

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
 Data File : VN068554.D
 Acq On : 18 Sep 2021 6:53
 Operator : JC/MD
 Sample : M3798-07
 Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DUPLICATE-2

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: VN068554.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	2224	2248	2259	rBV2	337638	818435	6.04%	0.606%
2	8.083	2260	2272	2304	rVB	723899	1639100	12.09%	1.213%
3	8.434	2382	2403	2429	rBV	329380	768457	5.67%	0.569%
4	8.965	2581	2601	2641	rBV	871114	1799706	13.28%	1.332%
5	10.443	3133	3152	3190	rBV	1342892	2611262	19.26%	1.932%
6	11.055	3364	3380	3396	rVB2	93731	170691	1.26%	0.126%
7	11.157	3402	3418	3434	rBV3	97116	213590	1.58%	0.158%
8	11.347	3478	3489	3501	rVB	209325	348727	2.57%	0.258%
9	11.460	3518	3531	3539	rBV3	227964	397820	2.93%	0.294%
10	11.521	3540	3554	3581	rVB4	507308	1581637	11.67%	1.170%
11	11.629	3582	3594	3618	rVB	811561	1441951	10.64%	1.067%
12	11.749	3618	3639	3655	rBV	1392738	2779500	20.51%	2.057%
13	11.816	3657	3664	3677	rVB	142823	223436	1.65%	0.165%
14	11.881	3677	3688	3696	rBV2	273718	462457	3.41%	0.342%
15	11.937	3697	3709	3717	rBV4	364930	710460	5.24%	0.526%
16	11.991	3719	3729	3739	rBV2	1108815	1808528	13.34%	1.338%
17	12.122	3757	3778	3785	rBV3	448749	1094483	8.07%	0.810%
18	12.178	3788	3799	3811	rVB3	1603749	2847967	21.01%	2.107%
19	12.256	3812	3828	3840	rBV4	4254101	8935791	65.92%	6.612%
20	12.372	3862	3871	3882	rVB	5202836	8156723	60.18%	6.035%
21	12.455	3882	3902	3904	rBV7	3052982	6146711	45.35%	4.548%
22	12.661	3974	3979	3997	rVB	8121171	13231546	97.61%	9.790%
23	12.739	3997	4008	4015	rBV4	2877402	4836227	35.68%	3.578%
24	12.900	4061	4068	4083	rVB4	4932057	9027125	66.60%	6.679%
25	12.983	4083	4099	4108	rBV7	2757497	6620731	48.84%	4.899%
26	13.061	4114	4128	4139	rBV4	6354889	13363116	98.59%	9.888%
27	13.200	4171	4180	4188	rBV3	4184405	6023806	44.44%	4.457%
28	13.249	4189	4198	4204	rVV4	3941028	6218443	45.88%	4.601%
29	13.286	4205	4212	4226	rVB2	9000958	13554918	100.00%	10.030%
30	13.415	4252	4260	4269	rVB2	2697820	3767407	27.79%	2.788%
31	13.608	4327	4332	4339	rVB	2590773	2911796	21.48%	2.155%
32	14.002	4467	4479	4489	rBV4	3152827	5716829	42.18%	4.230%
33	14.321	4589	4598	4611	rVB6	535491	965116	7.12%	0.714%
34	14.386	4614	4622	4636	rVB10	550624	1010443	7.45%	0.748%
35	14.512	4662	4669	4701	rVB5	1024808	2615257	19.29%	1.935%
36	14.624	4703	4711	4718	rBV7	190032	327565	2.42%	0.242%

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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

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Peak separation: 5

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

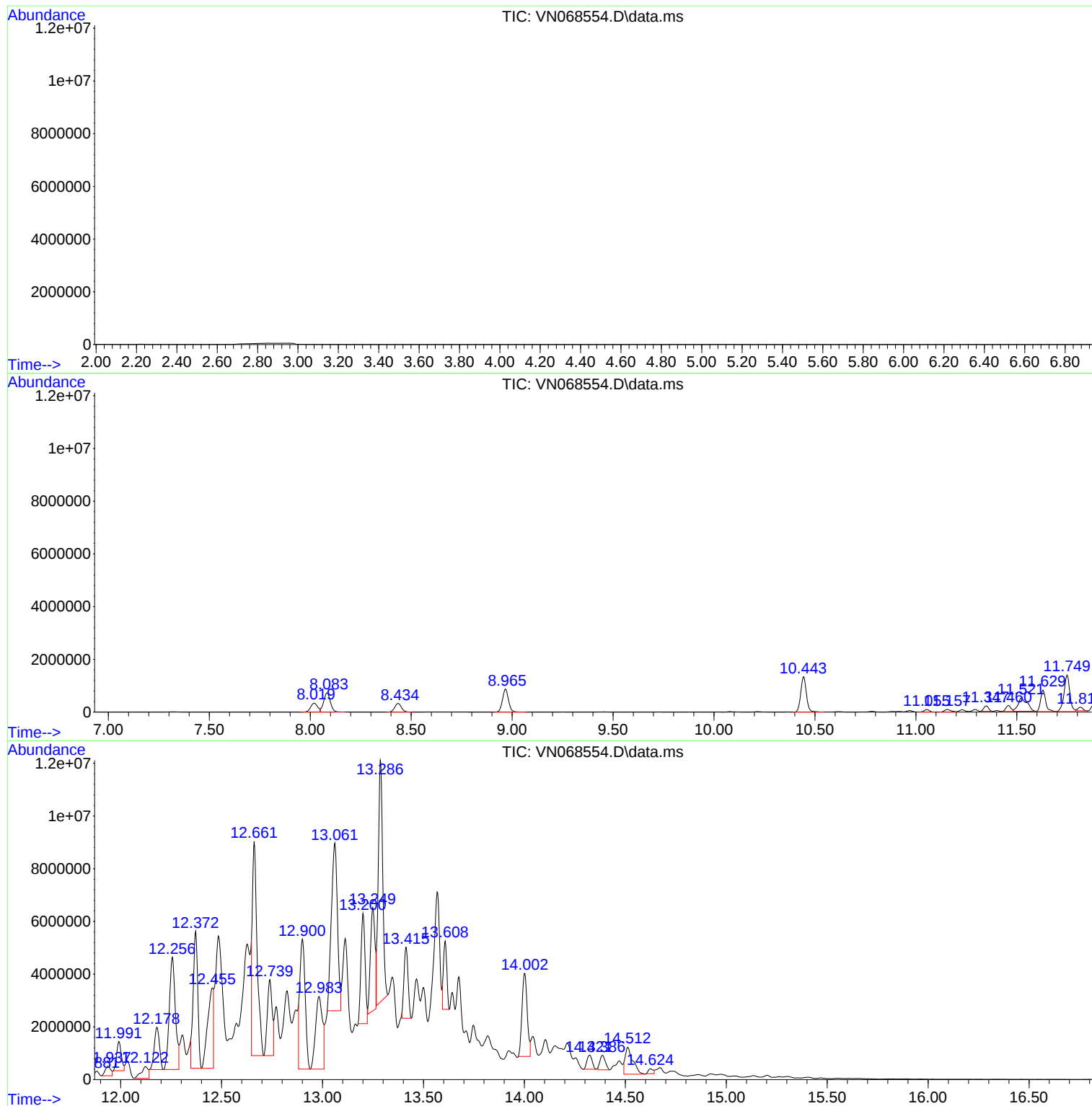
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
DUPLICATE-2

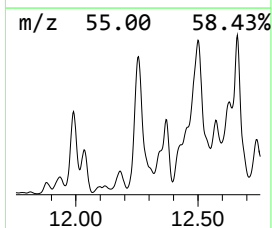
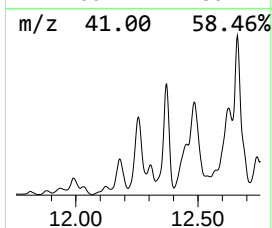
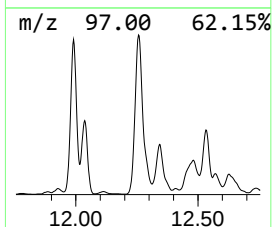
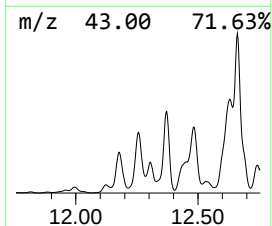
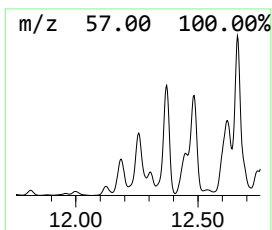
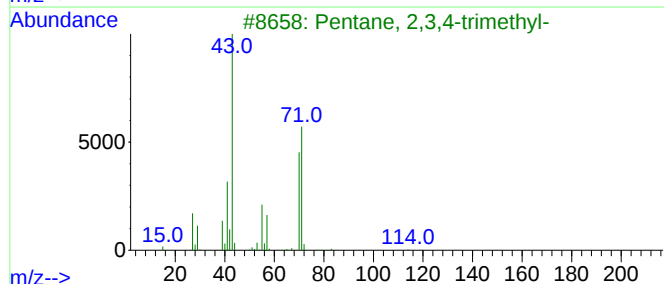
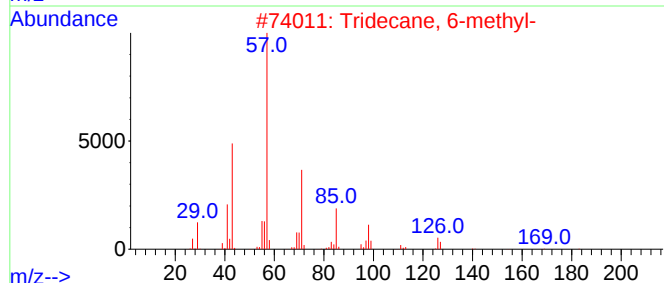
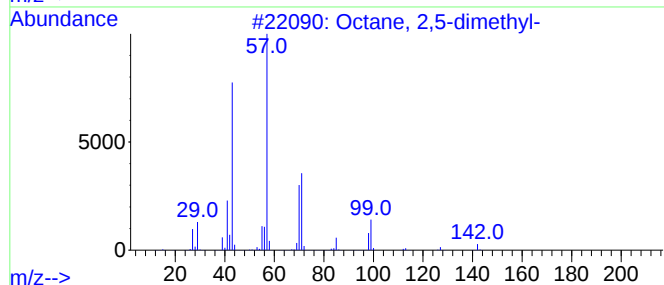
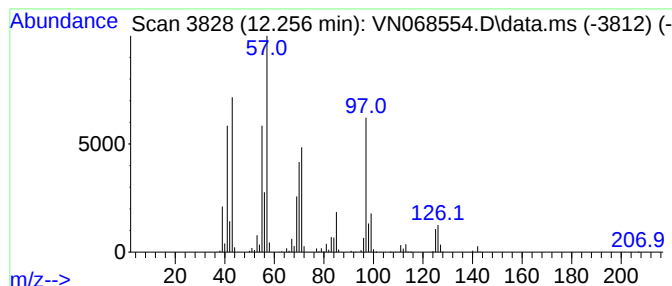
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	160.75 ug/l	8935790	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	52
2			Tridecane, 6-methyl-	198	C14H30	013287-21-3	38
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	35
4			Hexamethylenimine	99	C6H13N	000111-49-9	30
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	30



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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUPLICATE-2

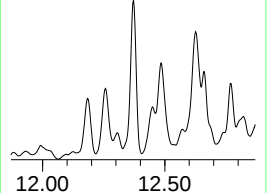
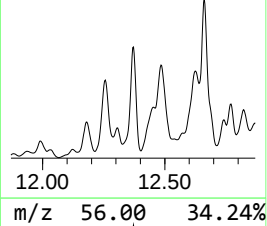
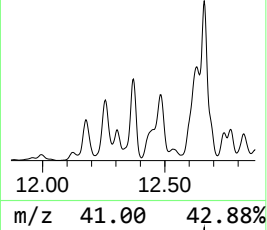
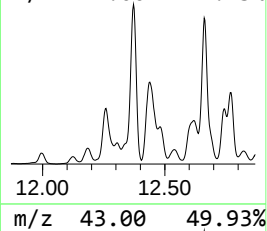
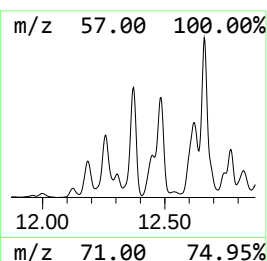
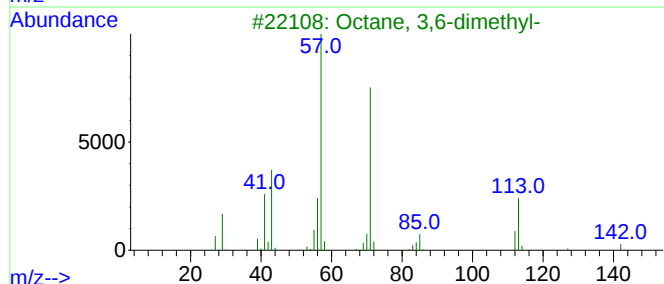
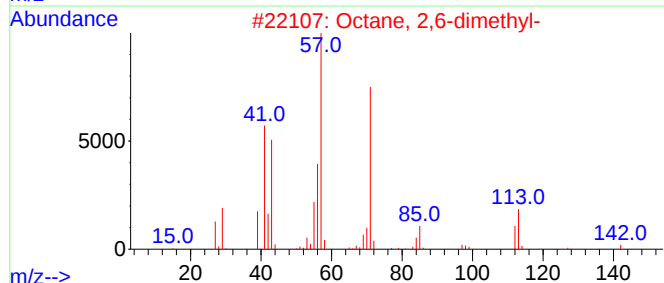
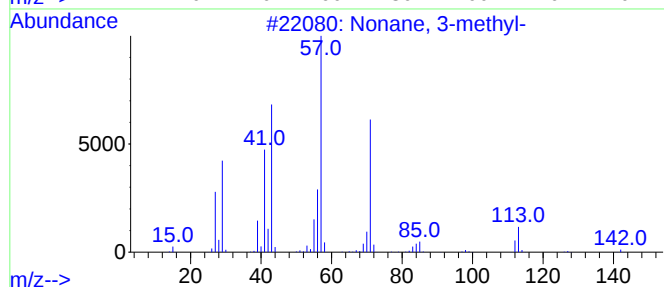
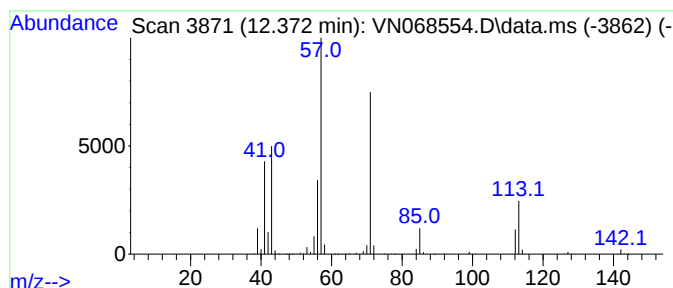
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Nonane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.371	146.73 ug/l	8156720	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	83
4			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	80
5			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	78



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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUPLICATE-2

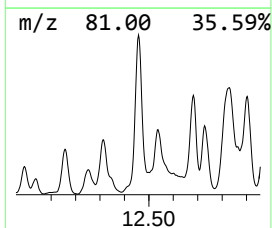
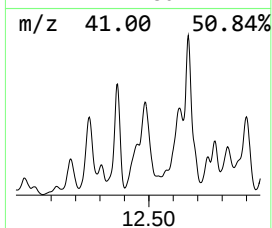
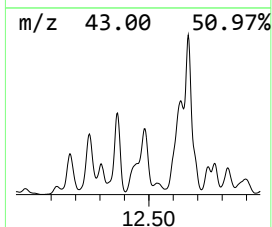
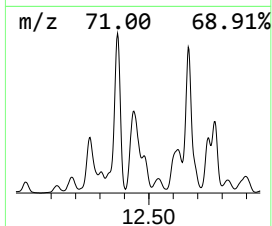
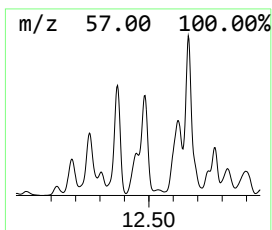
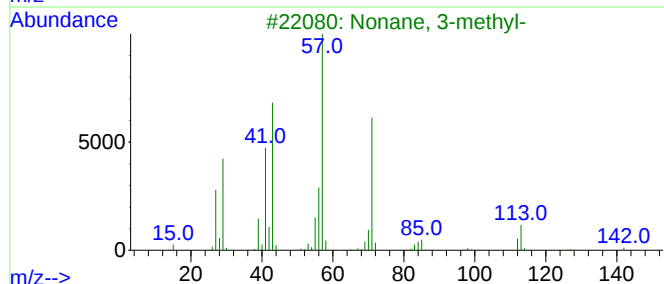
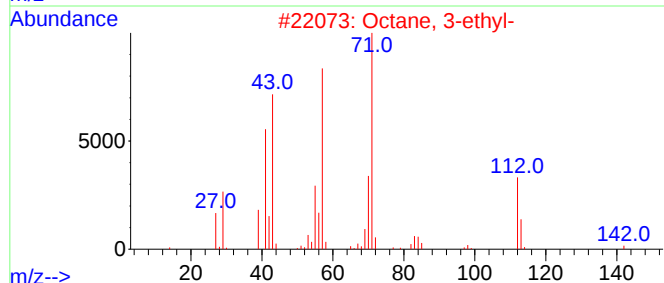
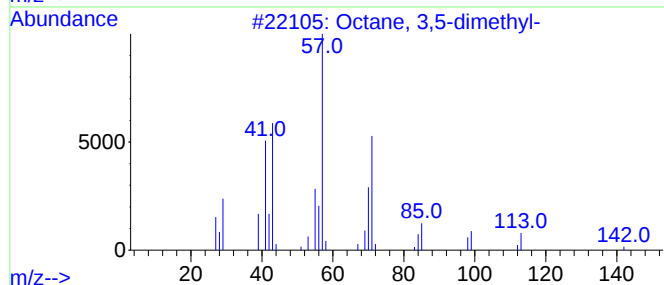
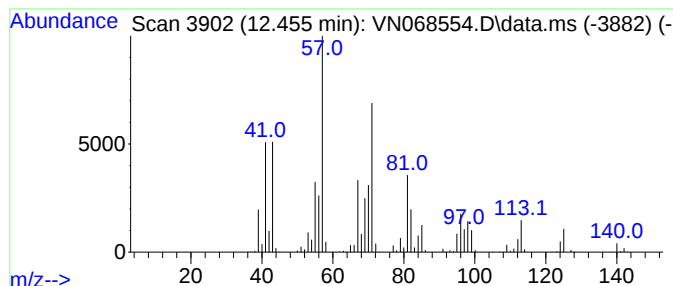
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 3,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	110.57 ug/l	6146710	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			Octane, 3-ethyl-	142	C10H22	005881-17-4	43
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	38
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	35
5			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	35



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Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

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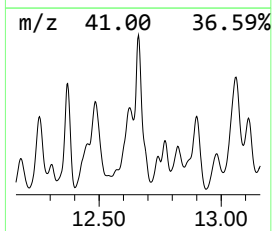
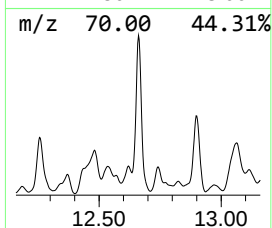
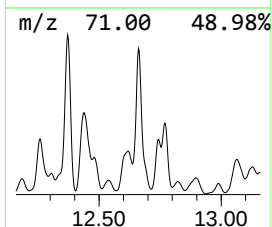
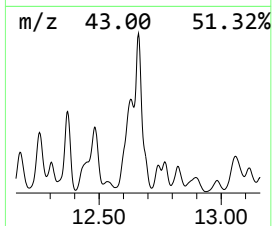
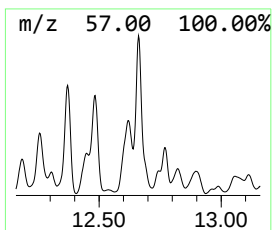
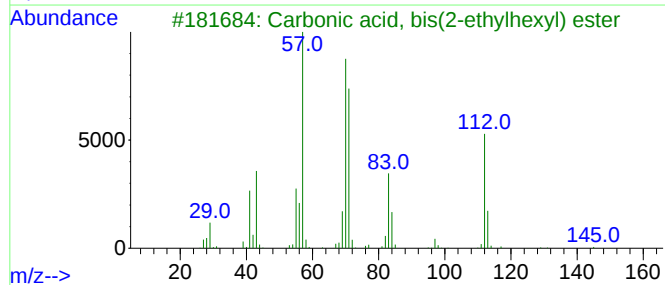
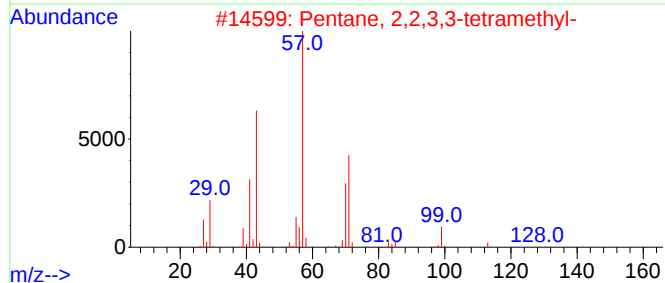
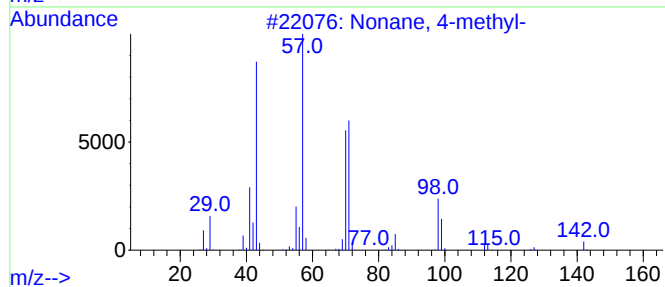
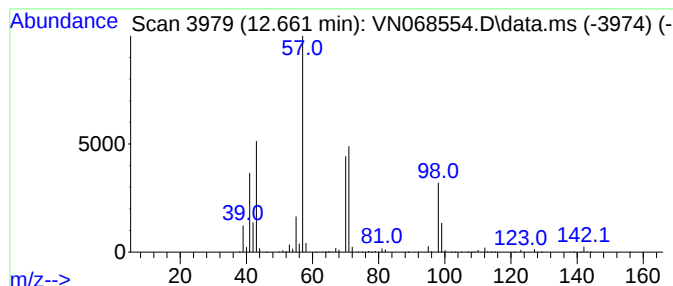
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.661	238.02 ug/l	13231500	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4-methyl-	142	C10H22	017301-94-9	80
2			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	59
3			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	53
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	50
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	47



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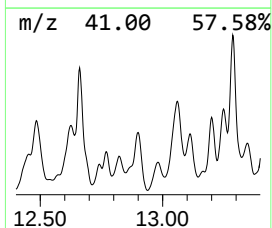
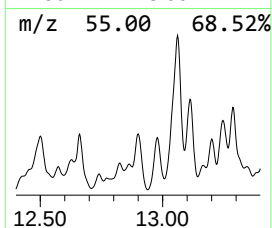
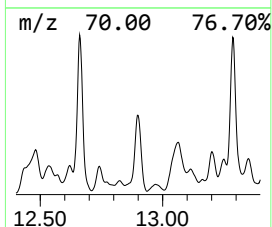
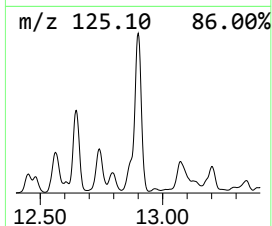
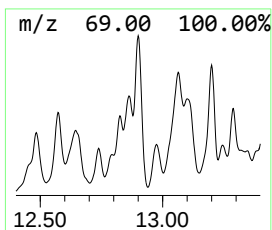
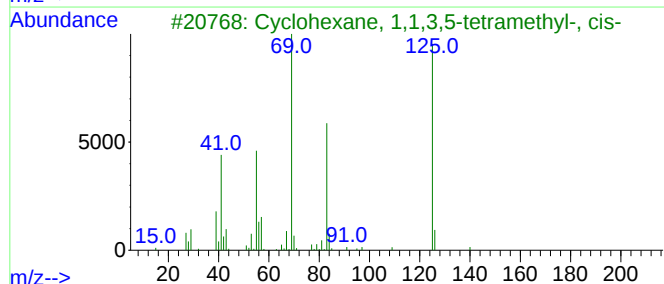
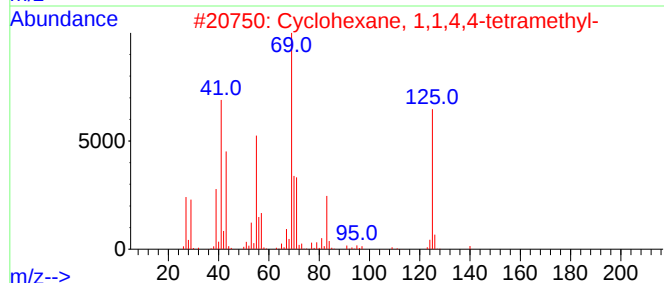
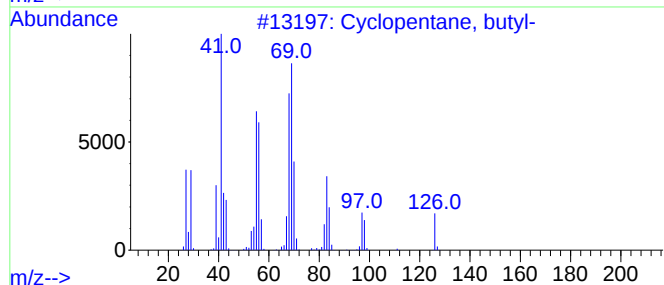
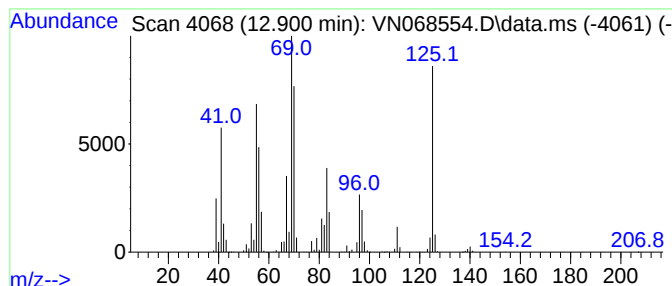
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown12.900 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.900	155.01 ug/l	9027130	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, butyl-	126	C9H18	002040-95-1	49
2			Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	46
3			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	43
4			(1,2,4-Trimethylcyclohexyl)metha...	156	C10H20O	1000499-04-1	43
5			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068554.D
Acq On : 18 Sep 2021 6:53
Operator : JC/MD
Sample : M3798-07
Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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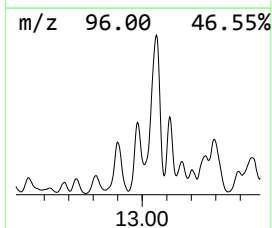
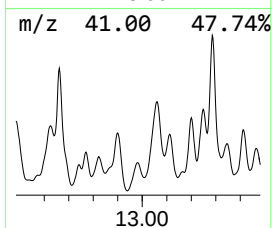
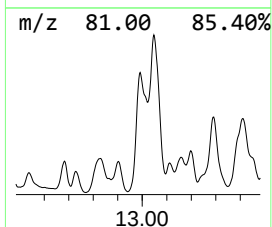
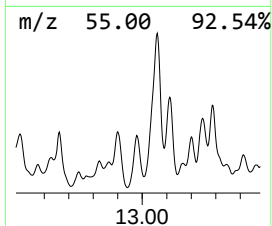
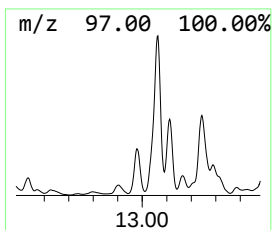
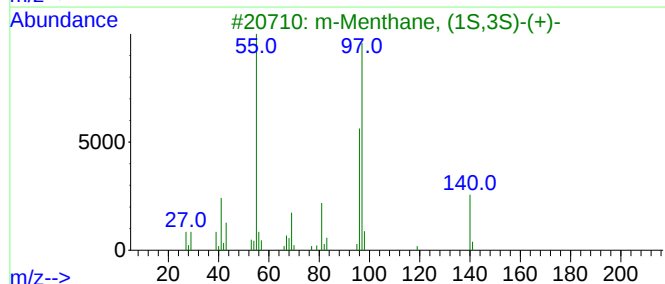
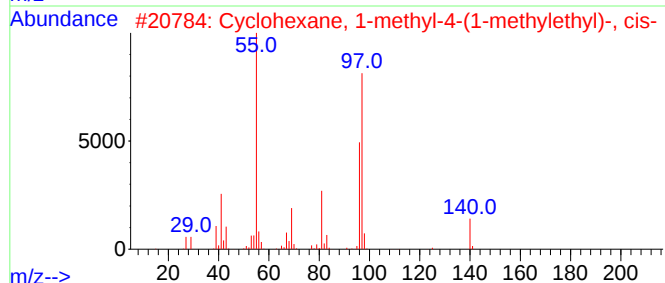
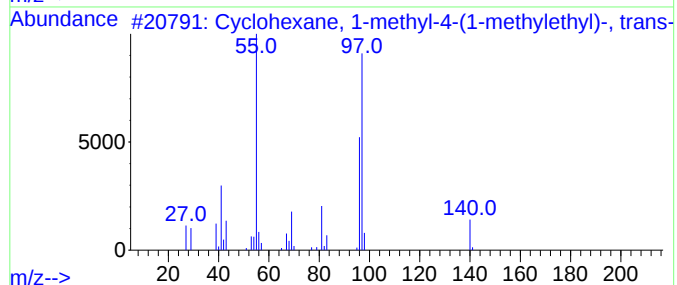
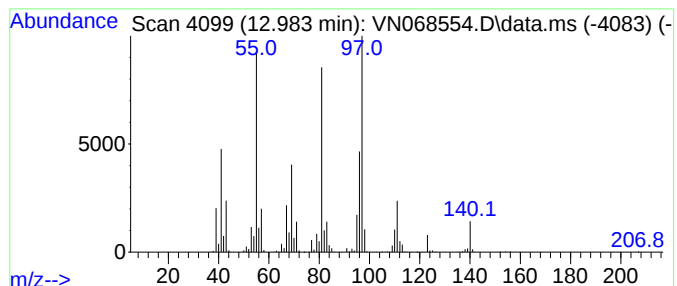
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Quant Title : SW846 8260

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

Peak Number 6 unknown12.983 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	113.69 ug/l	6620730	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	49
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	49
3			m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	47
4			Oxalic acid, butyl cyclohexylmet...	242	C13H22O4	1000309-68-2	43
5			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068554.D
Acq On : 18 Sep 2021 6:53
Operator : JC/MD
Sample : M3798-07
Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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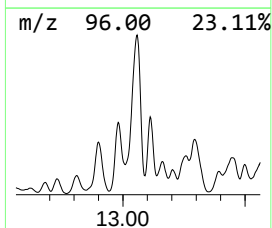
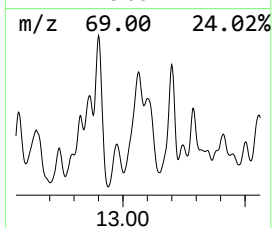
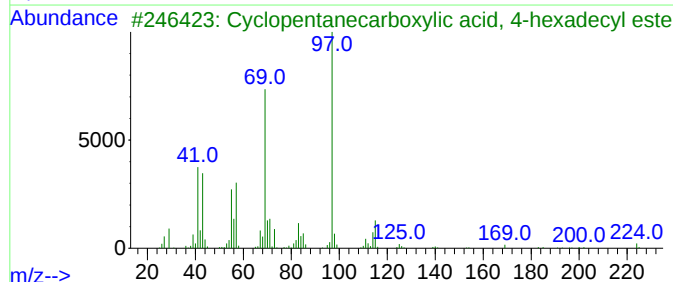
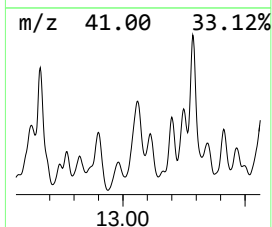
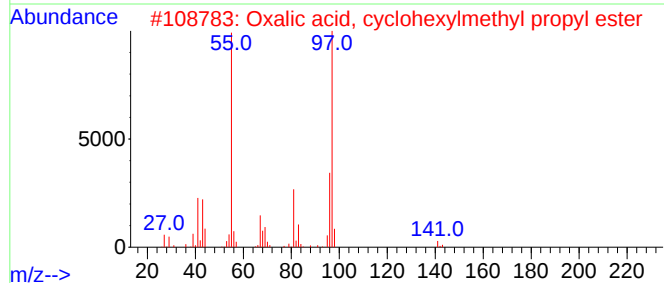
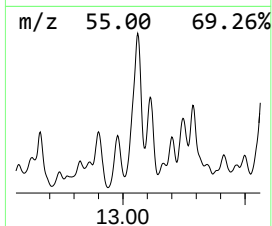
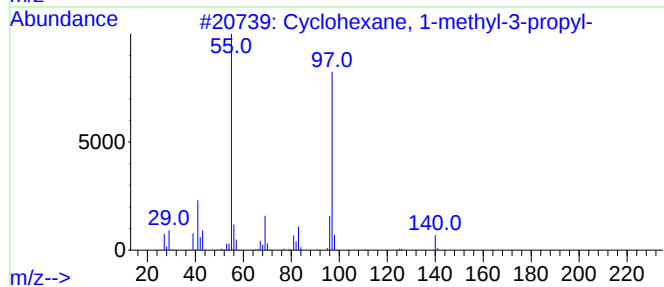
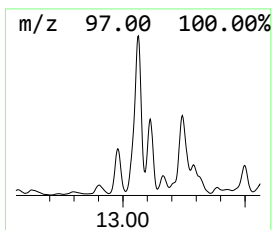
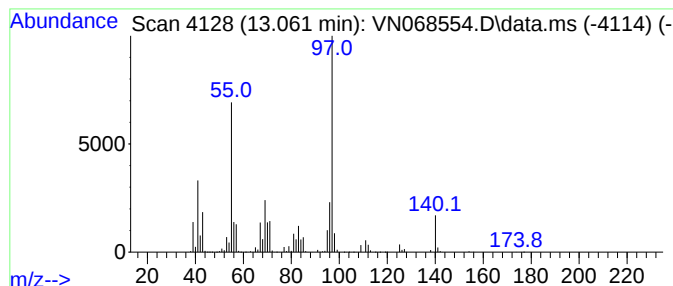
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1-methyl-3-pro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.061	229.47 ug/l	13363100	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	81
2			Oxalic acid, cyclohexylmethyl pr...	228	C12H20O4	1010309-68-1	64
3			Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	59
4			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	58
5			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068554.D
Acq On : 18 Sep 2021 6:53
Operator : JC/MD
Sample : M3798-07
Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUPLICATE-2

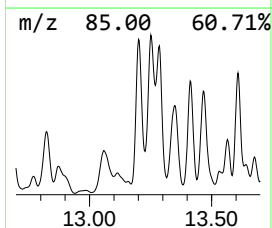
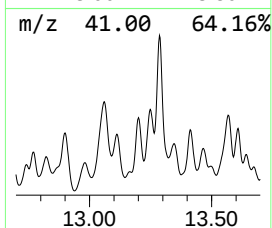
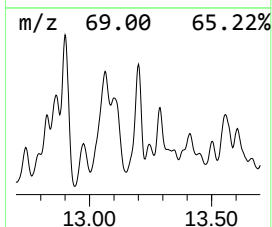
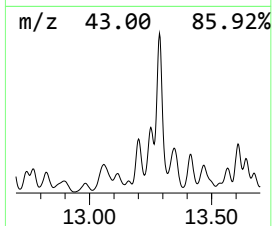
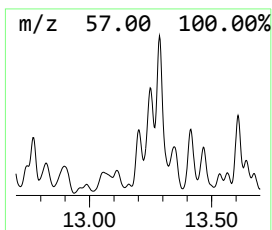
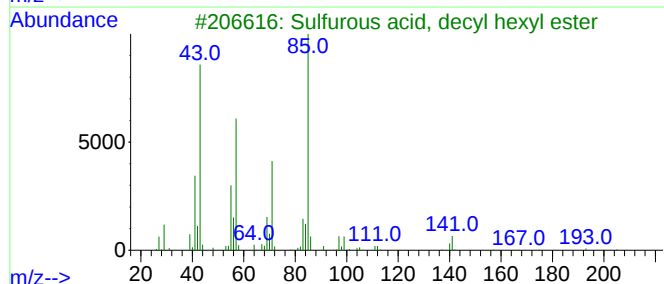
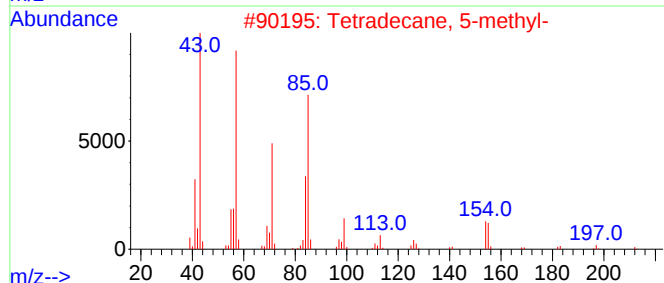
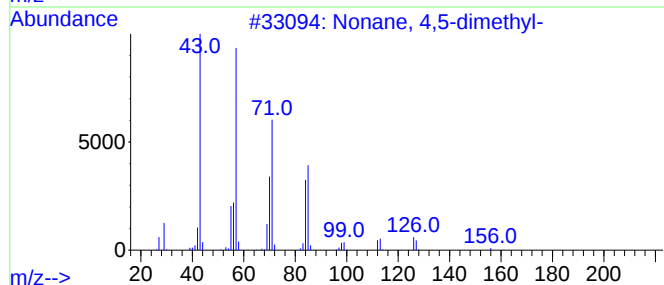
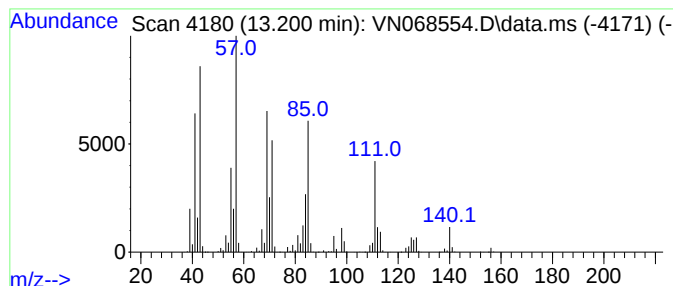
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.200 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.200	103.44 ug/l	6023810	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			Sulfurous acid, decyl hexyl ester	306	C16H34O3S	1000309-13-2	43
4			Decane, 4-methyl-	156	C11H24	002847-72-5	38
5			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068554.D
Acq On : 18 Sep 2021 6:53
Operator : JC/MD
Sample : M3798-07
Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUPLICATE-2

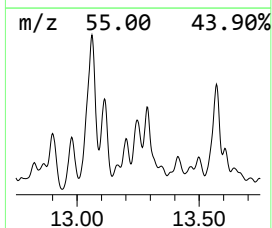
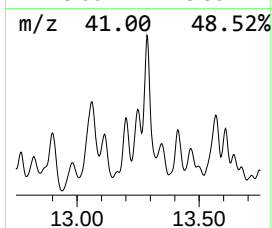
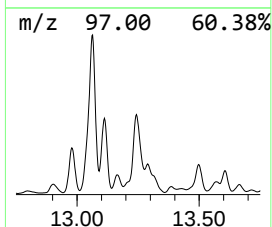
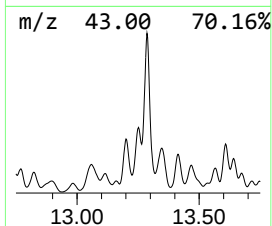
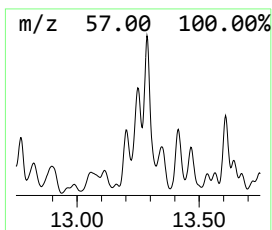
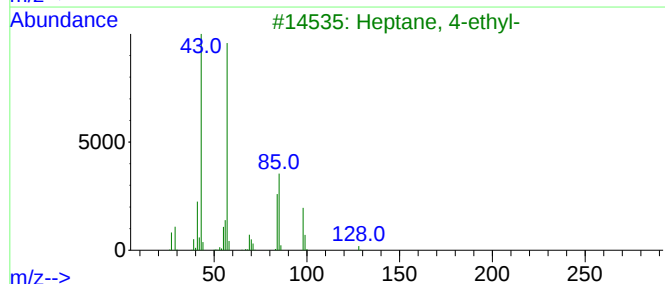
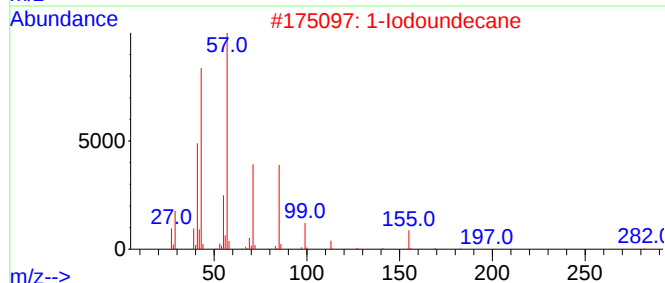
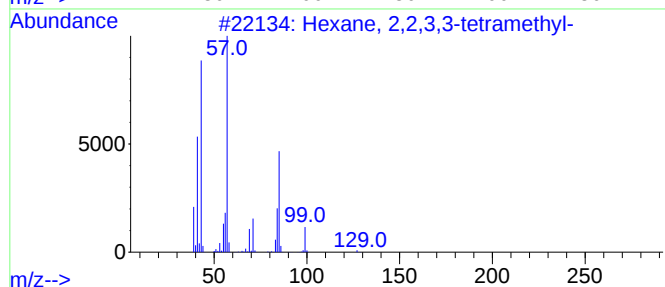
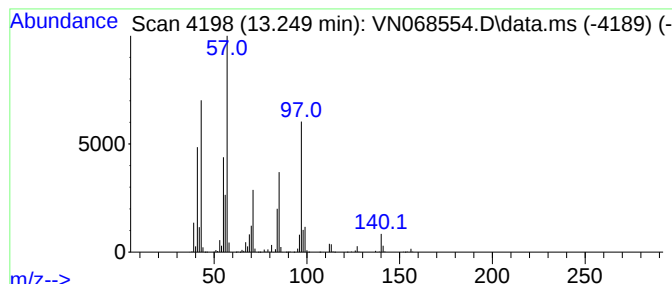
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Quant Title : SW846 8260

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

Peak Number 9 unknown13.249 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.249	106.78 ug/l	6218440	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	38
2			1-Iodoundecane	282	C11H23I	004282-44-4	38
3			Heptane, 4-ethyl-	128	C9H20	002216-32-2	38
4			Decane, 5-methyl-	156	C11H24	013151-35-4	38
5			Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068554.D
Acq On : 18 Sep 2021 6:53
Operator : JC/MD
Sample : M3798-07
Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUPLICATE-2

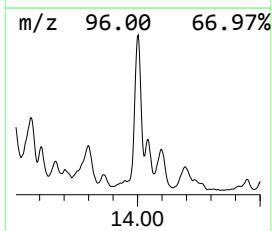
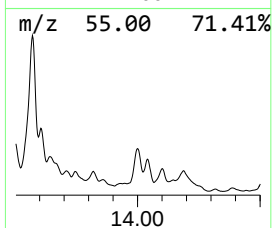
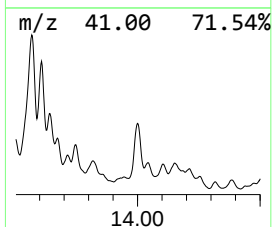
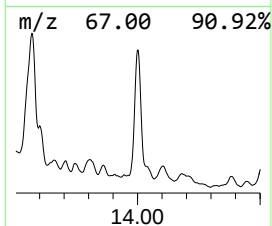
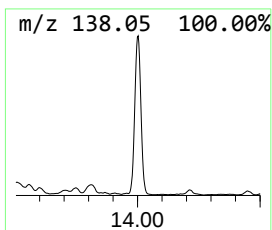
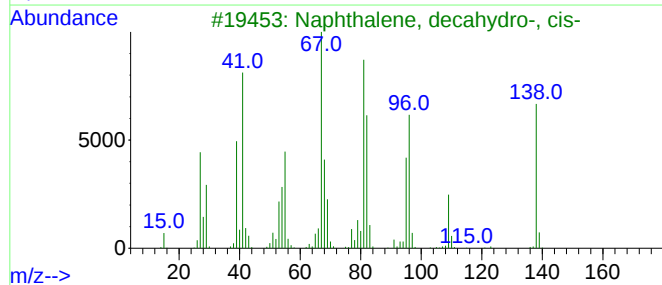
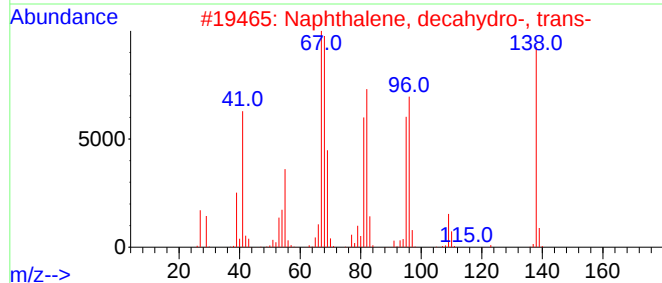
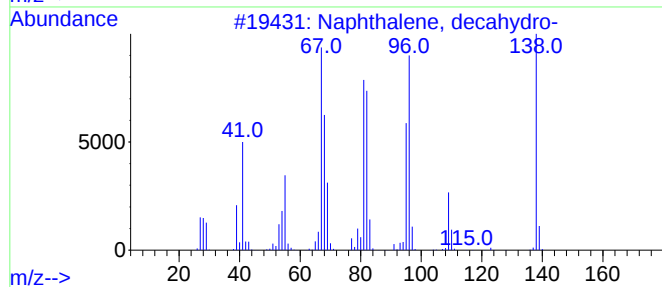
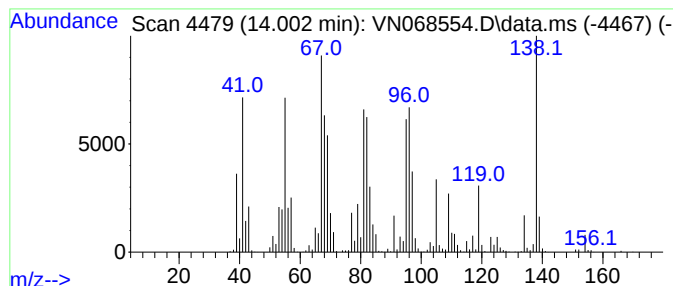
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, decahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.002	98.17 ug/l	5716830	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	87
4			Cyclodecene	138	C10H18	003618-12-0	83
5			Spiro[4.5]decane	138	C10H18	000176-63-6	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068554.D
Acq On : 18 Sep 2021 6:53
Operator : JC/MD
Sample : M3798-07
Misc : 6.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUPLICATE-2

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Nonane, 3-methyl-	12.371	146.7	ug/l	8156720	3	11.749	2779500	50.0
Octane, 3,5-dim...	12.455	110.6	ug/l	6146710	3	11.749	2779500	50.0
Nonane, 4-methyl-	12.661	238.0	ug/l	13231500	3	11.749	2779500	50.0
unknown12.900	12.900	155.0	ug/l	9027130	4	13.678	2911800	50.0
unknown12.983	12.983	113.7	ug/l	6620730	4	13.678	2911800	50.0
Cyclohexane, 1-...	13.061	229.5	ug/l	13363100	4	13.678	2911800	50.0
unknown13.200	13.200	103.4	ug/l	6023810	4	13.678	2911800	50.0
unknown13.249	13.249	106.8	ug/l	6218440	4	13.678	2911800	50.0
Naphthalene, de...	14.002	98.2	ug/l	5716830	4	13.678	2911800	50.0