

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
 Data File : VN068552.D
 Acq On : 18 Sep 2021 6:03
 Operator : JC/MD
 Sample : M3798-05
 Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SUB-SLAB-01-(5-8)

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\82N090721W.M
 Title : SW846 8260

Signal : TIC: VN068552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.019	2226	2248	2259	rBV	324804	771089	4.72%	0.548%
2	8.083	2260	2272	2296	rVB2	631961	1451679	8.89%	1.032%
3	8.434	2383	2403	2427	rBV	299265	685170	4.20%	0.487%
4	8.968	2581	2602	2640	rBV	779038	1674470	10.26%	1.190%
5	10.443	3133	3152	3189	rBV	1272617	2480974	15.20%	1.764%
6	11.055	3365	3380	3396	rVB3	114626	208625	1.28%	0.148%
7	11.157	3396	3418	3435	rBV3	125614	278584	1.71%	0.198%
8	11.229	3435	3445	3456	rBV3	101123	165394	1.01%	0.118%
9	11.347	3478	3489	3501	rVB	256348	432750	2.65%	0.308%
10	11.457	3519	3530	3539	rBV2	289563	490666	3.01%	0.349%
11	11.524	3540	3555	3562	rBV	521775	1045220	6.40%	0.743%
12	11.629	3582	3594	3618	rVB	1003255	1789906	10.97%	1.272%
13	11.747	3619	3638	3655	rBV	1296347	2684360	16.45%	1.908%
14	11.816	3656	3664	3677	rVB	169437	269432	1.65%	0.192%
15	11.881	3678	3688	3696	rBV2	340239	567705	3.48%	0.404%
16	11.937	3697	3709	3717	rBV6	456875	892809	5.47%	0.635%
17	11.991	3719	3729	3739	rBV2	1401849	2317669	14.20%	1.648%
18	12.122	3757	3778	3785	rBV3	584394	1438739	8.82%	1.023%
19	12.181	3788	3800	3811	rVB4	2074915	3664643	22.45%	2.605%
20	12.256	3812	3828	3840	rBV4	5135590	10840993	66.42%	7.707%
21	12.372	3861	3871	3882	rVB	6469365	10435213	63.94%	7.418%
22	12.455	3882	3902	3904	rBV7	3961063	7821973	47.93%	5.560%
23	12.739	3997	4008	4015	rBV5	3219533	5451199	33.40%	3.875%
24	12.900	4062	4068	4083	rVB4	5516736	9582469	58.71%	6.812%
25	12.983	4083	4099	4108	rBV7	3080788	7505182	45.98%	5.335%
26	13.061	4115	4128	4139	rBV4	6392915	12948583	79.34%	9.205%
27	13.200	4172	4180	4188	rBV3	4283183	5867093	35.95%	4.171%
28	13.249	4189	4198	4204	rVV4	4977786	7977380	48.88%	5.671%
29	13.286	4205	4212	4228	rVB2	10346021	16321230	100.00%	11.602%
30	13.415	4253	4260	4269	rVB	3538862	4569964	28.00%	3.249%
31	13.675	4351	4357	4366	rVB2	2194446	2910459	17.83%	2.069%
32	13.999	4467	4478	4489	rBV3	4476930	7901060	48.41%	5.617%
33	14.324	4589	4599	4611	rVV6	741579	1307173	8.01%	0.929%
34	14.386	4614	4622	4636	rVB9	781697	1401485	8.59%	0.996%
35	14.512	4661	4669	4701	rVB6	1571720	4179855	25.61%	2.971%
36	14.624	4704	4711	4716	rBV5	240864	339174	2.08%	0.241%

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SUB-SLAB-01-(5-8)

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\82N090721W.M
Title : SW846 8260

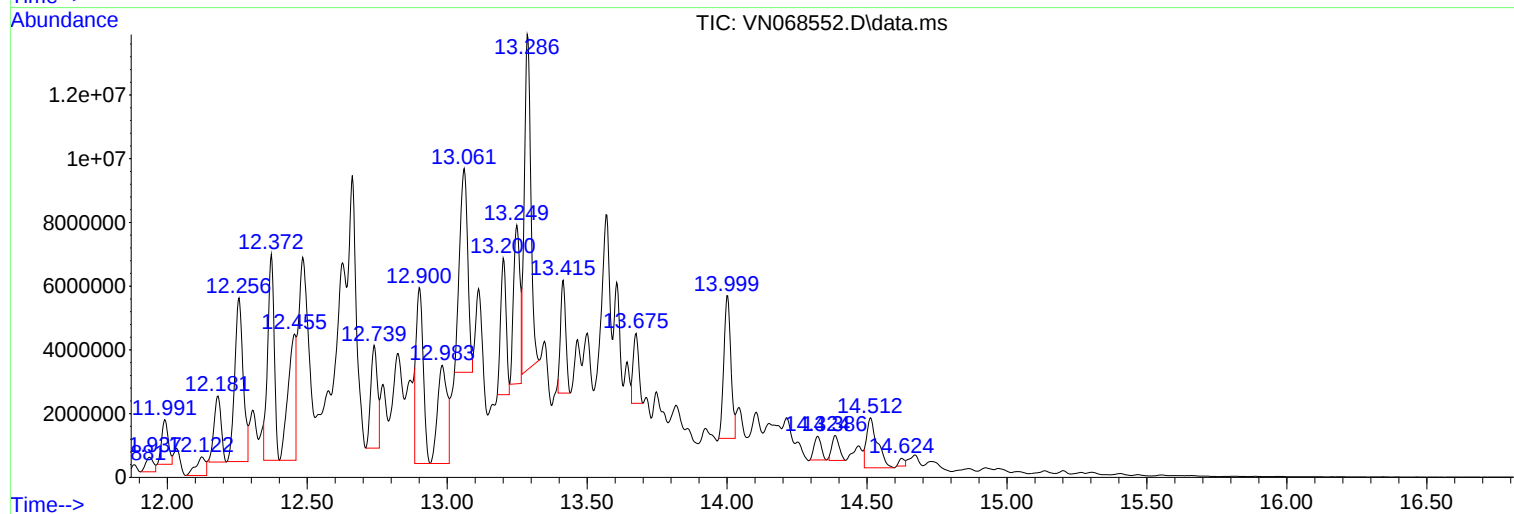
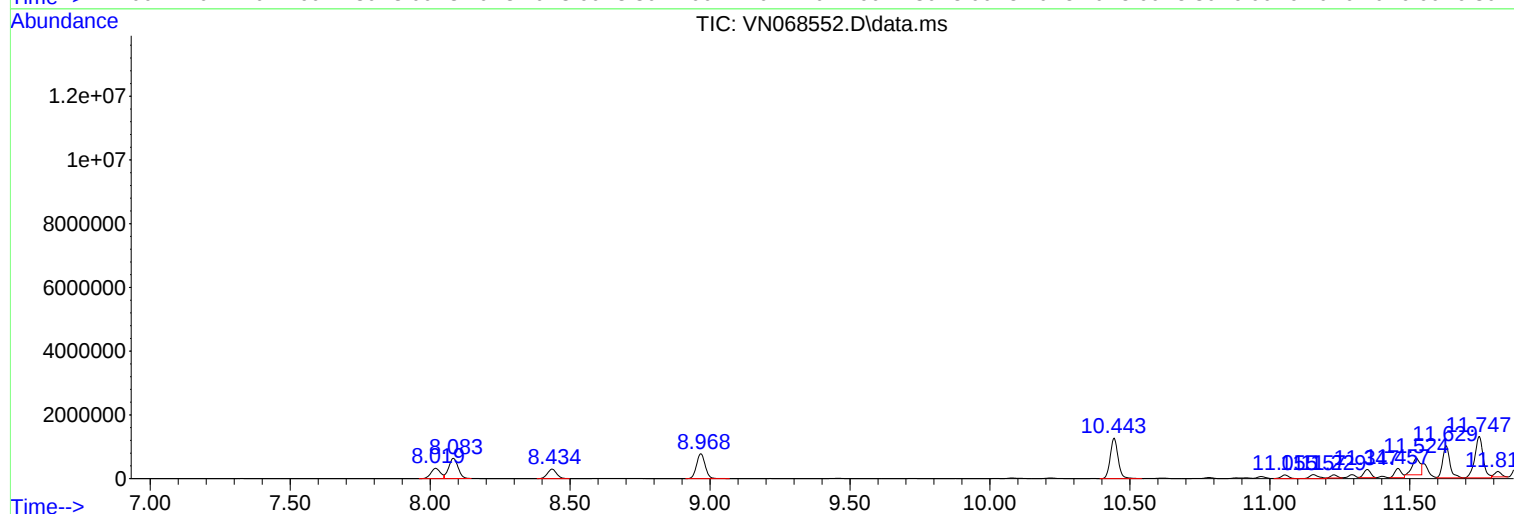
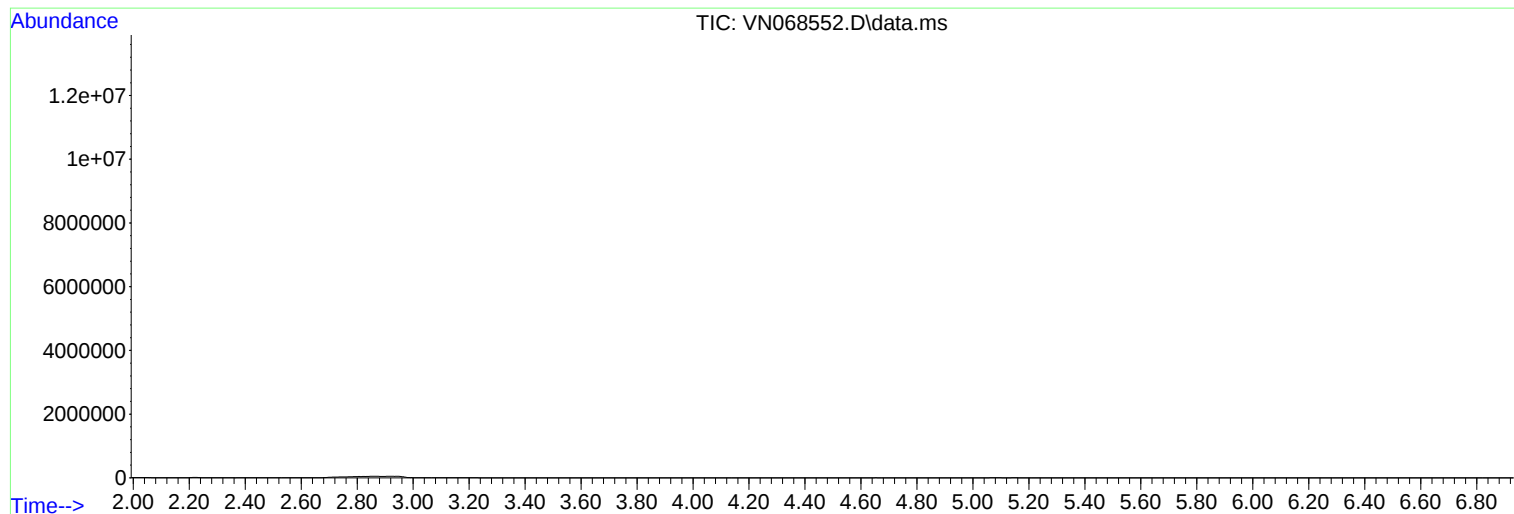
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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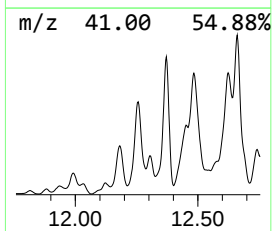
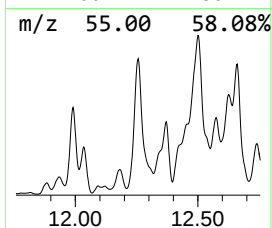
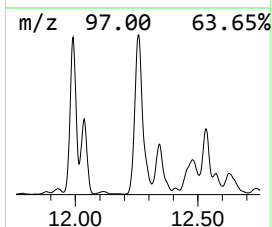
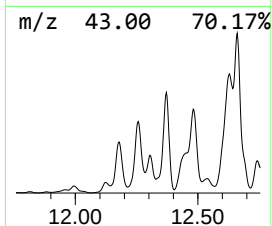
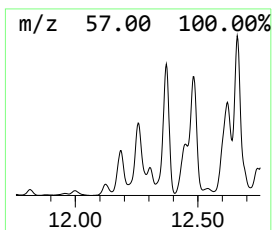
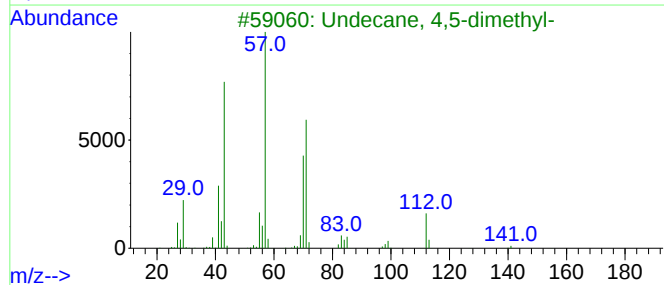
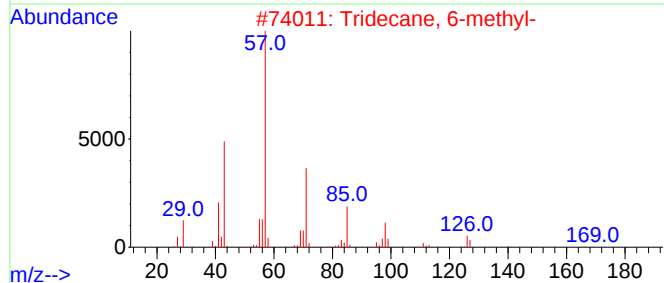
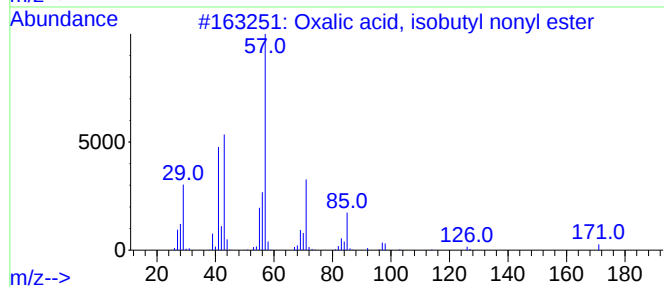
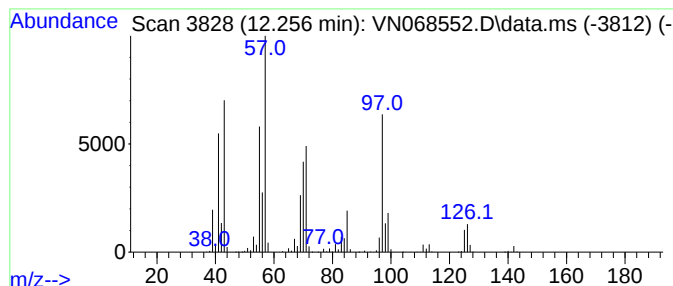
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.256 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	201.93 ug/l	10841000	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	43
2			Tridecane, 6-methyl-	198	C14H30	013287-21-3	43
3			Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	38
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	30
5			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	30



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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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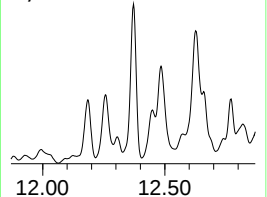
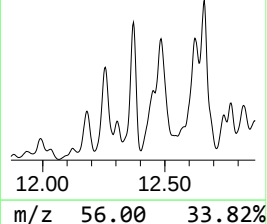
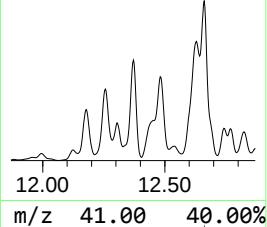
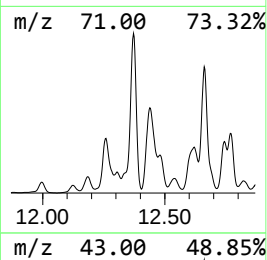
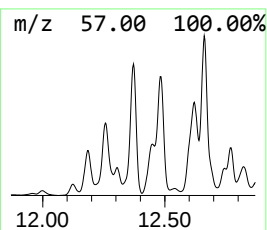
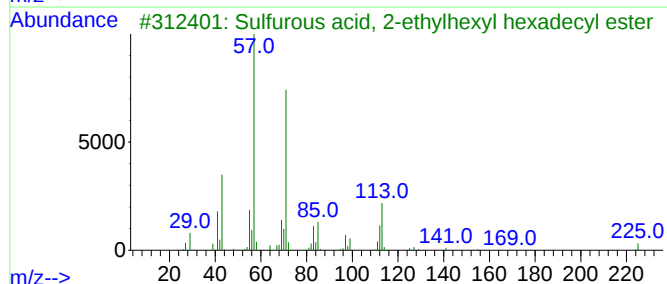
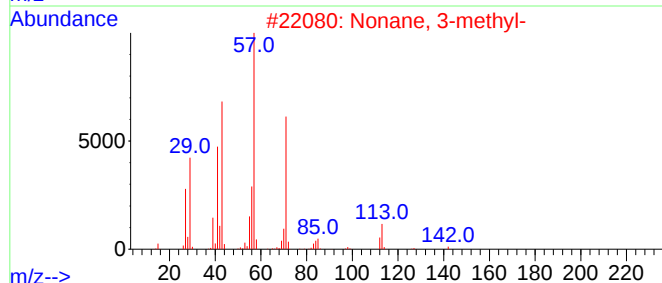
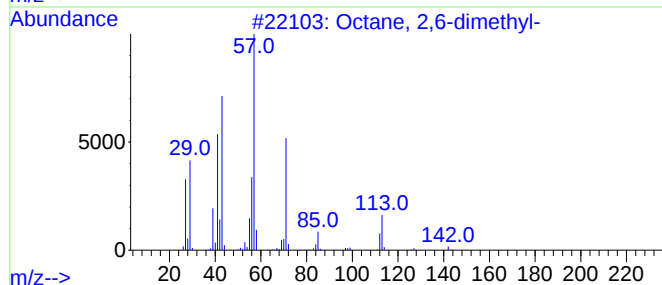
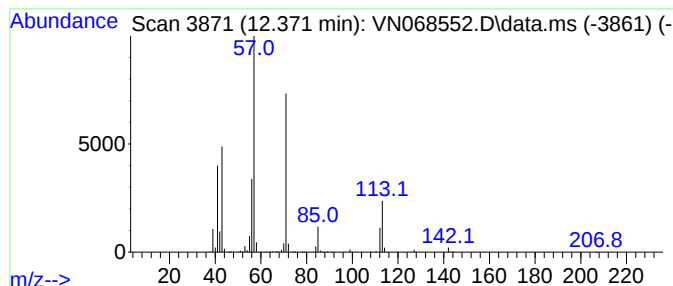
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.371	194.37 ug/l	10435200	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	90
3			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	78
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	78
5			Octyl thioglycolate	204	C10H20O2S	007664-80-4	72



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Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

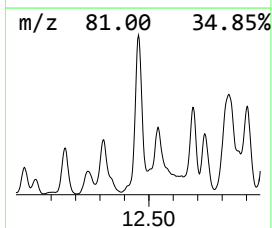
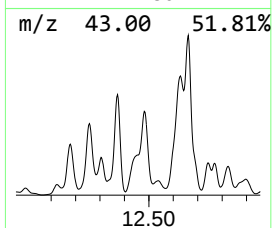
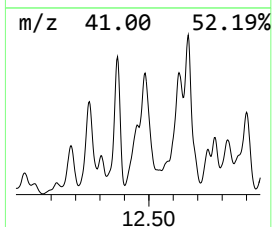
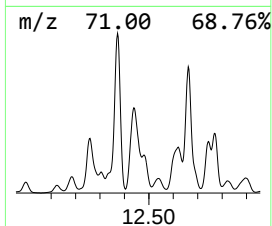
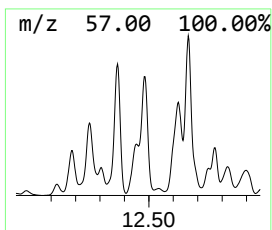
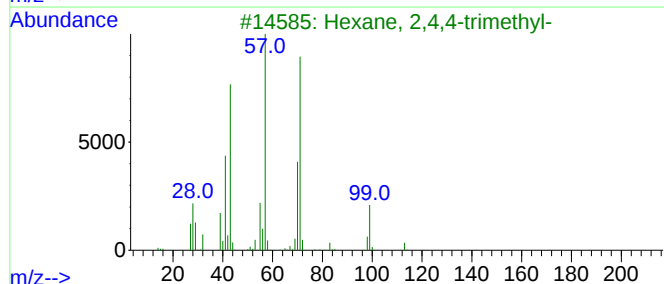
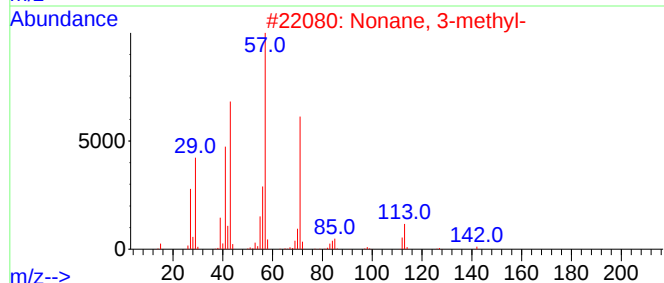
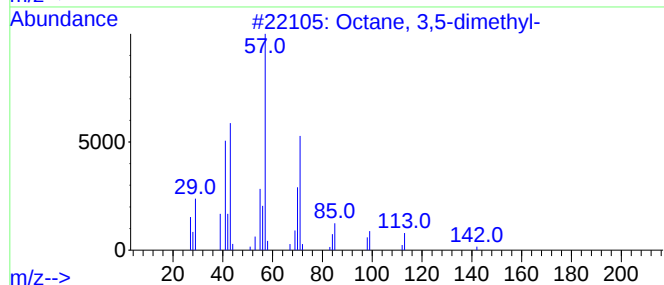
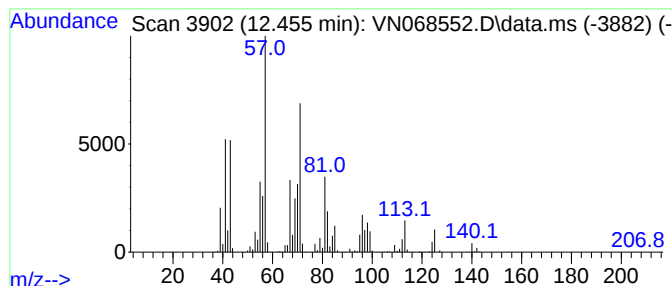
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 3,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	145.69 ug/l	7821970	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	60
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	42
3			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	35
4			Pyrrolidine, 1-(1-oxobutyl)-	141	C8H15NO	033527-93-4	35
5			Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	35



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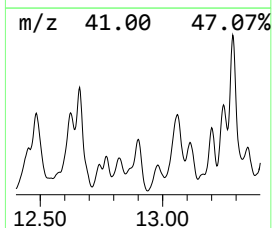
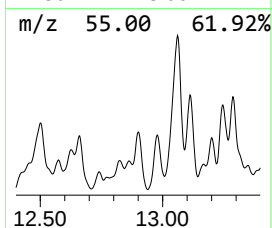
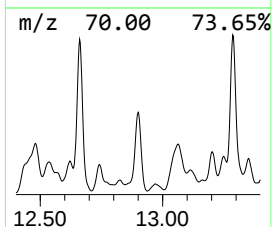
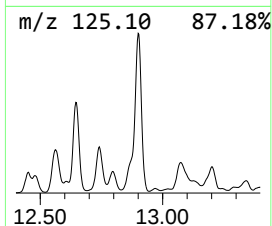
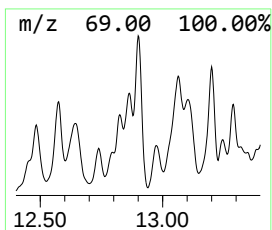
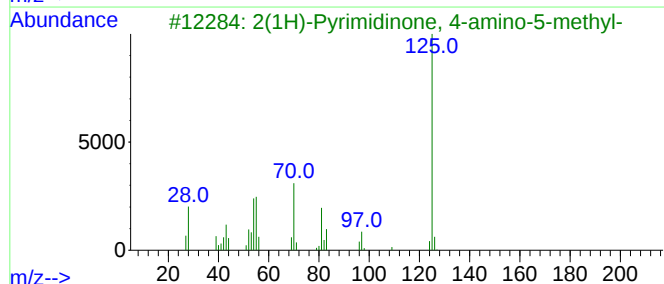
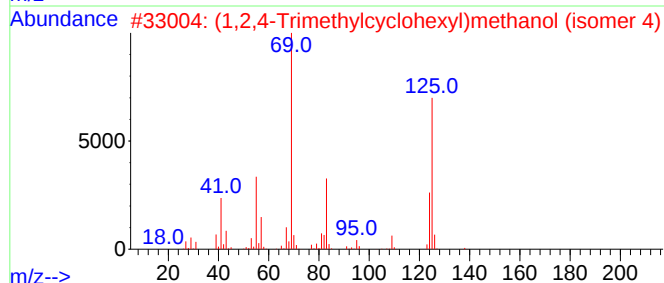
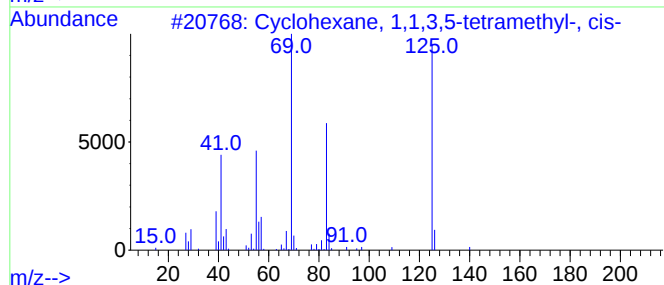
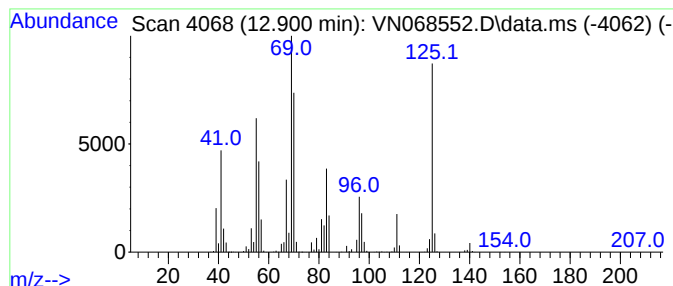
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.900 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.900	164.62 ug/l	9582470	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	43
2			(1,2,4-Trimethylcyclohexyl)metha...	156	C10H20O	1000499-04-1	43
3			2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	43
4			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	43
5			trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	41



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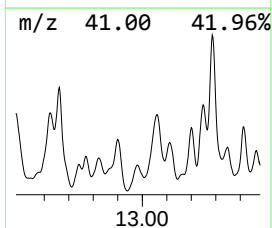
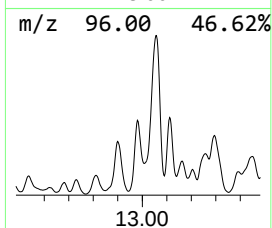
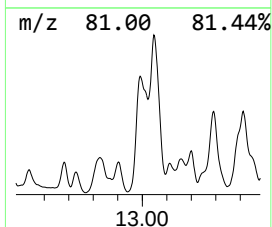
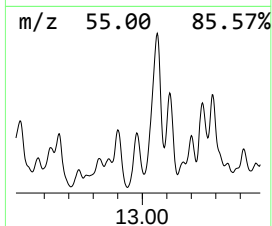
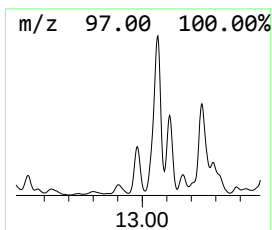
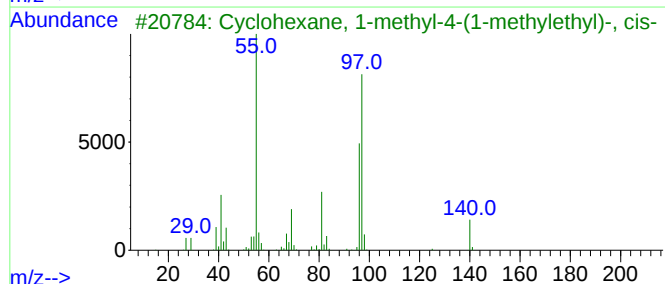
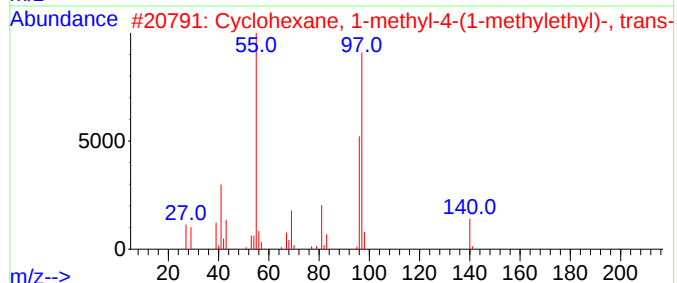
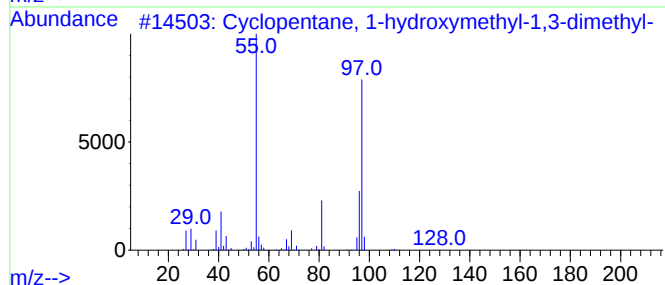
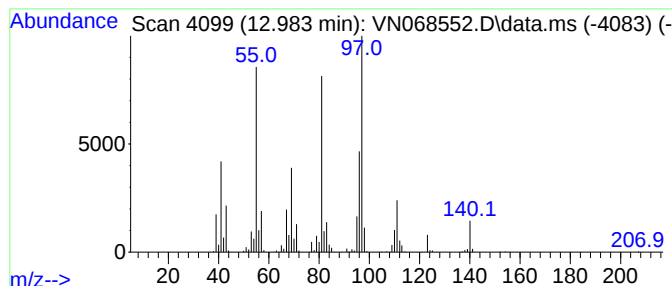
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1-hydroxymeth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	128.94 ug/l	7505180	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	64
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	53
3			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	49
4			Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	47
5			m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068552.D
Acq On : 18 Sep 2021 6:03
Operator : JC/MD
Sample : M3798-05
Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

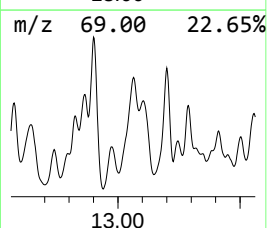
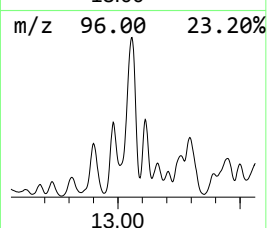
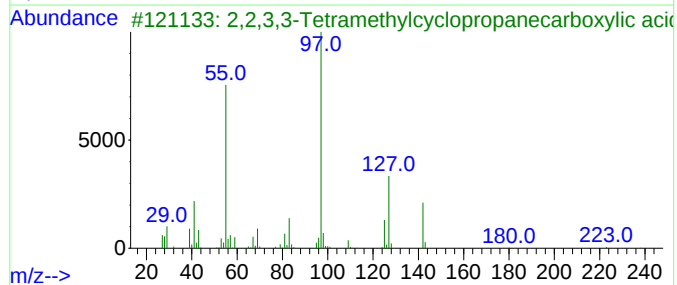
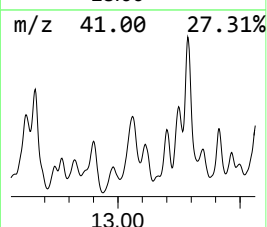
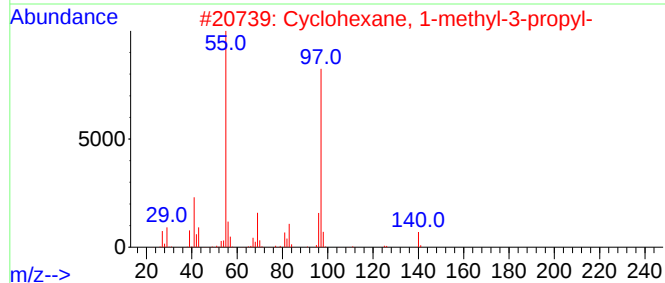
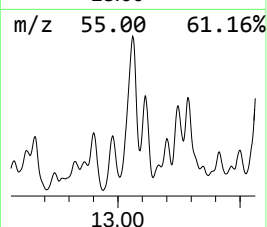
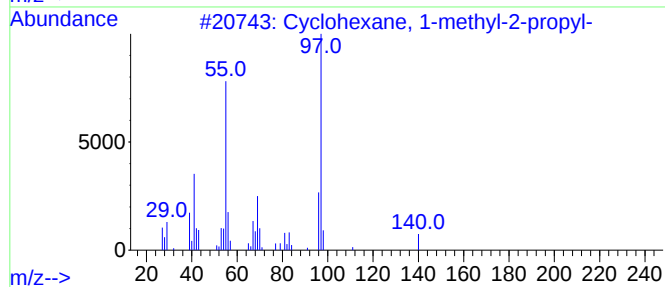
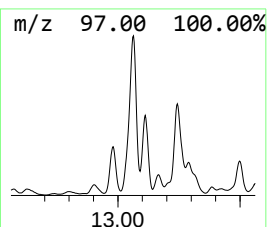
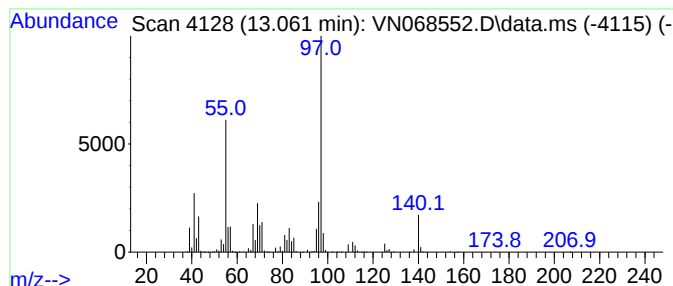
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1-methyl-2-pro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.061	222.45 ug/l	12948600	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	74
2			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	64
3			2,2,3,3-Tetramethylcyclopropanec...	238	C15H26O2	1010221-97-5	53
4			Thiophene, 2-butyl-	140	C8H12S	001455-20-5	53
5			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068552.D
Acq On : 18 Sep 2021 6:03
Operator : JC/MD
Sample : M3798-05
Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

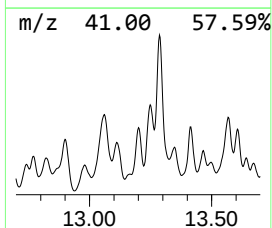
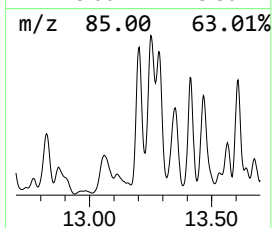
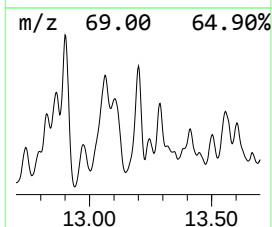
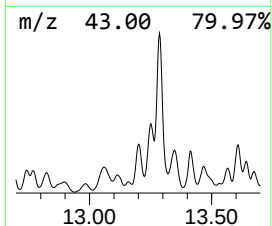
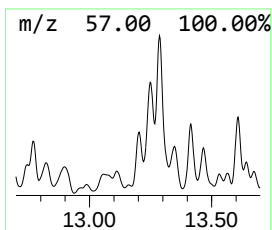
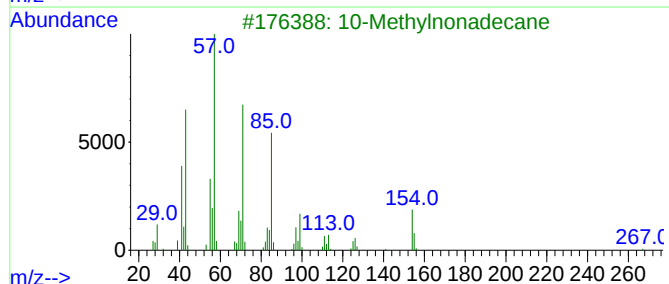
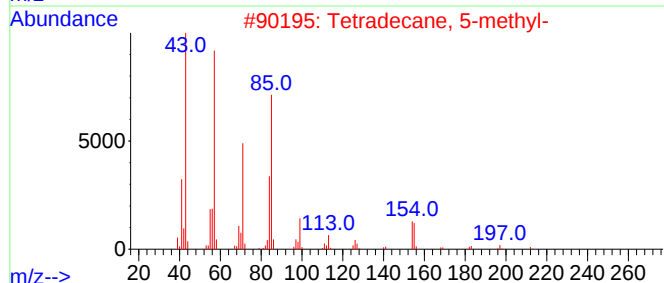
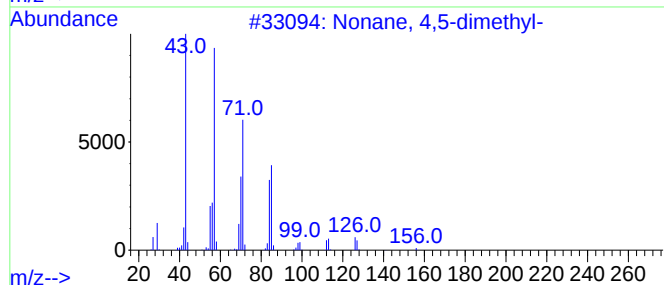
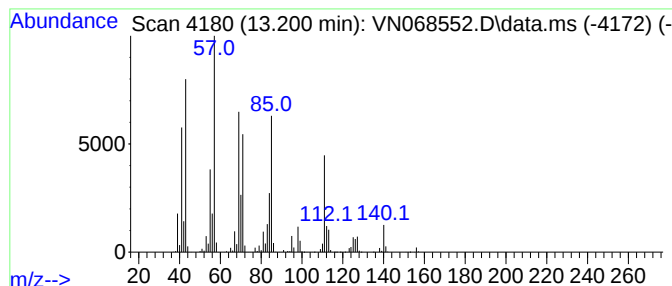
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.200 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.200	100.79 ug/l	5867090	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	49
2			Tetradecane, 5-methyl-	212	C15H32	025117-32-2	47
3			10-Methylnonadecane	282	C20H42	056862-62-5	47
4			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	43
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068552.D
Acq On : 18 Sep 2021 6:03
Operator : JC/MD
Sample : M3798-05
Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

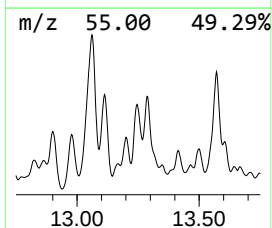
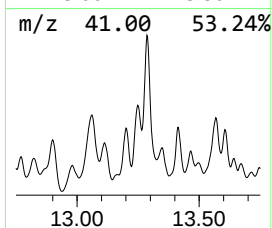
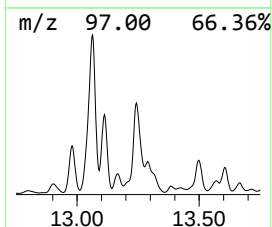
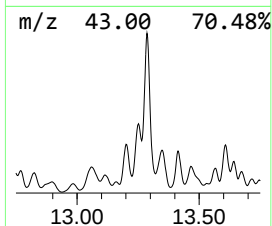
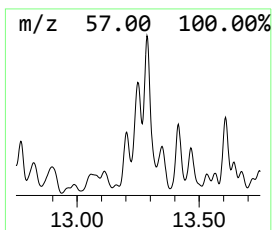
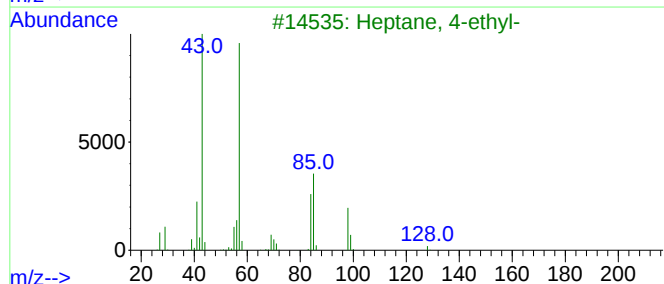
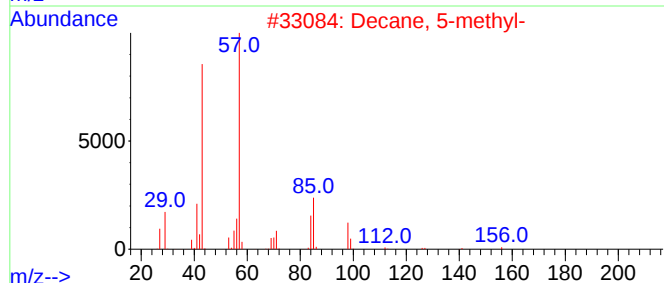
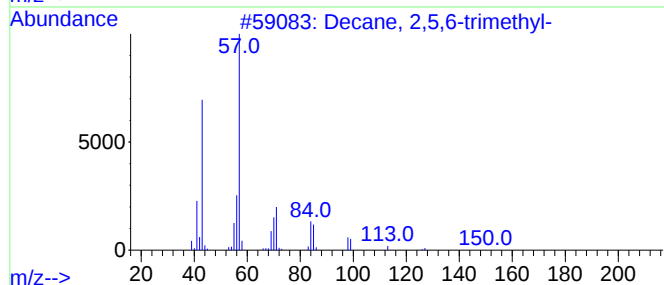
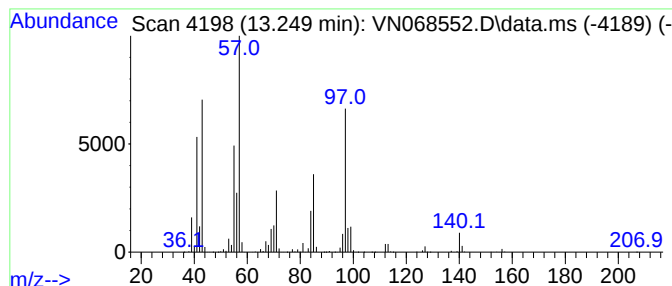
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.249 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.249	137.05 ug/l	7977380	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	47
2			Decane, 5-methyl-	156	C11H24	013151-35-4	43
3			Heptane, 4-ethyl-	128	C9H20	002216-32-2	38
4			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	38
5			1-Iodoundecane	282	C11H23I	004282-44-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068552.D
Acq On : 18 Sep 2021 6:03
Operator : JC/MD
Sample : M3798-05
Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

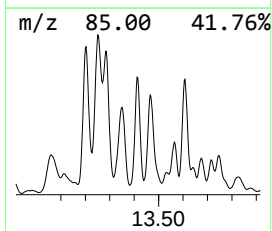
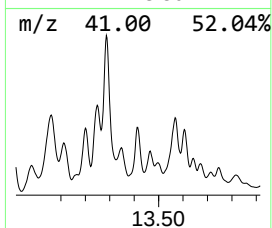
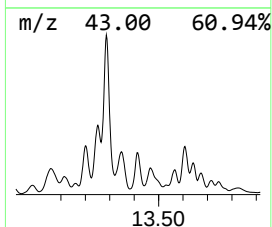
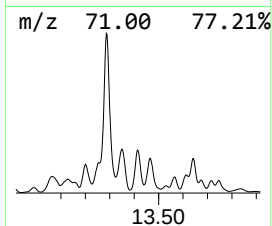
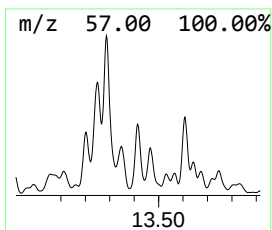
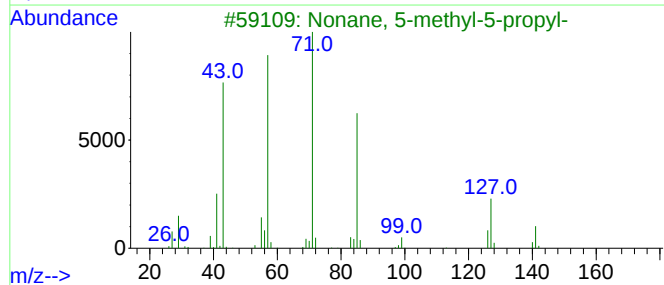
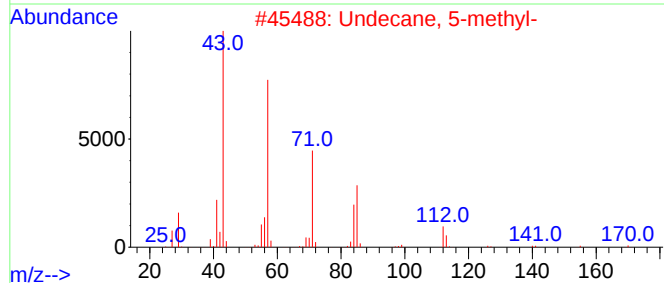
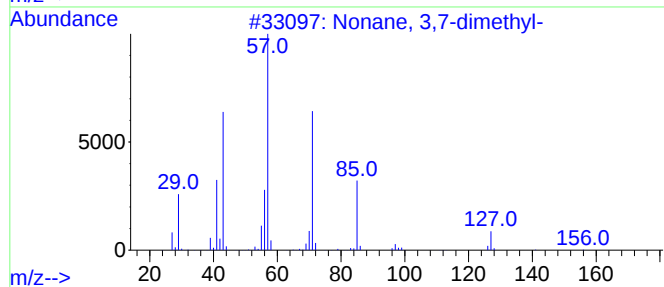
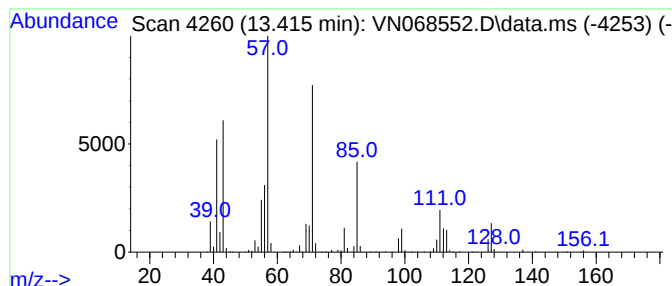
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Quant Title : SW846 8260

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

Peak Number 9 Nonane, 3,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.415	78.51 ug/l	4569960	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	76
2			Undecane, 5-methyl-	170	C12H26	001632-70-8	53
3			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	50
4			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	50
5			Sulfurous acid, decyl pentyl ester	292	C15H32O3S	1000309-14-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068552.D
Acq On : 18 Sep 2021 6:03
Operator : JC/MD
Sample : M3798-05
Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

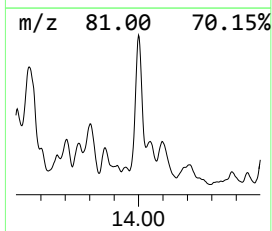
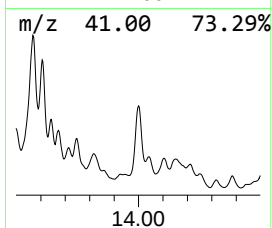
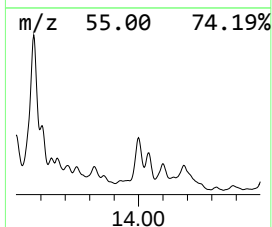
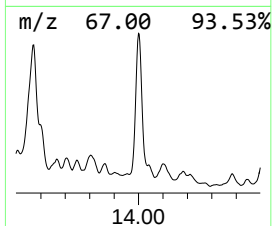
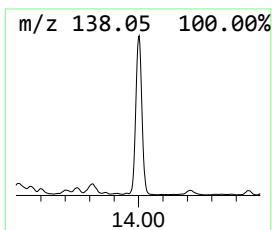
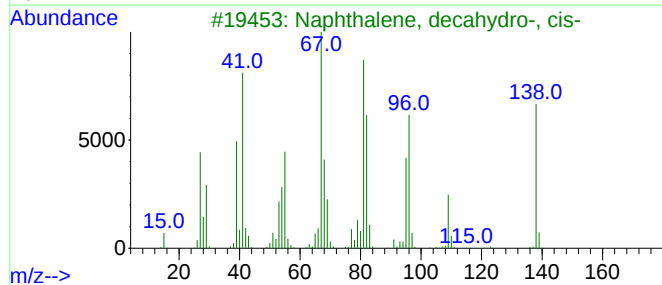
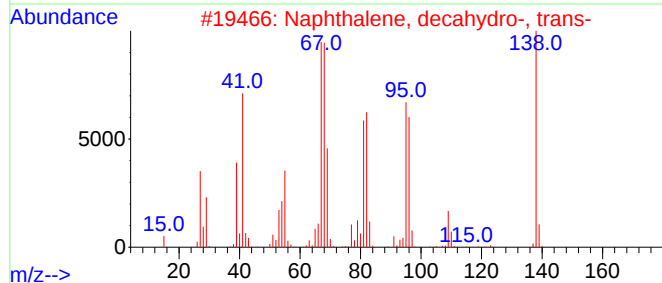
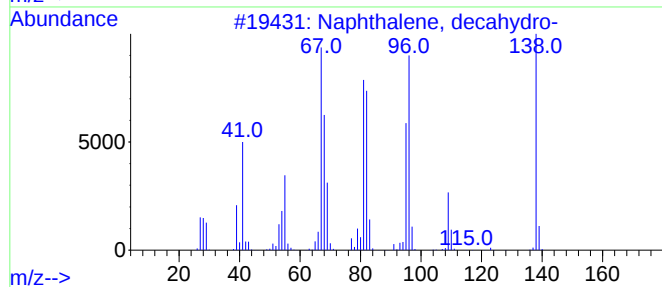
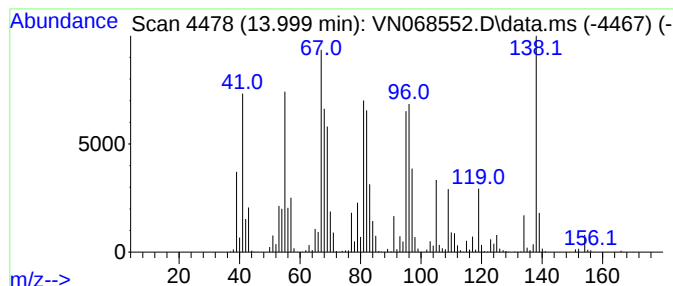
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, decahydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	135.74 ug/l	7901060	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	97
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	81
4			Spiro[4.5]decane	138	C10H18	000176-63-6	74
5			Cyclodecene	138	C10H18	003618-12-0	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068552.D
Acq On : 18 Sep 2021 6:03
Operator : JC/MD
Sample : M3798-05
Misc : 6.64g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SUB-SLAB-01-(5-8)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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Octane, 3,5-dim...	12.455	145.7	ug/l	7821970	3	11.749	2684360	50.0
unknown12.900	12.900	164.6	ug/l	9582470	4	13.678	2910460	50.0
Cyclopentane, 1...	12.983	128.9	ug/l	7505180	4	13.678	2910460	50.0
Cyclohexane, 1-...	13.061	222.4	ug/l	12948600	4	13.678	2910460	50.0
unknown13.200	13.200	100.8	ug/l	5867090	4	13.678	2910460	50.0
unknown13.249	13.249	137.1	ug/l	7977380	4	13.678	2910460	50.0
Nonane, 3,7-dim...	13.415	78.5	ug/l	4569960	4	13.678	2910460	50.0
Naphthalene, de...	13.999	135.7	ug/l	7901060	4	13.678	2910460	50.0