

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN123021\
 Data File : VN070397.D
 Acq On : 30 Dec 2021 14:16
 Operator : JC/MD
 Sample : M5223-01
 Misc : 5.00g/5mL/100uL/5.00mL01/MSVOA_N/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DB-19-(10-15)-12-22-21

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	80	91	122	rVB3	173605	542250	4.97%	0.797%
2	8.019	2224	2248	2258	rBV	1382833	3287831	30.10%	4.830%
3	8.080	2259	2271	2302	rVB	2386370	5471907	50.10%	8.038%
4	8.434	2382	2403	2428	rBV	1729310	3987235	36.51%	5.857%
5	8.965	2581	2601	2643	rVB	3642179	7578295	69.39%	11.132%
6	10.440	3131	3151	3184	rBV	5715709	10675673	97.75%	15.682%
7	11.344	3477	3488	3501	rVB2	156965	276243	2.53%	0.406%
8	11.551	3558	3565	3582	rVB4	75924	142535	1.31%	0.209%
9	11.747	3620	3638	3663	rBV	4536257	8082296	74.00%	11.873%
10	11.988	3718	3728	3738	rBV3	96053	189935	1.74%	0.279%
11	12.253	3811	3827	3841	rBV7	201425	484354	4.43%	0.711%
12	12.366	3863	3869	3879	rVB	193007	271512	2.49%	0.399%
13	12.457	3880	3903	3904	rBV6	246363	431343	3.95%	0.634%
14	12.731	3990	4005	4024	rBV2	6312255	10921443	100.00%	16.043%
15	12.897	4057	4067	4082	rVB5	444871	815509	7.47%	1.198%
16	12.975	4084	4096	4107	rBV6	175297	406303	3.72%	0.597%
17	13.061	4113	4128	4139	rBV10	314329	778924	7.13%	1.144%
18	13.197	4172	4179	4188	rVB4	179347	247323	2.26%	0.363%
19	13.286	4204	4212	4227	rBV5	356968	561451	5.14%	0.825%
20	13.675	4344	4357	4377	rVB	4323767	7264305	66.51%	10.671%
21	13.997	4467	4477	4488	rBV4	868440	1483134	13.58%	2.179%
22	14.506	4658	4667	4679	rVB5	994199	1530575	14.01%	2.248%
23	14.670	4719	4728	4740	rVB5	841705	1329175	12.17%	1.953%
24	15.469	5018	5026	5042	rVB3	774094	1315690	12.05%	1.933%

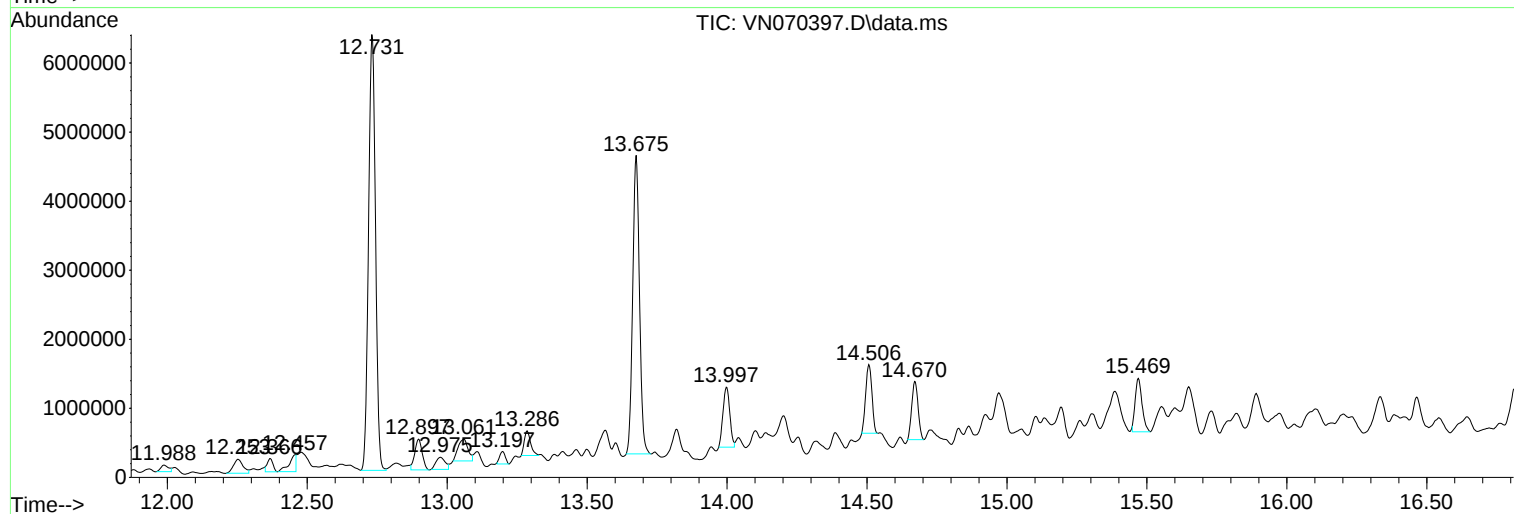
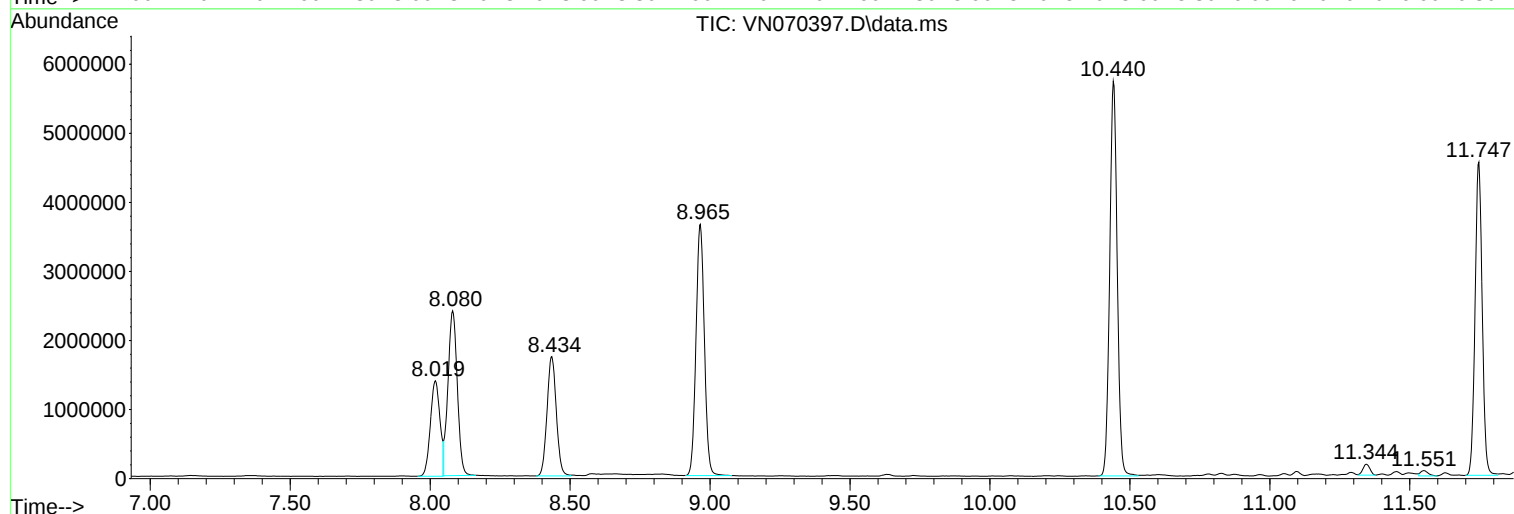
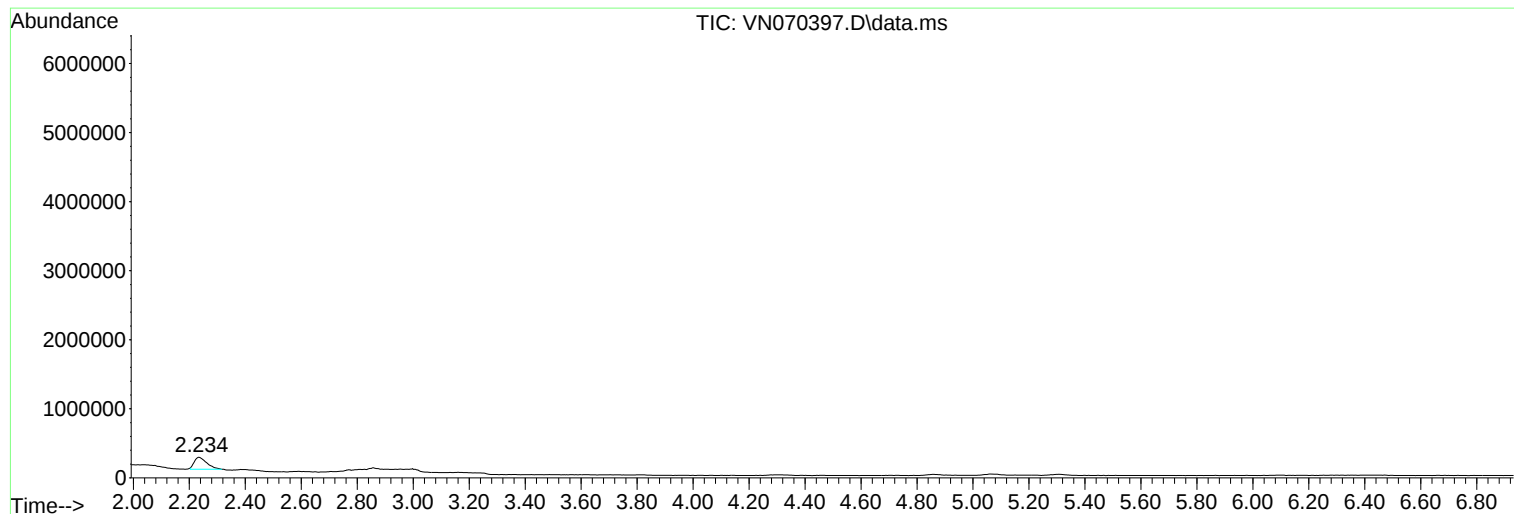
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DB-19-(10-15)-12-22-21

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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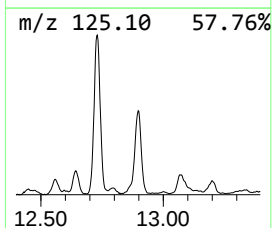
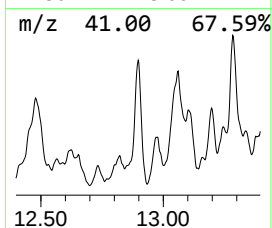
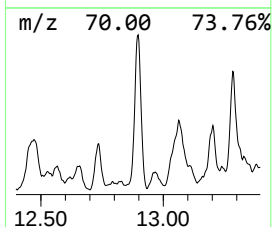
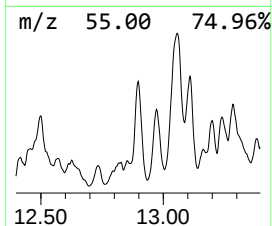
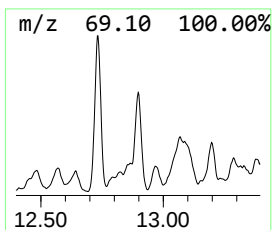
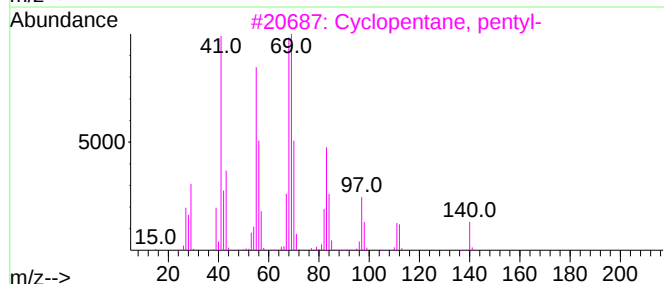
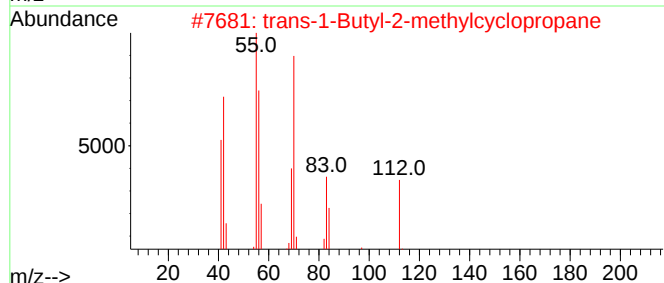
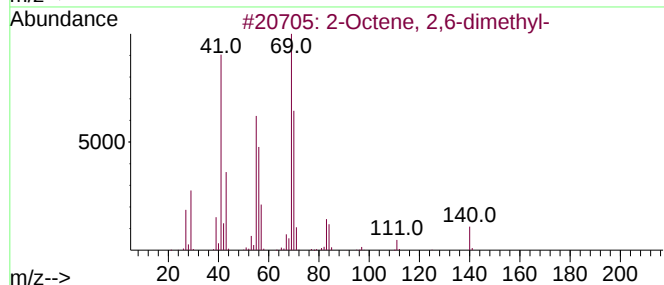
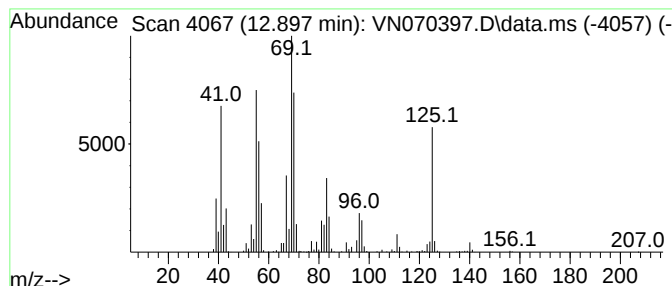
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Octene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.897	5.61 ug/l	815509	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene, 2,6-dimethyl-			140	C10H20	004057-42-5	70
2	trans-1-Butyl-2-methylcyclopropane			112	C8H16	038851-70-6	55
3	Cyclopentane, pentyl-			140	C10H20	003741-00-2	53
4	4-Octene, 2,6-dimethyl-, [S-(E)]-			140	C10H20	062960-76-3	47
5	cis-1-Butyl-2-methylcyclopropane			112	C8H16	038851-69-3	45



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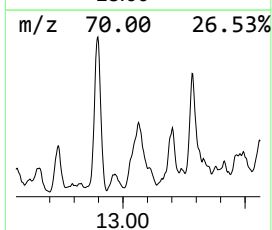
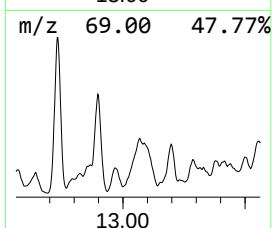
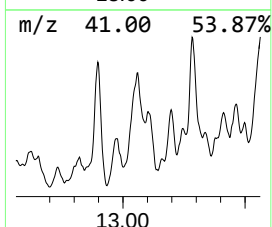
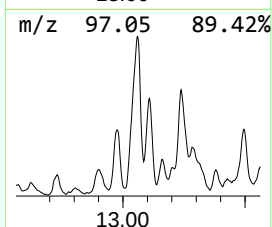
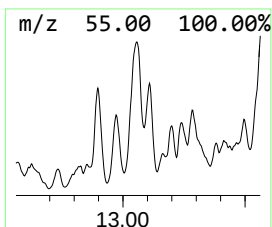
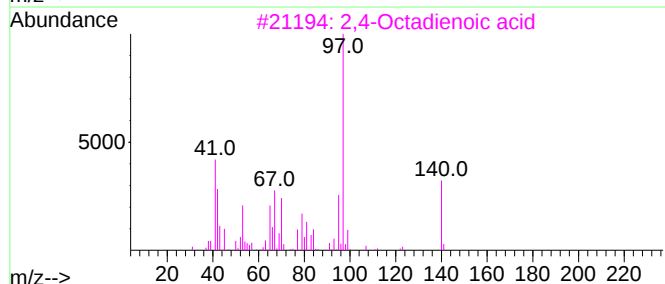
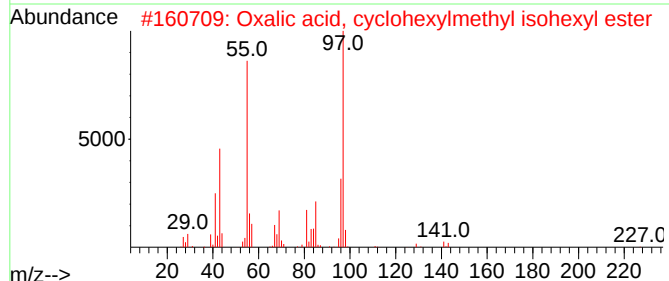
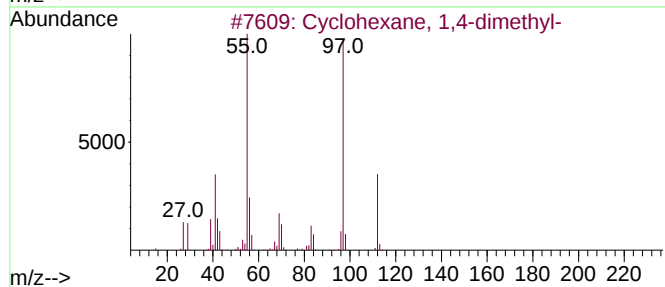
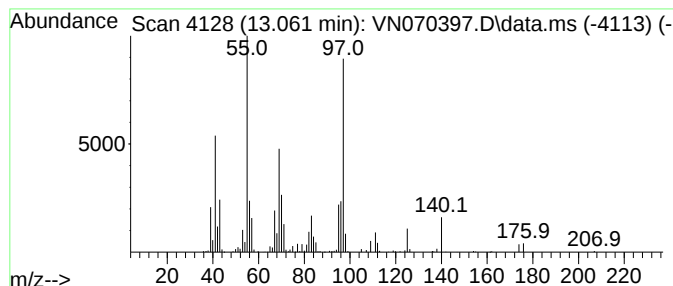
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown13.061 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.061	5.36 ug/l	778924	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	49
2			Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	47
3			2,4-Octadienoic acid	140	C8H12O2	083615-26-3	47
4			3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	46
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	46



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Instrument :
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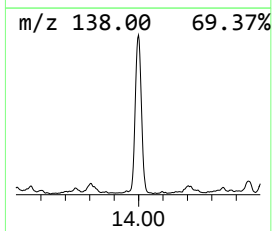
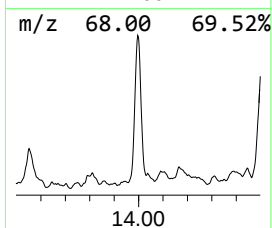
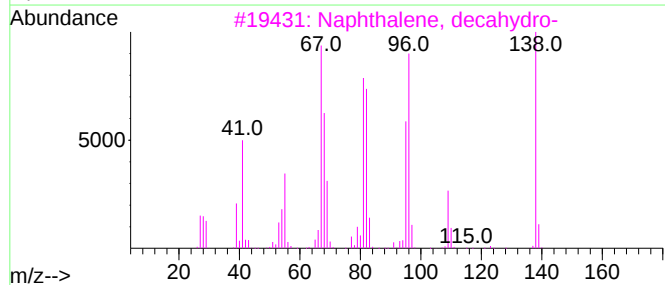
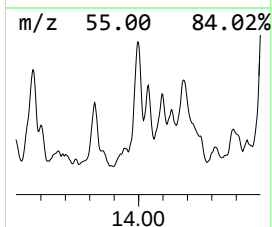
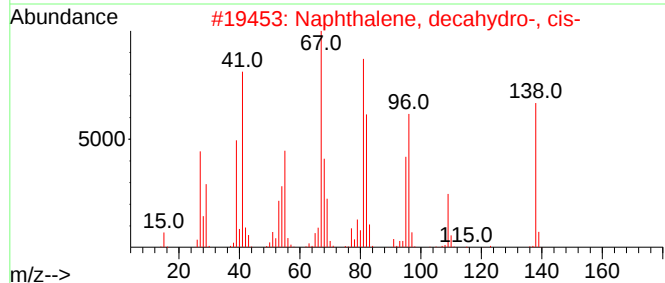
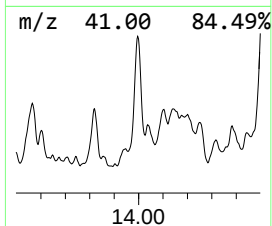
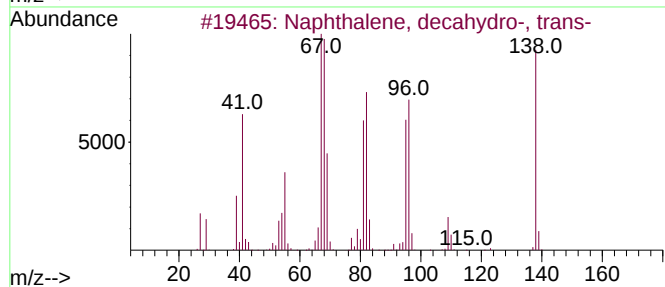
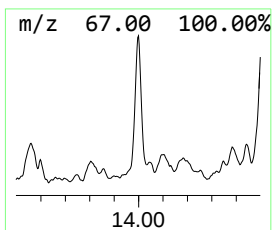
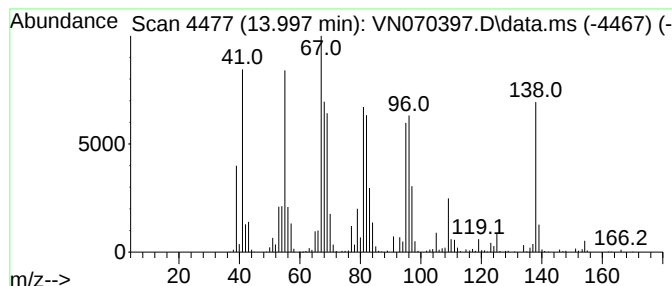
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, decahydro-, tr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	10.21 ug/l	1483130	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	95
3			Naphthalene, decahydro-	138	C10H18	000091-17-8	93
4			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	91
5			Cyclodecene	138	C10H18	003618-12-0	90



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ALS Vial : 11 Sample Multiplier: 1

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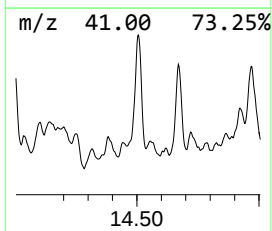
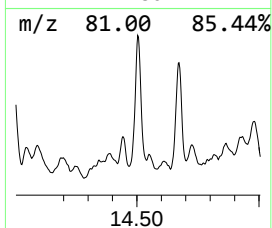
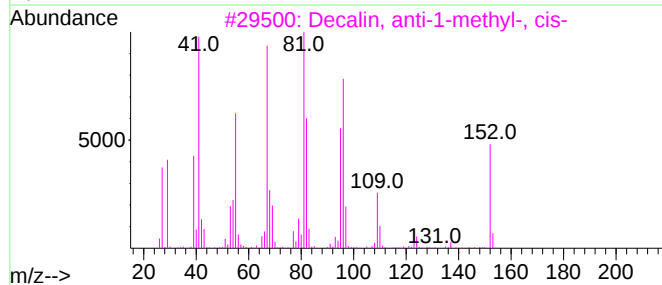
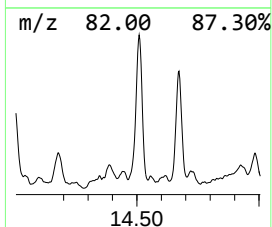
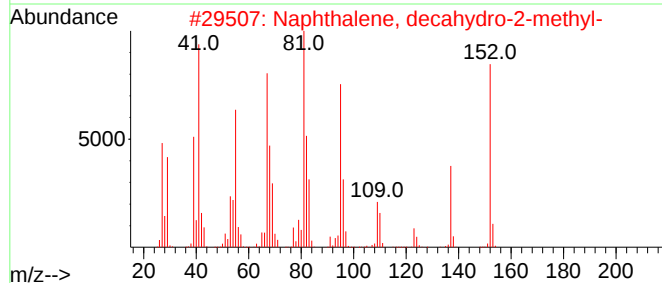
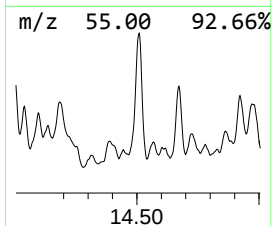
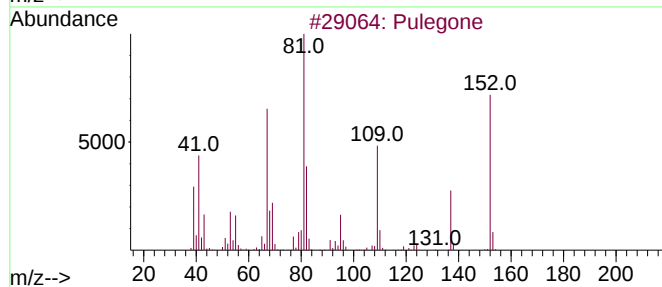
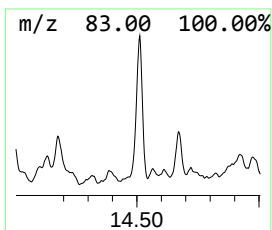
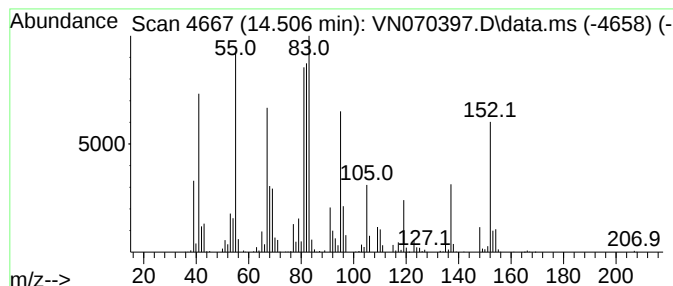
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pulegone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.506	10.53 ug/l	1530580	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pulegone	152	C10H16O	000089-82-7	50
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	46
3			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	46
4			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	46
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	43



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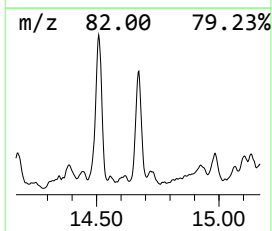
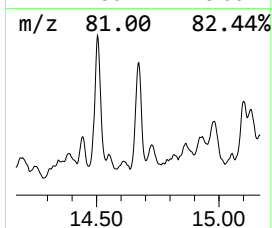
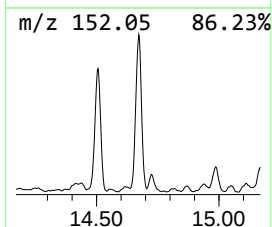
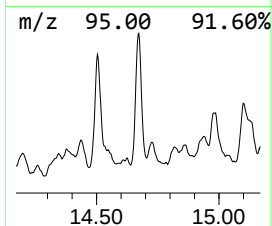
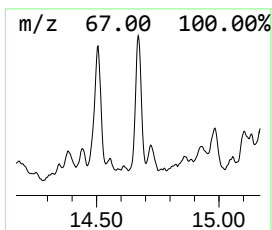
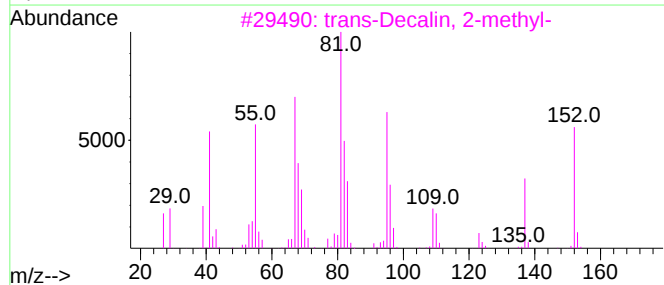
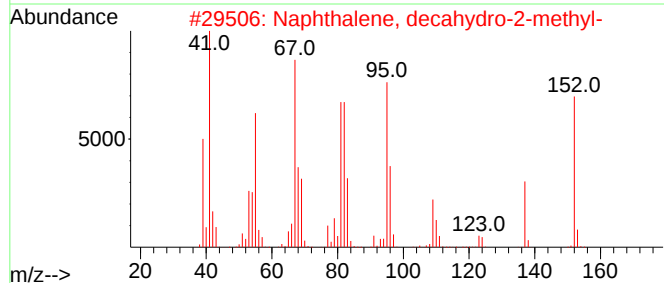
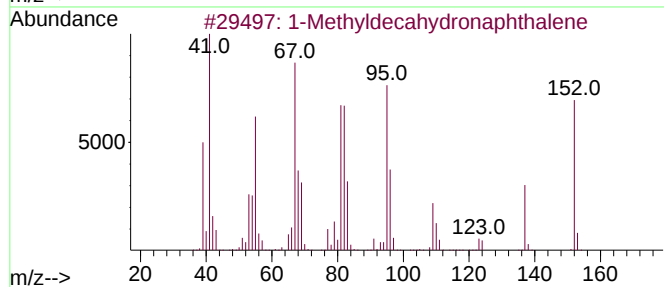
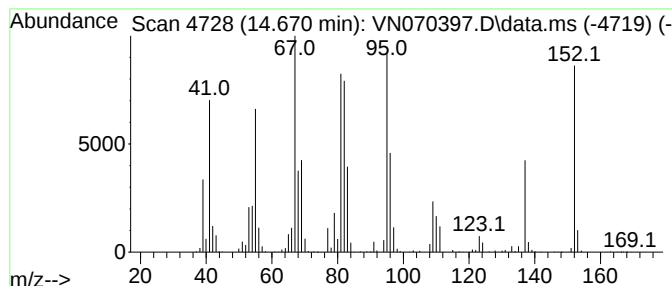
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Methyldecahydronaphthalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	9.15 ug/l	1329180	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	97
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	97
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	91
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	89
5			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	83



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DB-19-(10-15)-12-22-21

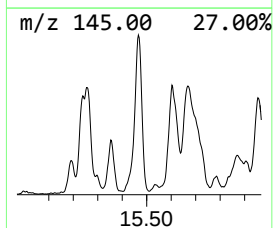
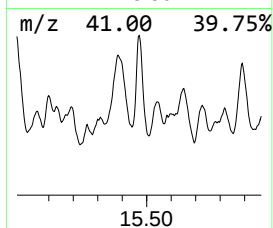
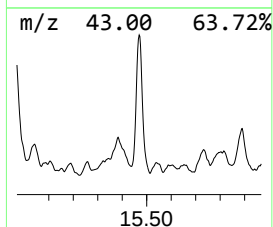
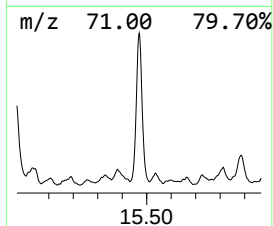
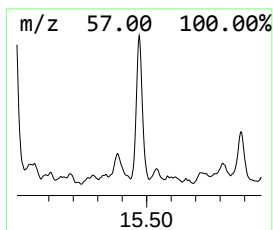
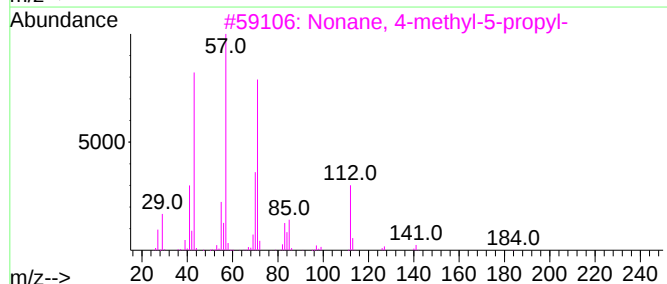
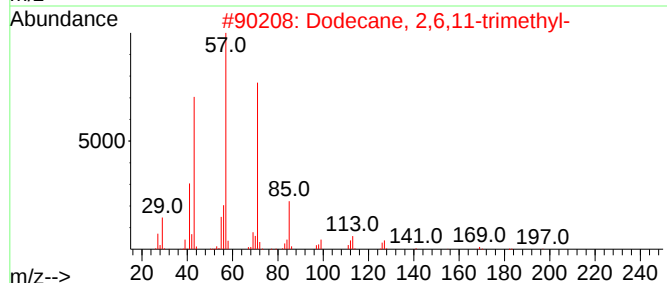
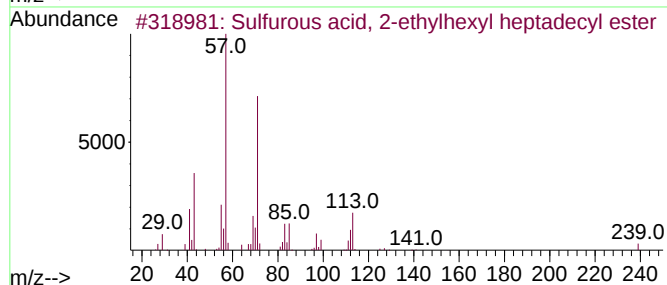
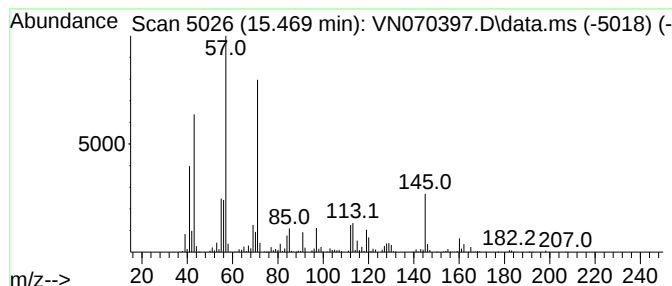
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, 2-ethylhexy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.469	9.06 ug/l	1315690	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	59
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	53
3			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	52
4			Octane, 3-ethyl-	142	C10H22	005881-17-4	52
5			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN123021\
Data File : VN070397.D
Acq On : 30 Dec 2021 14:16
Operator : JC/MD
Sample : M5223-01
Misc : 5.00g/5mL/100uL/5.00mL01/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DB-19-(10-15)-12-22-21

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
2-Octene, 2,6-d...	12.897	5.6	ug/l	815509	4	13.675	7264310	50.0
unknown13.061	13.061	5.4	ug/l	778924	4	13.675	7264310	50.0
Naphthalene, de...	13.997	10.2	ug/l	1483130	4	13.675	7264310	50.0
Pulegone	14.506	10.5	ug/l	1530580	4	13.675	7264310	50.0
1-Methyldecahyd...	14.670	9.2	ug/l	1329180	4	13.675	7264310	50.0
Sulfurous acid,...	15.469	9.1	ug/l	1315690	4	13.675	7264310	50.0