

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
 Data File : VN066984.D
 Acq On : 5 May 2021 13:23
 Operator : JC/MD
 Sample : M2238-01
 Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 HR-02-043021

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\82N050421W.M

Title : SW846 8260

Signal : TIC: VN066984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.509	2116	2145	2158	rBV2	314369	811776	3.95%	0.412%
2	7.584	2159	2173	2196	rVB	559842	1368408	6.66%	0.695%
3	7.949	2288	2309	2340	rBV3	418692	1057571	5.14%	0.537%
4	8.515	2497	2520	2546	rBV	857893	1860819	9.05%	0.945%
5	10.030	3065	3085	3103	rBV	1423935	2719385	13.23%	1.381%
6	10.226	3141	3158	3177	rVB	128595	238012	1.16%	0.121%
7	10.947	3416	3427	3439	rVB4	124602	219239	1.07%	0.111%
8	11.146	3481	3501	3523	rVB6	483548	1108048	5.39%	0.563%
9	11.245	3524	3538	3563	rBV2	390358	738233	3.59%	0.375%
10	11.352	3563	3578	3601	rBV	1159319	2230016	10.85%	1.133%
11	11.580	3636	3663	3679	rBV4	2761531	5580177	27.14%	2.835%
12	11.798	3735	3744	3754	rBV5	161988	247775	1.21%	0.126%
13	11.883	3754	3776	3789	rBV7	652022	2316014	11.26%	1.177%
14	11.991	3807	3816	3832	rBV	765997	1055342	5.13%	0.536%
15	12.066	3834	3844	3849	rBV4	461951	724422	3.52%	0.368%
16	12.106	3851	3859	3881	rVB7	1054110	2120223	10.31%	1.077%
17	12.283	3919	3925	3930	rBV	646326	707183	3.44%	0.359%
18	12.353	3943	3951	3958	rBV2	655636	996879	4.85%	0.506%
19	12.393	3959	3966	3976	rVB	1324103	1806173	8.78%	0.918%
20	12.506	4001	4008	4027	rVB3	678395	1420303	6.91%	0.722%
21	12.599	4029	4043	4051	rBV3	1521013	2815684	13.69%	1.430%
22	12.675	4060	4071	4083	rVV3	11234379	17250136	83.90%	8.763%
23	12.726	4085	4090	4102	rVB3	1172983	1629343	7.92%	0.828%
24	12.838	4117	4132	4140	rBV5	898238	2174476	10.58%	1.105%
25	12.908	4150	4158	4172	rVB2	2543807	4212098	20.49%	2.140%
26	12.983	4174	4186	4198	rBV	4114742	7047076	34.27%	3.580%
27	13.096	4219	4228	4231	rBV4	821404	1157786	5.63%	0.588%
28	13.181	4245	4260	4270	rBV4	3388121	6764948	32.90%	3.437%
29	13.230	4272	4278	4286	rVV3	1924278	2906059	14.13%	1.476%
30	13.267	4287	4292	4295	rVV3	1406086	1584659	7.71%	0.805%
31	13.299	4298	4304	4321	rVV3	2867201	6457701	31.41%	3.280%
32	13.369	4323	4330	4339	rVB	1499128	1949061	9.48%	0.990%
33	13.485	4368	4373	4382	rVB2	1795624	2275948	11.07%	1.156%
34	13.530	4382	4390	4407	rVB4	2092664	3805892	18.51%	1.933%
35	13.619	4409	4423	4433	rBV	12610857	20560636	100.00%	10.445%
36	13.777	4477	4482	4493	rVB6	2182979	2989472	14.54%	1.519%

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37	13.833	4497	4503	4513	rVB2	2655408	3783799	18.40%	1.922%
38	13.938	4532	4542	4553	rVB2	3456922	5430673	26.41%	2.759%
39	14.109	4597	4606	4624	rBV10	3603368	8253982	40.14%	4.193%
40	14.241	4647	4655	4661	rBV2	2351290	3198072	15.55%	1.625%
41	14.276	4662	4668	4678	rVB2	2888821	3787801	18.42%	1.924%
42	14.469	4731	4740	4750	rVB2	8475289	11894836	57.85%	6.042%
43	14.528	4751	4762	4776	rVV6	5731409	12775585	62.14%	6.490%
44	14.584	4778	4783	4797	rVB3	3326019	5089187	24.75%	2.585%
45	15.265	5029	5037	5054	rVB4	5286968	8799629	42.80%	4.470%
46	15.542	5133	5140	5155	rVB	4438133	7255164	35.29%	3.686%
47	15.834	5237	5249	5262	rVB4	3408708	6503865	31.63%	3.304%
48	16.019	5310	5318	5331	rVB3	2838340	5174572	25.17%	2.629%

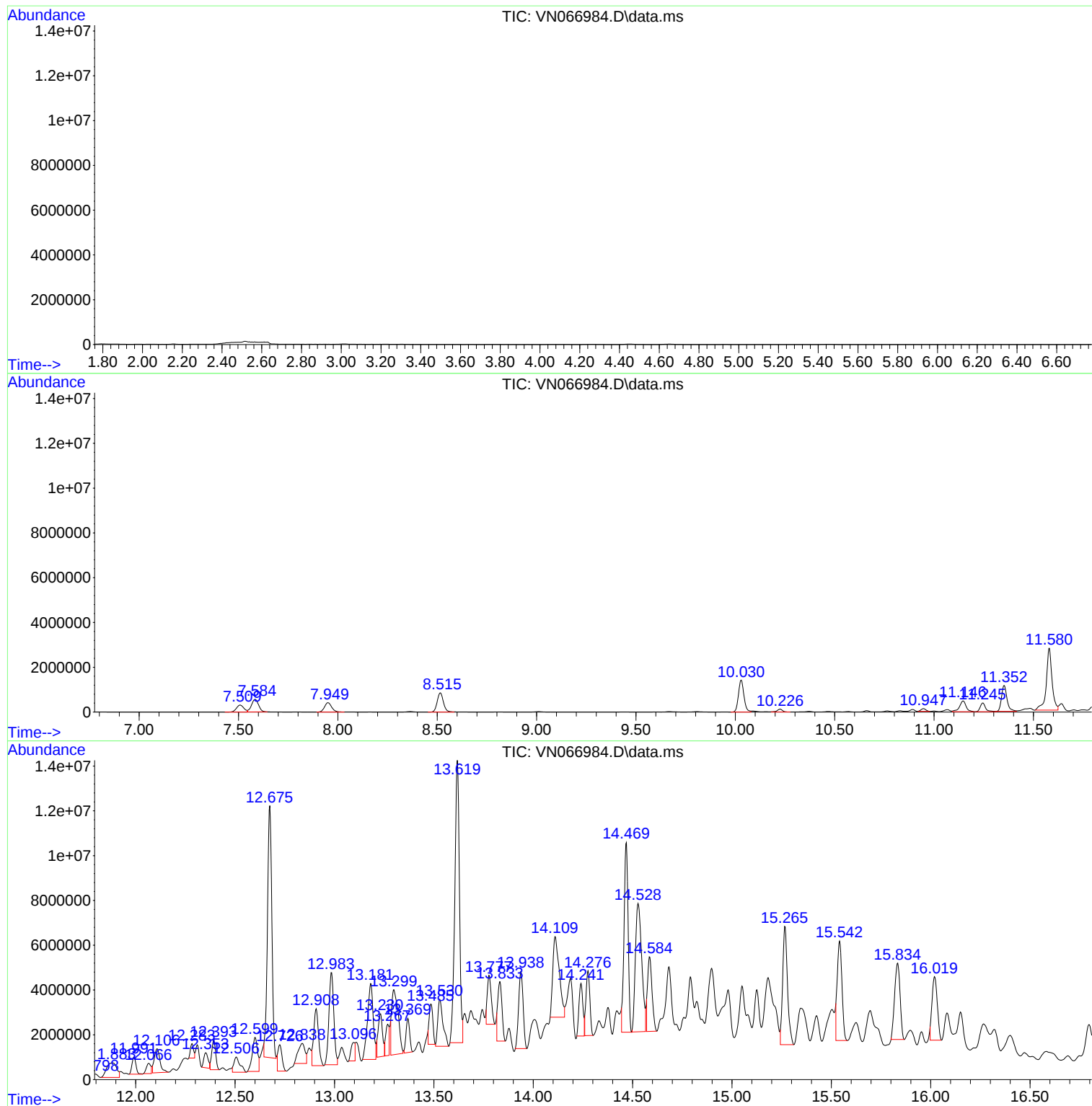
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N050421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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HR-02-043021

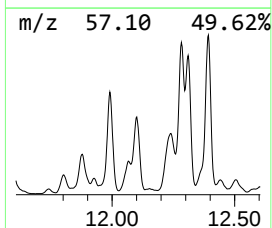
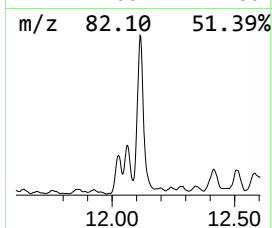
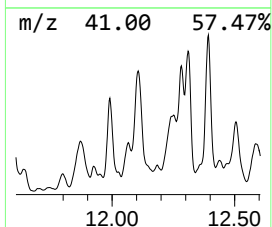
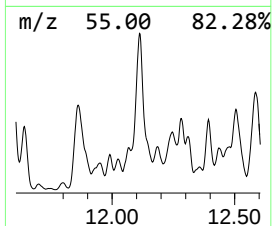
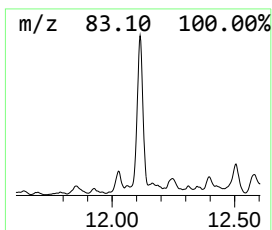
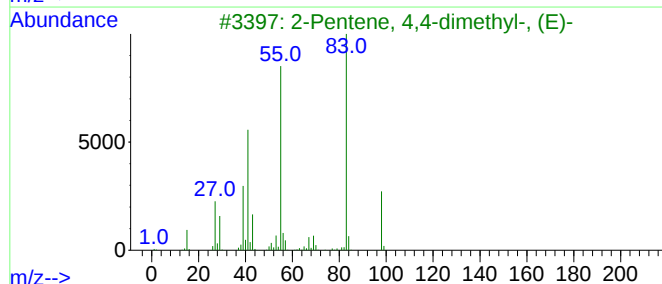
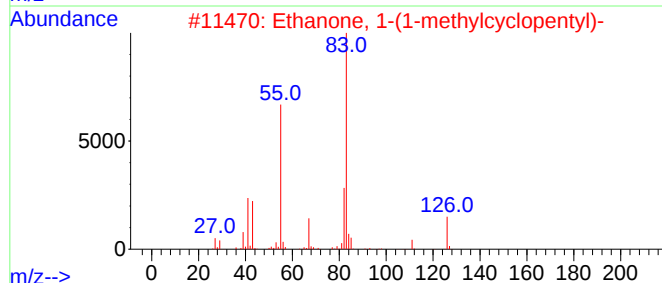
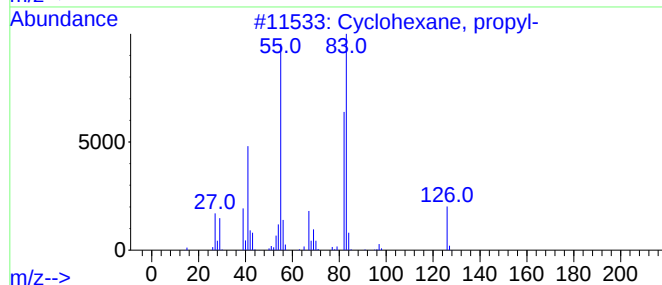
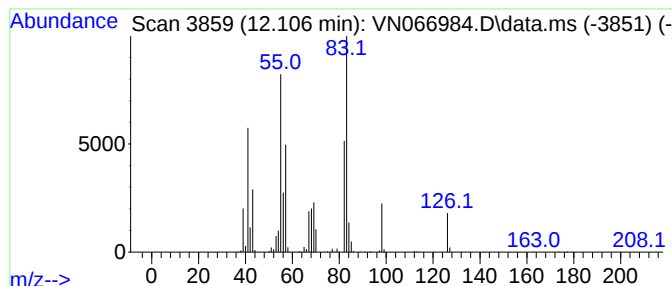
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N050421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclohexane, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.106	47.54 ug/l	2120220	Chlorobenzene-d5	11.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	76
2			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	49
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	43
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	43
5			Trichloroacetic acid, 6-chlorohe...	280	C8H12Cl4O2	1000330-89-2	43



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Instrument :
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ClientSampleId :
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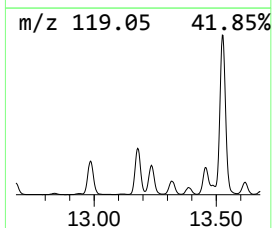
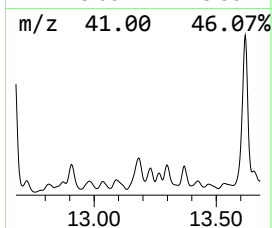
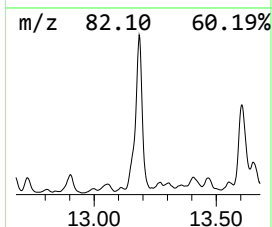
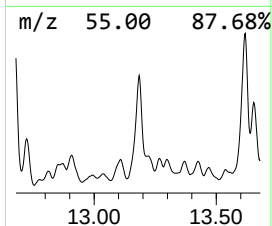
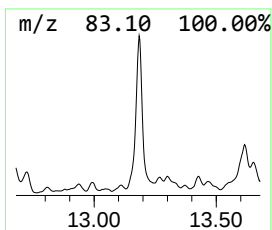
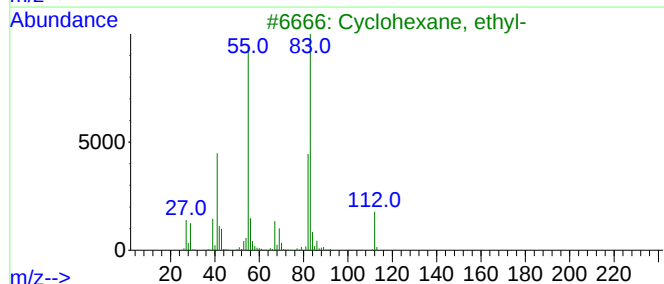
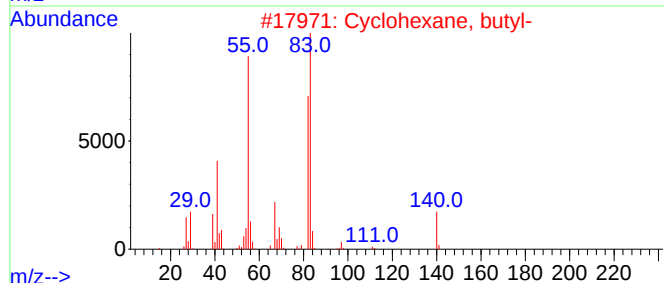
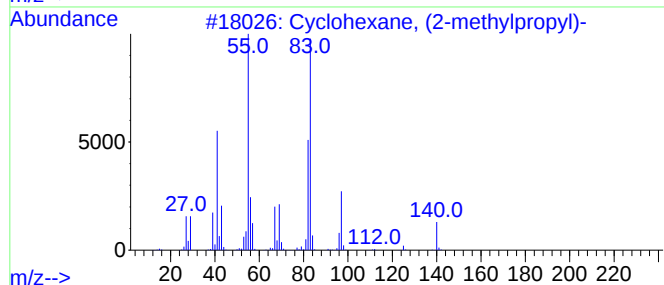
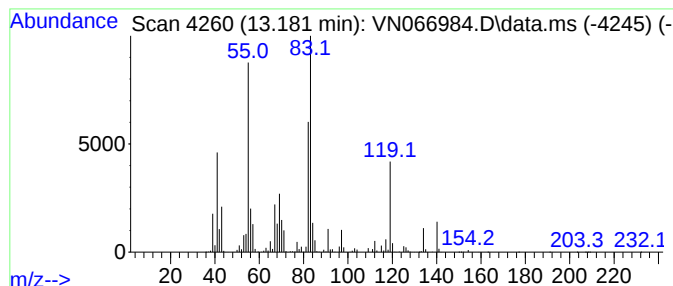
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N050421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, (2-methylpropyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.181	52.38 ug/l	6764950	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	76
2			Cyclohexane, butyl-	140	C10H20	001678-93-9	68
3			Cyclohexane, ethyl-	112	C8H16	001678-91-7	58
4			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	58
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	53



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Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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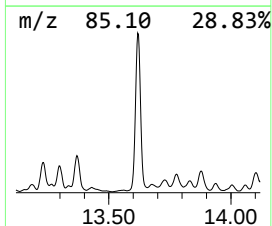
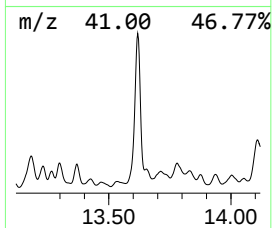
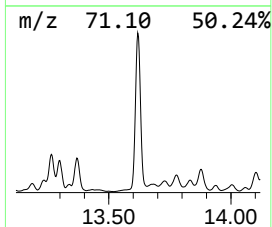
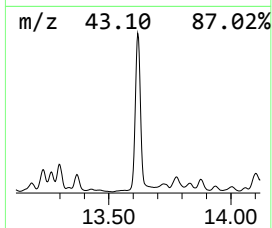
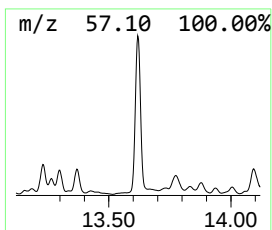
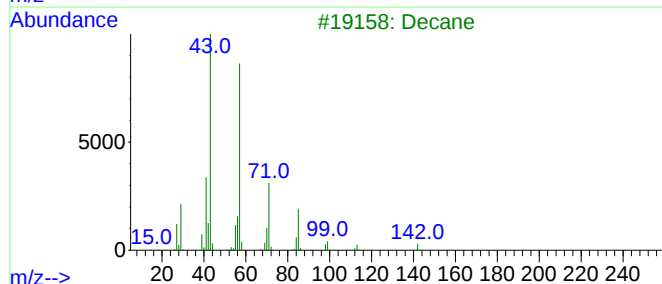
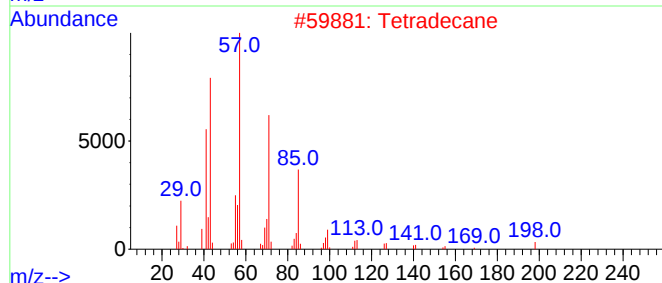
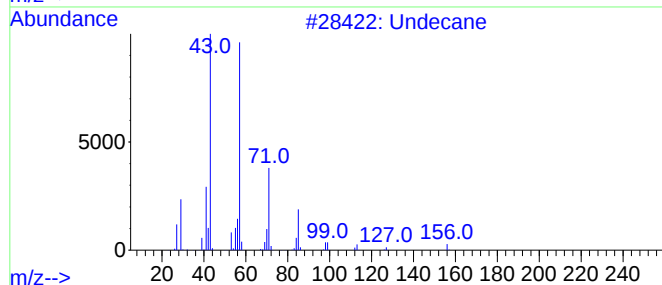
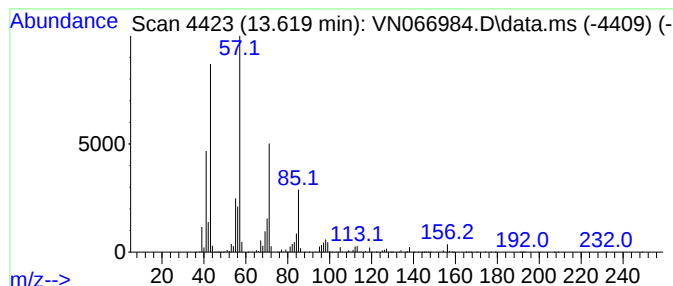
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.619	159.19 ug/l	20560600	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	91
2	Tetradecane			198	C14H30	000629-59-4	86
3	Decane			142	C10H22	000124-18-5	78
4	Tridecane			184	C13H28	000629-50-5	72
5	Hexadecane			226	C16H34	000544-76-3	64



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Instrument :
MSVOA_N
ClientSampleId :
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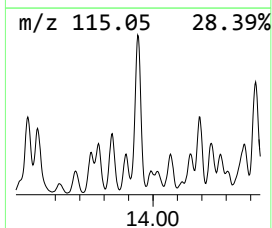
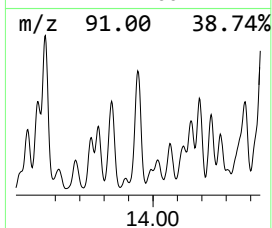
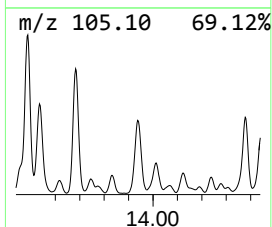
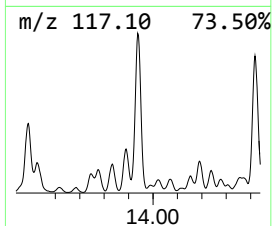
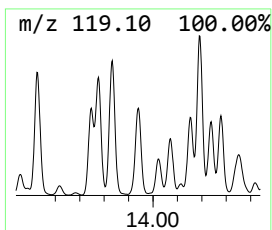
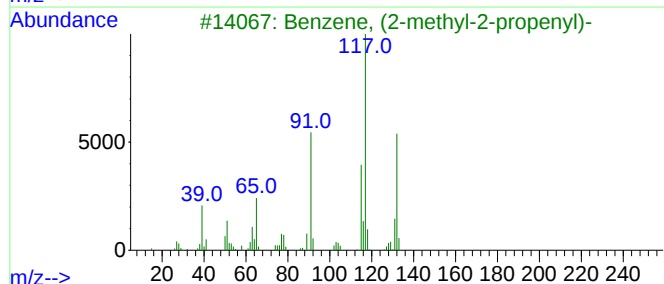
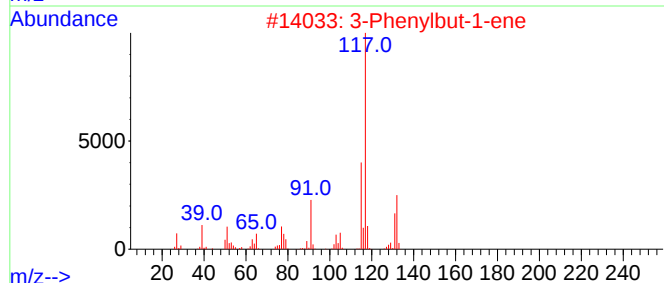
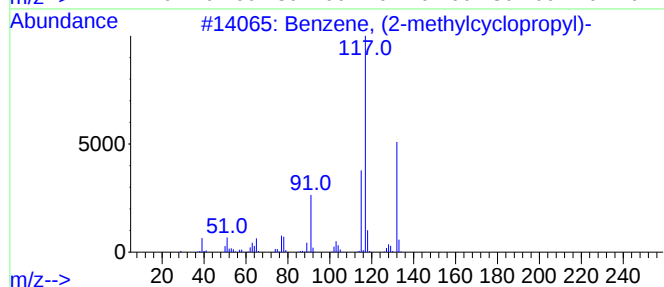
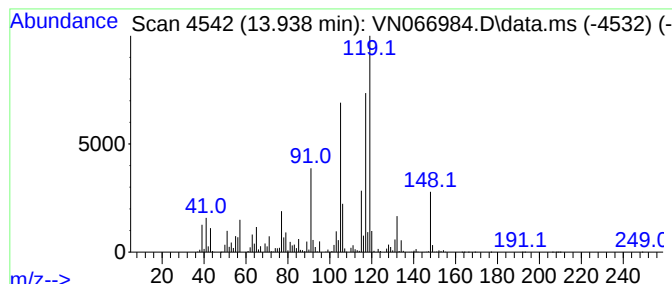
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, (2-methylcycloprop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.938	42.05 ug/l	5430670	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	50
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	50
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	46
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	46
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	46



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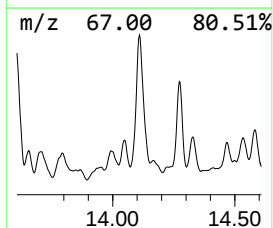
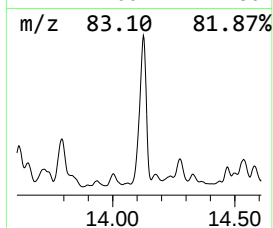
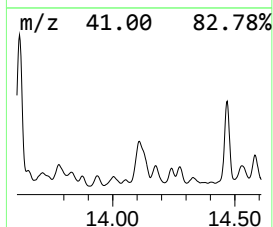
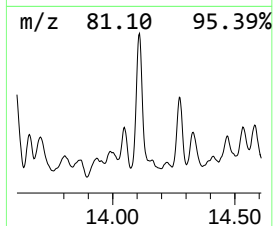
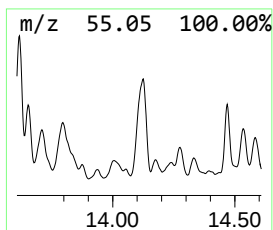
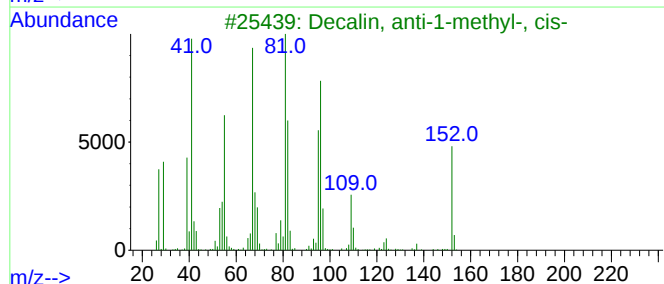
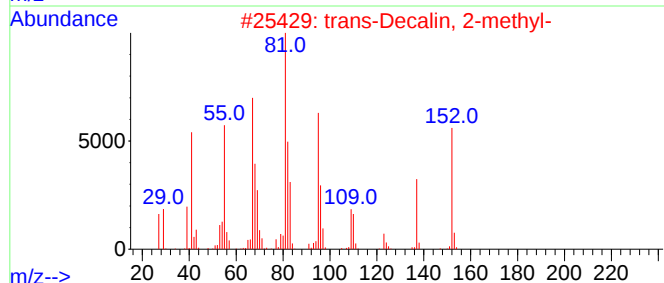
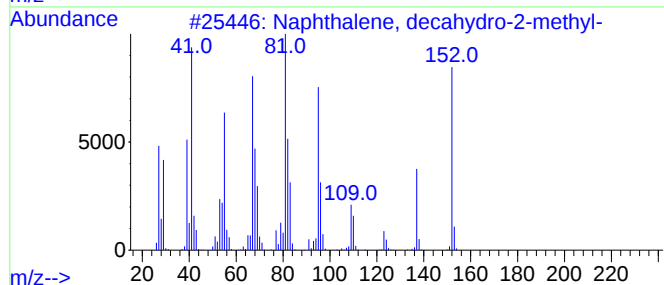
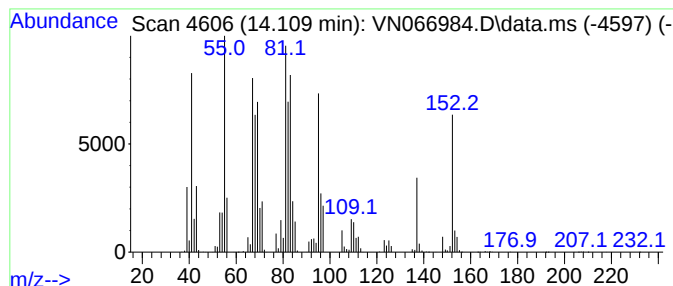
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, decahydro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.109	63.91 ug/l	8253980	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	92
3			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	70
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	70
5			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
Data File : VN066984.D
Acq On : 5 May 2021 13:23
Operator : JC/MD
Sample : M2238-01
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-02-043021

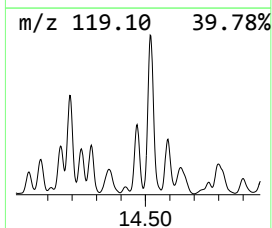
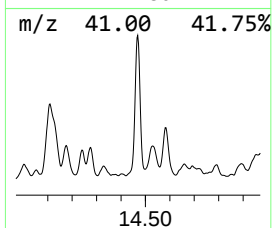
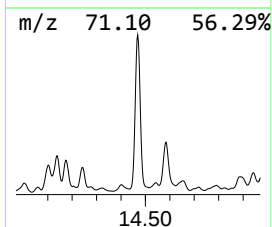
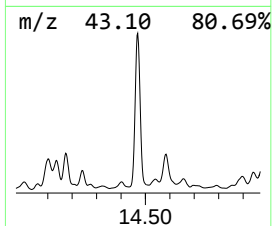
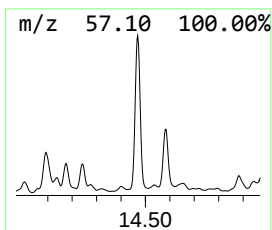
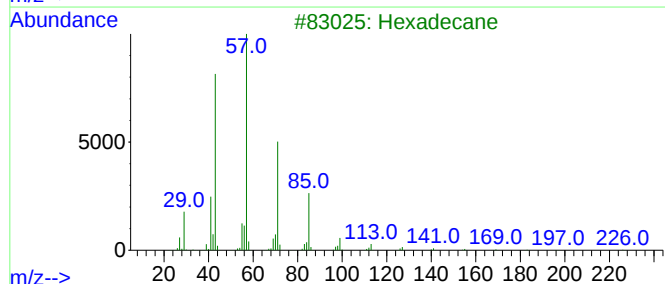
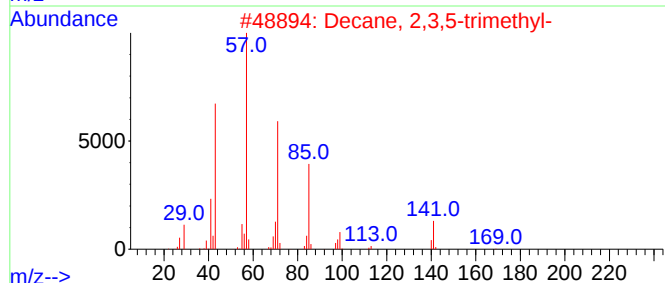
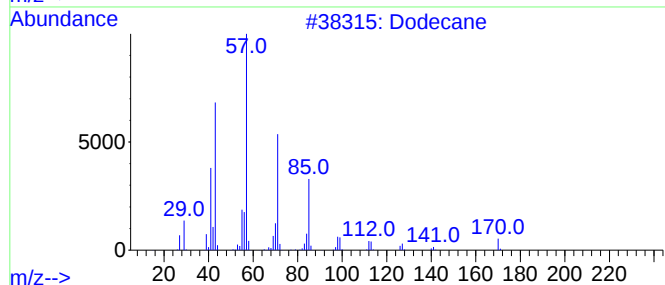
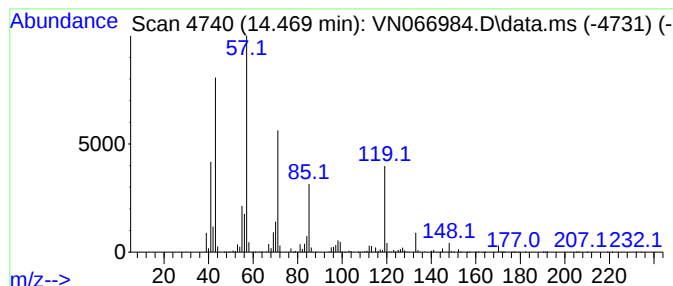
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.469	92.10 ug/l	11894800	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	49
3			Hexadecane	226	C16H34	000544-76-3	47
4			Tridecane	184	C13H28	000629-50-5	47
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
Data File : VN066984.D
Acq On : 5 May 2021 13:23
Operator : JC/MD
Sample : M2238-01
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-02-043021

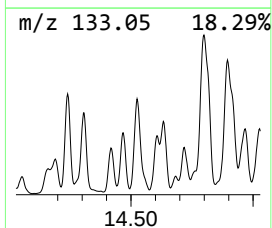
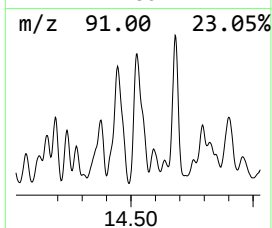
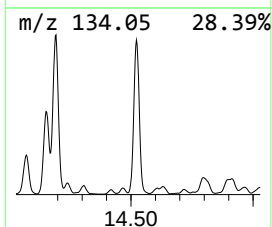
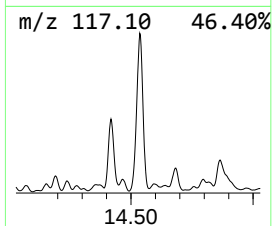
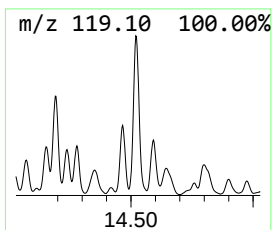
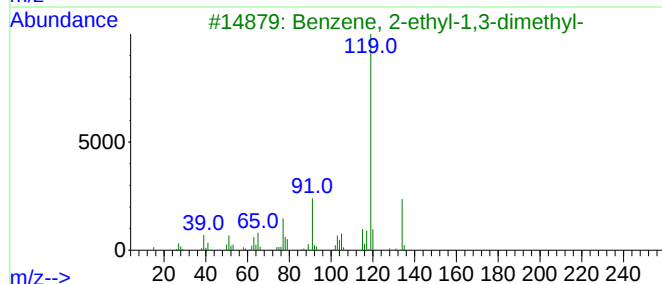
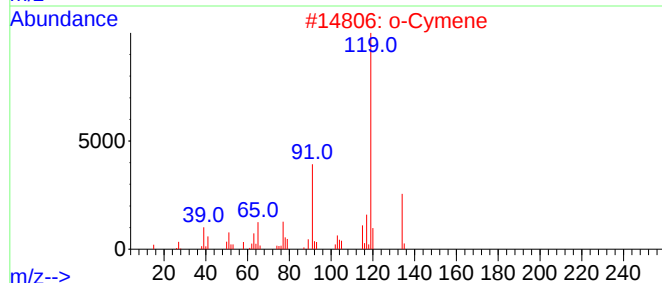
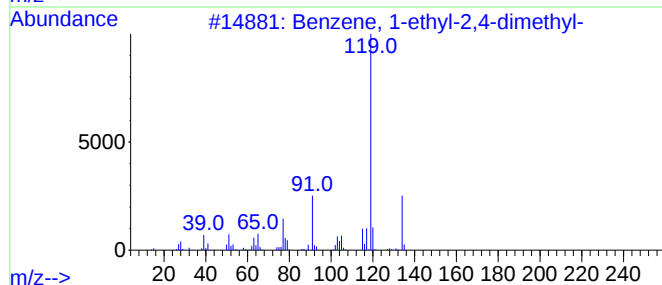
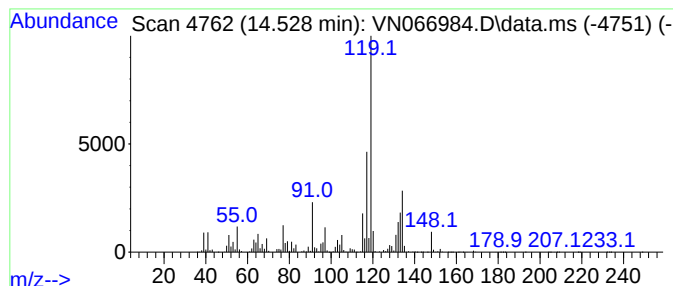
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.528	98.92 ug/l	12775600	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	87
2			o-Cymene	134	C10H14	000527-84-4	60
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	55
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	55
5			p-Cymene	134	C10H14	000099-87-6	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
Data File : VN066984.D
Acq On : 5 May 2021 13:23
Operator : JC/MD
Sample : M2238-01
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-02-043021

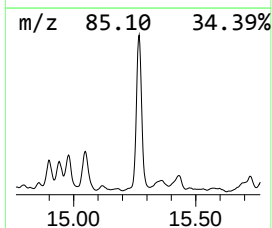
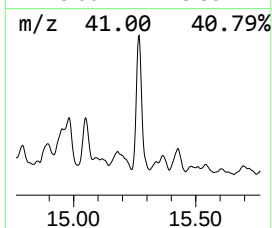
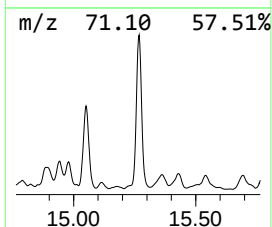
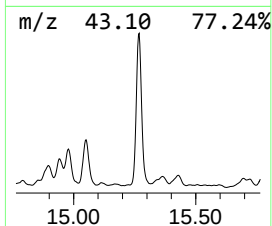
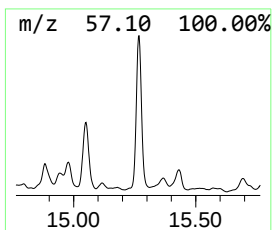
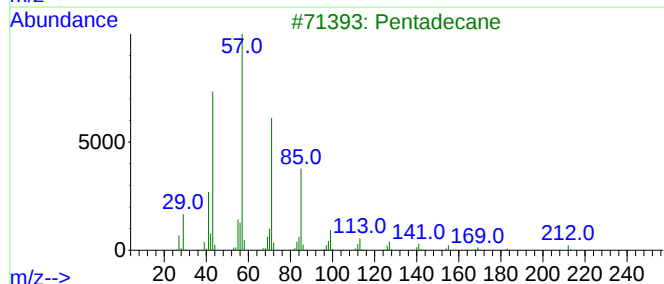
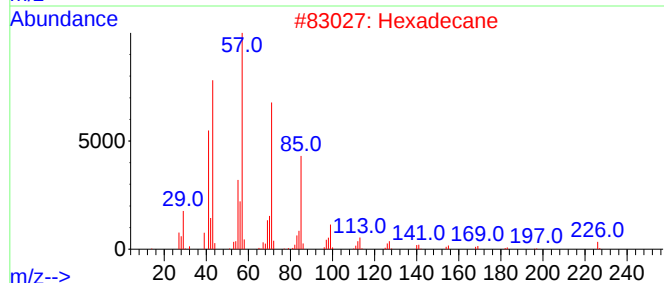
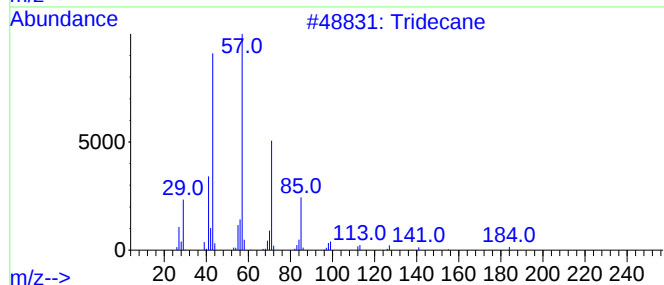
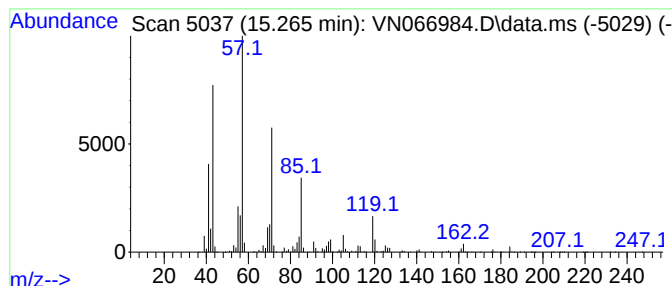
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.265	68.13 ug/l	8799630	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Hexadecane	226	C16H34	000544-76-3	74
3			Pentadecane	212	C15H32	000629-62-9	72
4			Tetradecane	198	C14H30	000629-59-4	72
5			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
Data File : VN066984.D
Acq On : 5 May 2021 13:23
Operator : JC/MD
Sample : M2238-01
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-02-043021

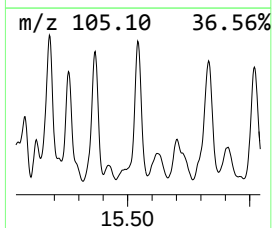
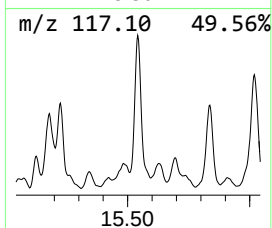
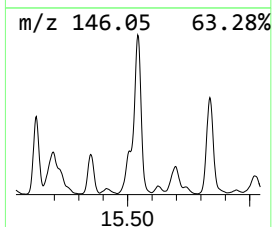
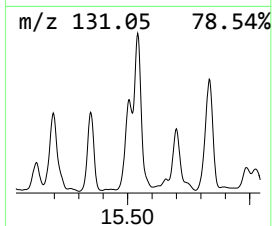
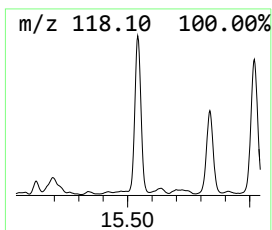
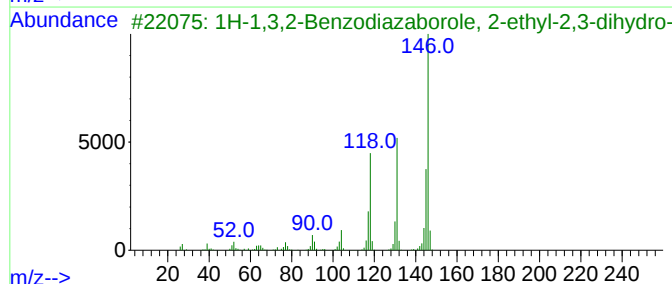
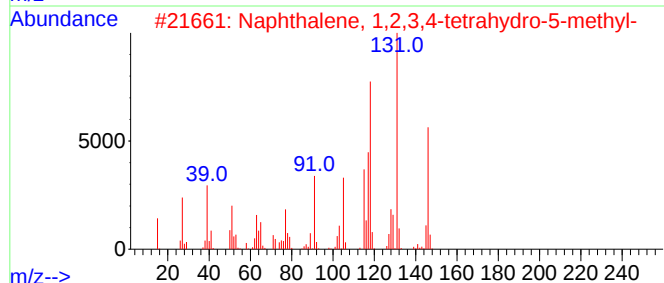
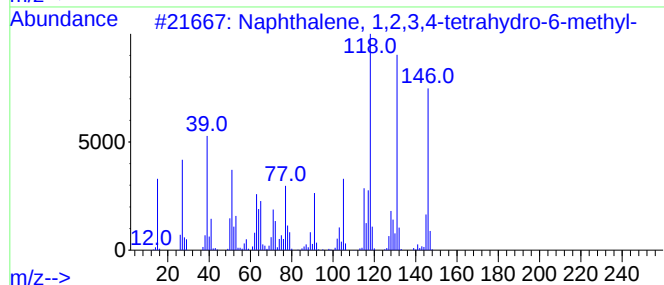
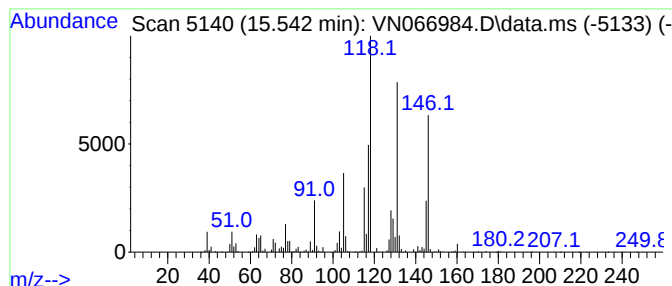
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	56.17 ug/l	7255160	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	83
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	62
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	55
5			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
Data File : VN066984.D
Acq On : 5 May 2021 13:23
Operator : JC/MD
Sample : M2238-01
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-02-043021

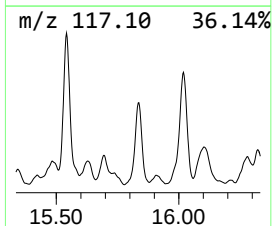
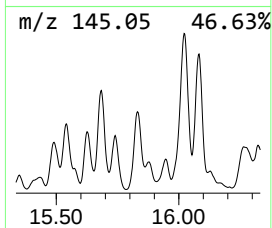
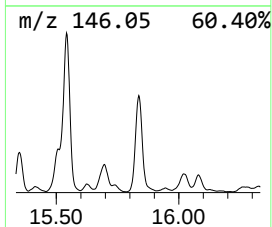
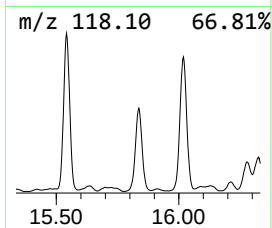
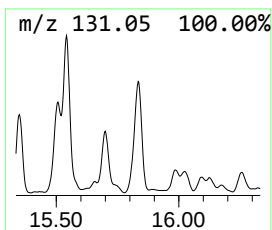
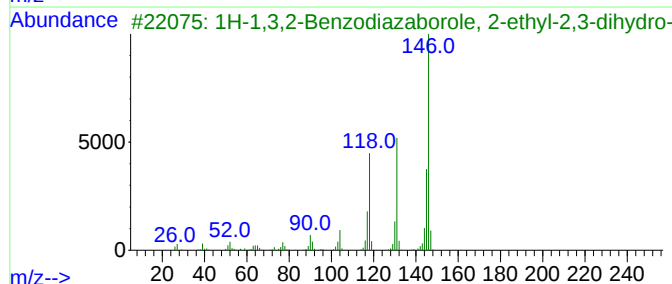
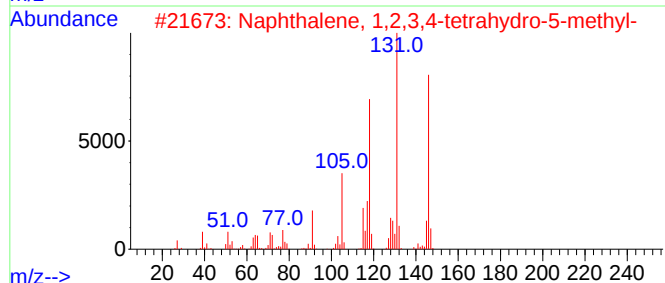
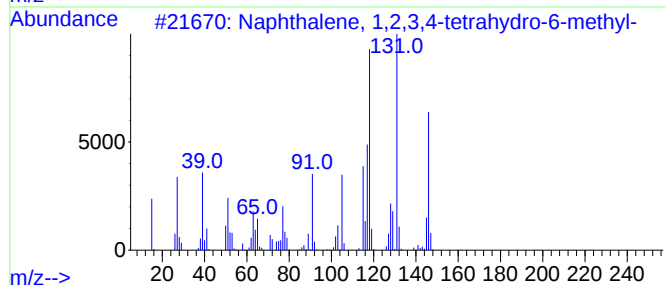
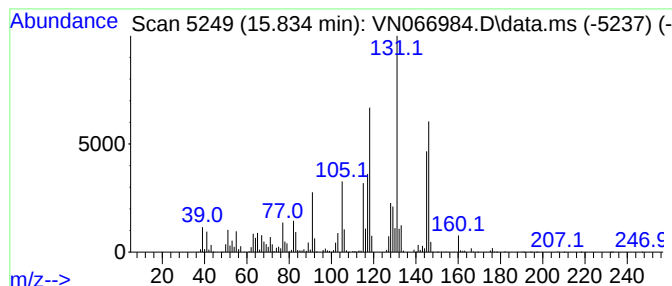
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N050421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.834	50.36 ug/l	6503870	1,4-Dichlorobenzene-d4	13.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	76
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	70
4			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	53
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050521\
Data File : VN066984.D
Acq On : 5 May 2021 13:23
Operator : JC/MD
Sample : M2238-01
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-02-043021

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N050421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, pr...	12.106	47.5	ug/l	2120220	3	11.352	2230020	50.0
Cyclohexane, (2...	13.181	52.4	ug/l	6764950	4	13.291	6457700	50.0
Undecane	13.619	159.2	ug/l	20560600	4	13.291	6457700	50.0
Benzene, (2-met...	13.938	42.0	ug/l	5430670	4	13.291	6457700	50.0
Naphthalene, de...	14.109	63.9	ug/l	8253980	4	13.291	6457700	50.0
Dodecane	14.469	92.1	ug/l	11894800	4	13.291	6457700	50.0
Benzene, 1-ethy...	14.528	98.9	ug/l	12775600	4	13.291	6457700	50.0
Tridecane	15.265	68.1	ug/l	8799630	4	13.291	6457700	50.0
Naphthalene, 1,...	15.542	56.2	ug/l	7255160	4	13.291	6457700	50.0
Naphthalene, 1,...	15.834	50.4	ug/l	6503870	4	13.291	6457700	50.0