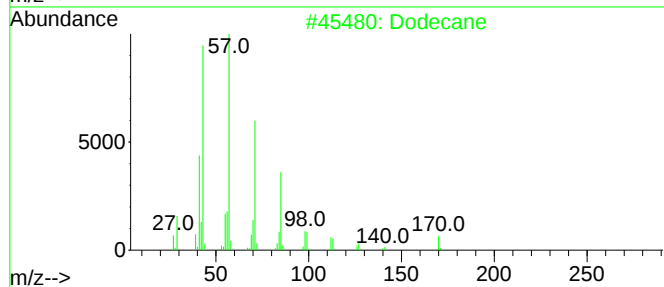
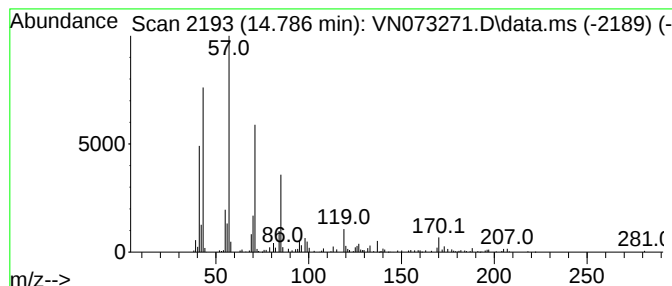
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Quant Title : SW846 8260

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

Peak Number 3 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	7.65 ug/l	239724	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	81
2			Tetradecane	198	C14H30	000629-59-4	64
3			Heptadecane	240	C17H36	000629-78-7	64
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	59
5			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	53



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Data File : VN073271.D
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Operator : JC\MD
Sample : N3524-04
Misc : 1.15g/10mL/100uL/5.0mL/MeOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31546

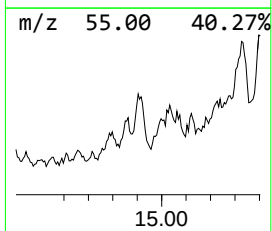
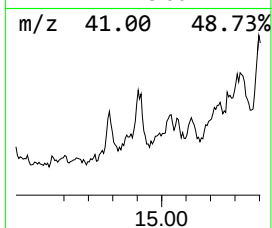
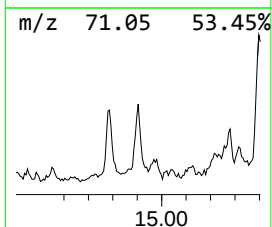
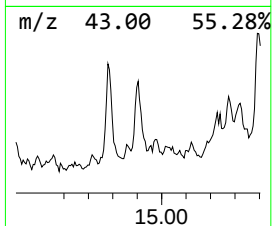
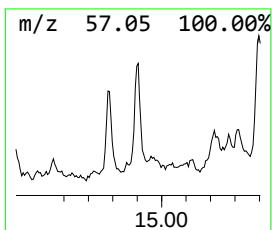
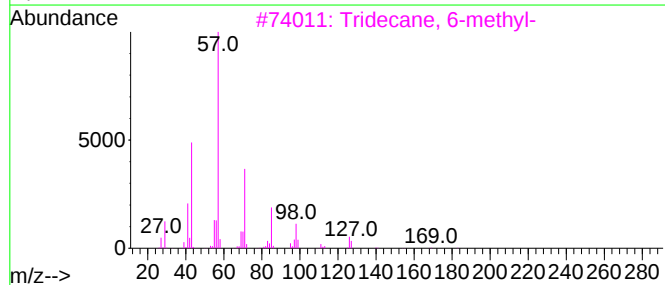
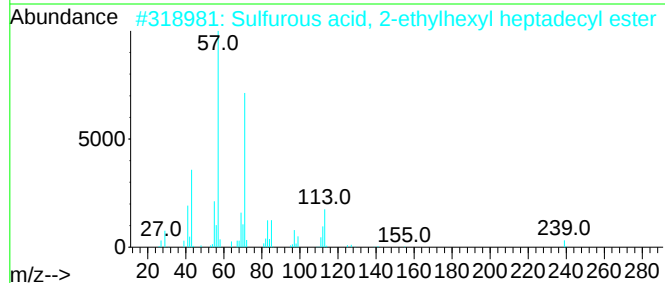
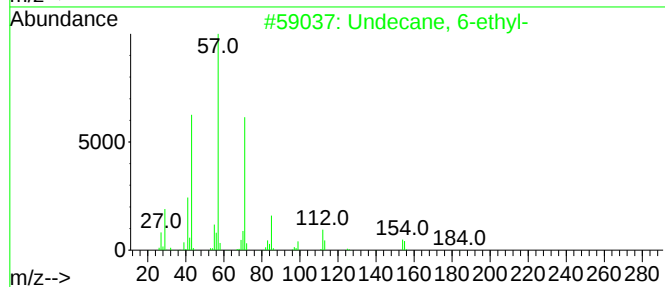
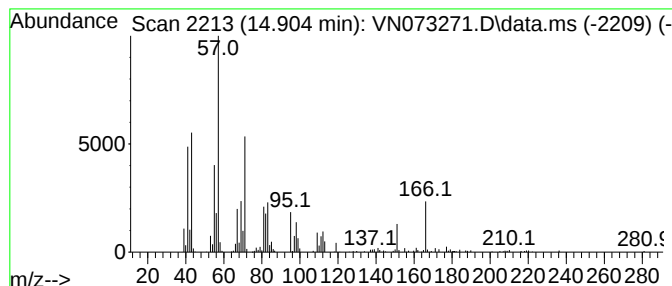
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown14.904 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	15.14 ug/l	474155	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 6-ethyl-	184	C13H28	017312-60-6	35
2			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	35
3			Tridecane, 6-methyl-	198	C14H30	013287-21-3	30
4			Nonane, 2-methyl-	142	C10H22	000871-83-0	27
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	27



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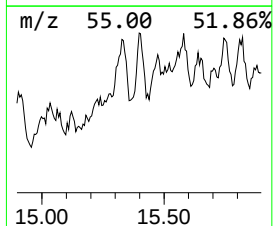
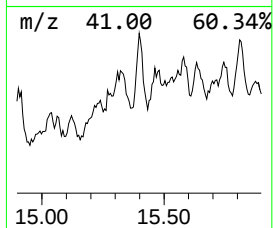
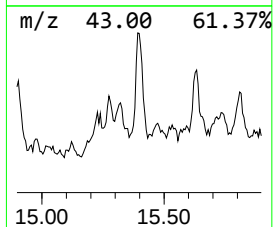
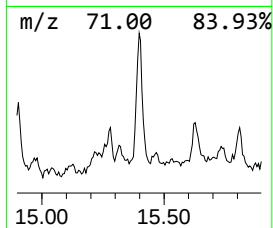
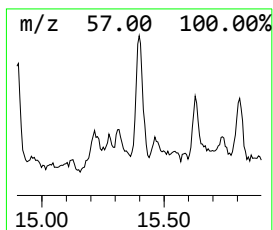
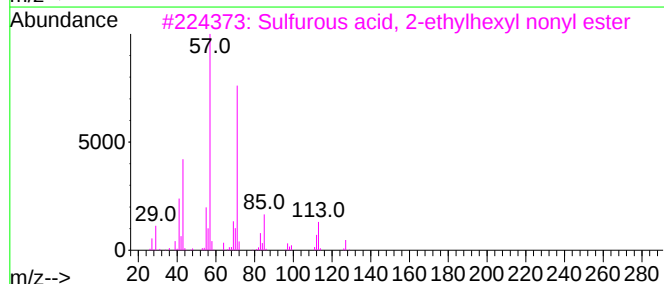
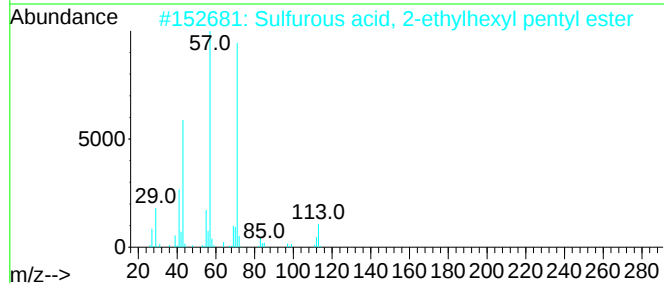
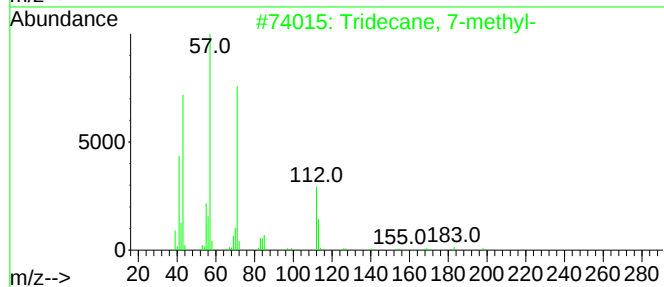
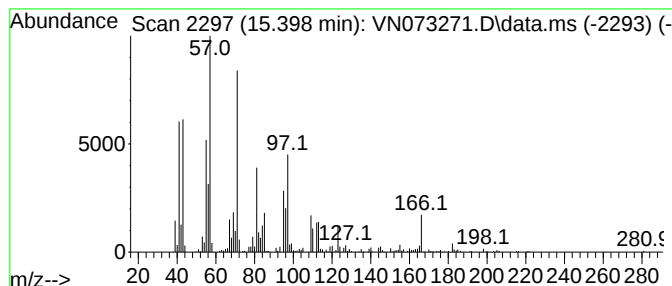
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Quant Title : SW846 8260

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

Peak Number 5 unknown15.398 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	18.16 ug/l	568799	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-methyl-	198	C14H30	026730-14-3	42
2			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	35
3			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	35
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	30
5			3-Bromooctane	192	C8H17Br	000999-64-4	30



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
D-Limonene	13.527	201.3	ug/l	6304100	4	13.615	1565930	50.0
Nonanal	14.386	13.9	ug/l	435148	4	13.615	1565930	50.0
Dodecane	14.786	7.7	ug/l	239724	4	13.615	1565930	50.0
unknown14.904	14.904	15.1	ug/l	474155	4	13.615	1565930	50.0
unknown15.398	15.398	18.2	ug/l	568799	4	13.615	1565930	50.0