

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
 Data File : VN067097.D
 Acq On : 17 May 2021 13:38
 Operator : JC/MD
 Sample : M2387-02
 Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30782

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\82N051421W.M
 Title : SW846 8260

Signal : TIC: VN067097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.516	2131	2154	2166	rBV2	344120	975993	17.04%	1.259%
2	7.592	2170	2182	2201	rVB	690667	1698548	29.66%	2.191%
3	7.803	2238	2261	2296	rBV2	194620	487018	8.50%	0.628%
4	7.956	2296	2318	2347	rBV	339393	838073	14.63%	1.081%
5	8.080	2347	2364	2382	rVB4	32276	79418	1.39%	0.102%
6	8.369	2453	2472	2494	rBV2	225095	470738	8.22%	0.607%
7	8.522	2509	2529	2559	rBV	912929	2012112	35.14%	2.595%
8	9.018	2685	2714	2729	rBV5	80822	214164	3.74%	0.276%
9	9.673	2945	2958	2984	rVB3	48982	124792	2.18%	0.161%
10	9.815	2990	3011	3037	rVB3	45684	115580	2.02%	0.149%
11	10.035	3075	3093	3105	rBV	1534381	2870075	50.12%	3.702%
12	10.099	3105	3117	3148	rVB	3036204	5726682	100.00%	7.386%
13	10.231	3157	3166	3183	rVB	162437	285484	4.99%	0.368%
14	10.378	3213	3221	3237	rVB3	37006	64722	1.13%	0.083%
15	10.475	3243	3257	3272	rBV3	54940	115513	2.02%	0.149%
16	10.670	3315	3330	3340	rBV3	60655	104674	1.83%	0.135%
17	10.772	3357	3368	3381	rBV	43056	80208	1.40%	0.103%
18	10.831	3382	3390	3397	rBV3	46390	69564	1.21%	0.090%
19	10.898	3408	3415	3425	rVB	102966	150897	2.63%	0.195%
20	10.955	3425	3436	3450	rVB5	101100	186283	3.25%	0.240%
21	11.073	3467	3480	3489	rBV5	71673	138099	2.41%	0.178%
22	11.153	3490	3510	3533	rVB6	393440	930720	16.25%	1.200%
23	11.252	3533	3547	3573	rBV	301325	585786	10.23%	0.756%
24	11.360	3573	3587	3610	rBV	1071186	2061904	36.01%	2.659%
25	11.464	3616	3626	3644	rBV3	210558	456297	7.97%	0.589%
26	11.585	3645	3671	3688	rBV5	1414978	3473788	60.66%	4.480%
27	11.805	3744	3753	3763	rBV6	75700	118112	2.06%	0.152%
28	11.902	3763	3789	3816	rBV3	735709	2278548	39.79%	2.939%
29	11.998	3817	3825	3835	rVV	281670	389465	6.80%	0.502%
30	12.073	3844	3853	3859	rBV5	238072	387185	6.76%	0.499%
31	12.116	3861	3869	3891	rVB6	422944	875271	15.28%	1.129%
32	12.202	3894	3901	3908	rBV3	120999	191505	3.34%	0.247%
33	12.293	3929	3935	3939	rBV	208537	218560	3.82%	0.282%
34	12.360	3952	3960	3969	rBV	603305	943050	16.47%	1.216%
35	12.400	3970	3975	3986	rVB2	463418	605609	10.58%	0.781%
36	12.610	4041	4053	4061	rBV	1566612	2643238	46.16%	3.409%

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37	12.685	4072	4081	4094	rVB3	2839803	4342747	75.83%	5.601%
38	12.846	4131	4141	4151	rBV	658653	1070193	18.69%	1.380%
39	12.915	4161	4167	4182	rVB4	608420	1001664	17.49%	1.292%
40	12.996	4183	4197	4209	rBV	2689373	4471713	78.09%	5.767%
41	13.122	4231	4244	4253	rBV6	283185	591088	10.32%	0.762%
42	13.192	4256	4270	4280	rBV3	689761	1244736	21.74%	1.605%
43	13.242	4282	4289	4296	rBV2	323800	387656	6.77%	0.500%
44	13.304	4298	4312	4317	rBV	1204084	2209193	38.58%	2.849%
45	13.497	4366	4384	4392	rBV2	1836795	3385090	59.11%	4.366%
46	13.540	4393	4400	4419	rVB4	1339076	2587112	45.18%	3.337%
47	13.629	4420	4433	4443	rBV2	1573305	2547671	44.49%	3.286%
48	13.757	4473	4481	4486	rBV	646375	899646	15.71%	1.160%
49	13.846	4504	4514	4524	rVB	1238764	1807211	31.56%	2.331%
50	13.951	4543	4553	4565	rVB	1225565	1947795	34.01%	2.512%
51	14.119	4610	4616	4625	rBV8	385905	542814	9.48%	0.700%
52	14.203	4642	4647	4657	rVB	917326	1248335	21.80%	1.610%
53	14.251	4658	4665	4672	rVV3	635486	889578	15.53%	1.147%
54	14.288	4674	4679	4689	rVB3	533477	696064	12.15%	0.898%
55	14.433	4725	4733	4742	rBV2	630260	1024911	17.90%	1.322%
56	14.482	4743	4751	4761	rVB2	1255896	1801856	31.46%	2.324%
57	14.546	4762	4775	4787	rBV5	1576451	3173898	55.42%	4.094%
58	14.600	4789	4795	4809	rVB2	583243	990707	17.30%	1.278%
59	14.696	4823	4831	4851	rVB	864093	1462788	25.54%	1.887%
60	15.066	4962	4969	4988	rVV7	295737	717332	12.53%	0.925%
61	15.141	4991	4997	5006	rVB	344650	455598	7.96%	0.588%
62	15.283	5042	5050	5067	rVB3	683894	1135797	19.83%	1.465%
63	15.560	5146	5153	5170	rVB	695640	1218565	21.28%	1.572%
64	15.852	5252	5262	5275	rVB5	380971	715573	12.50%	0.923%

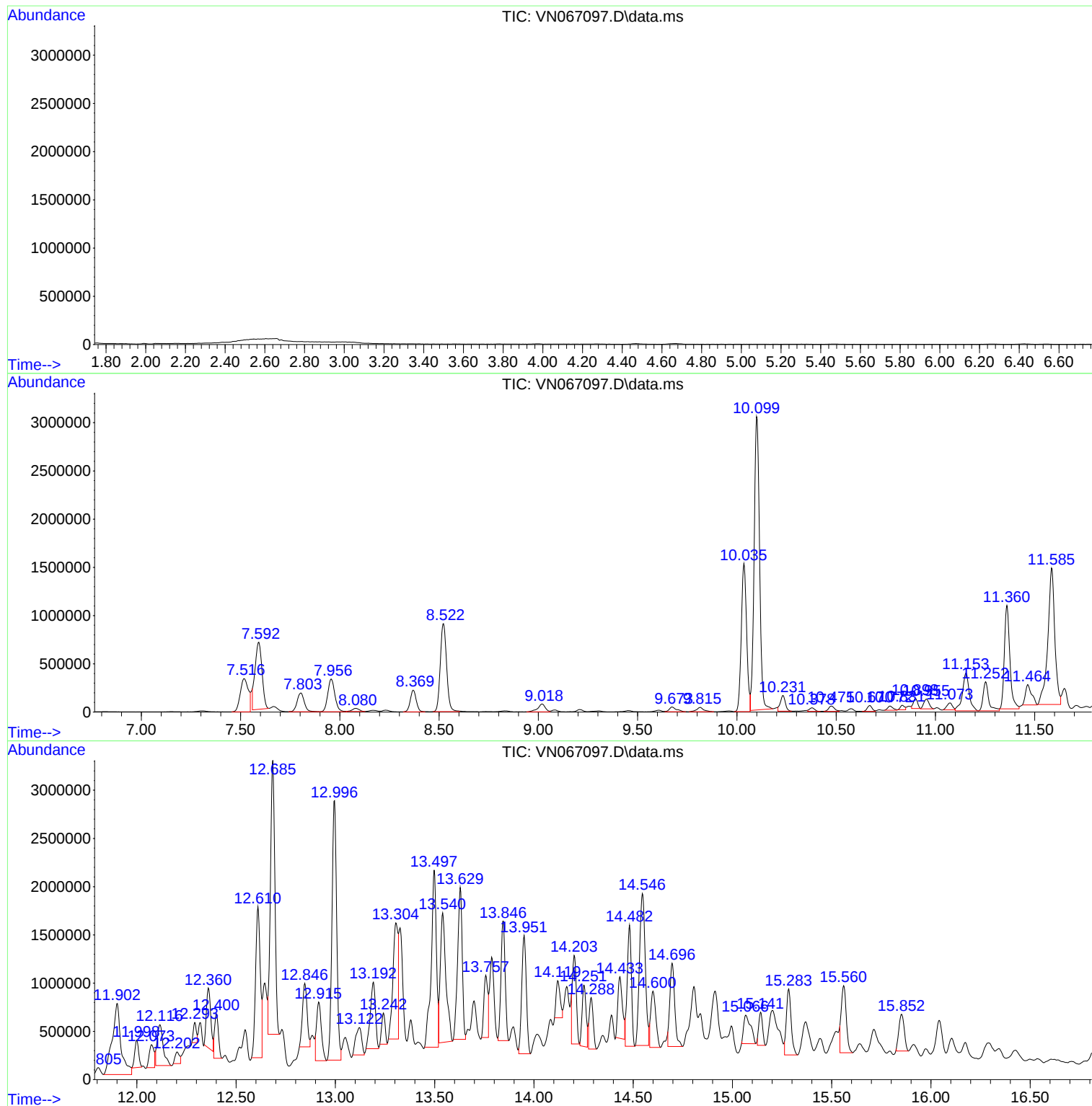
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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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



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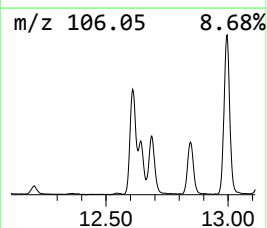
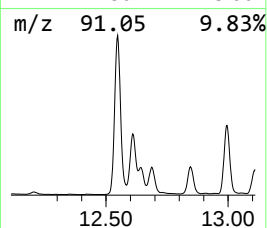
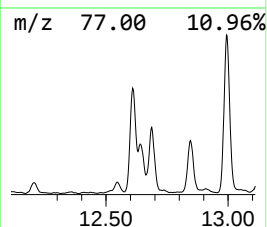
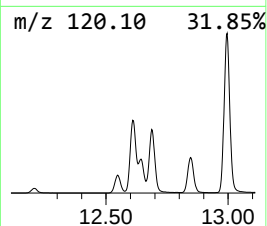
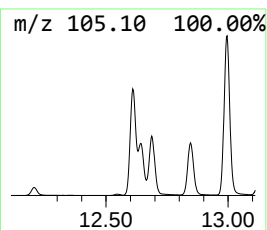
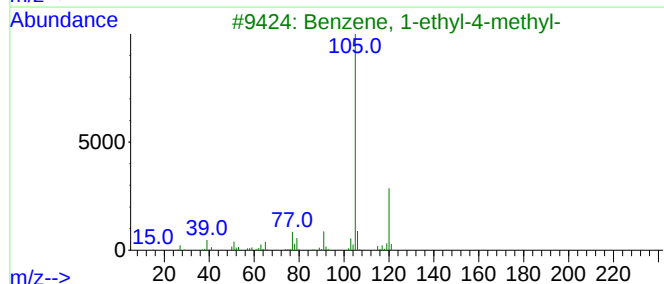
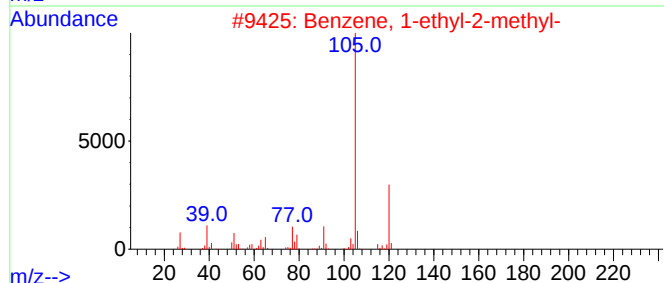
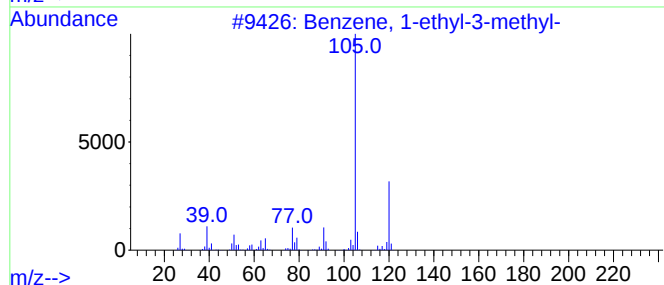
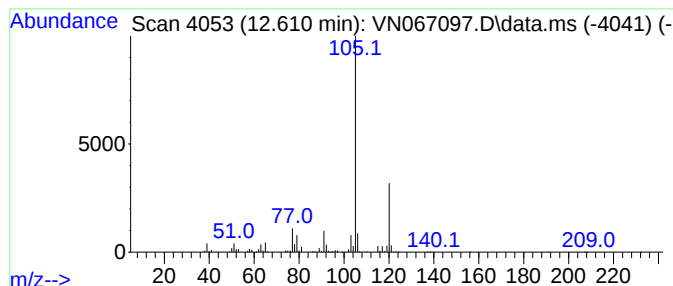
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	59.82 ug/l	2643240	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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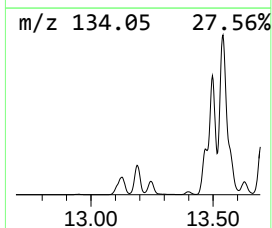
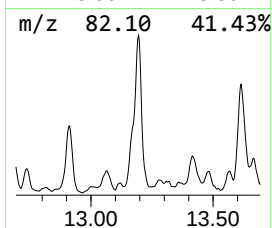
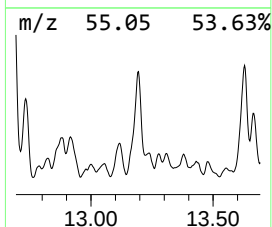
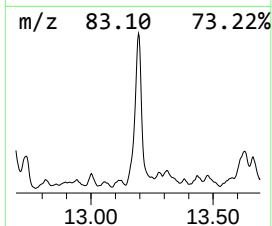
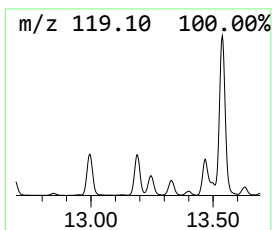
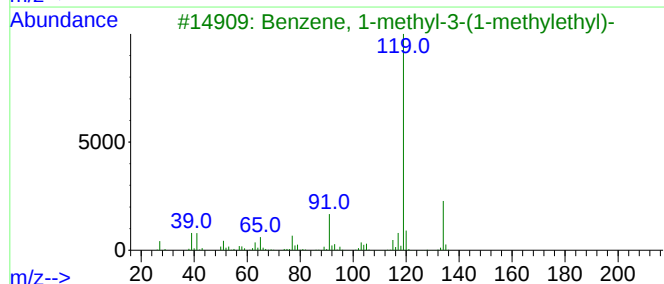
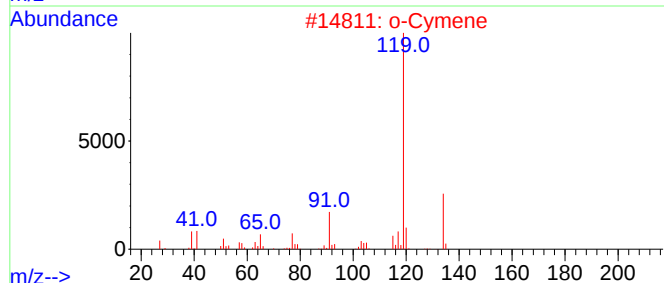
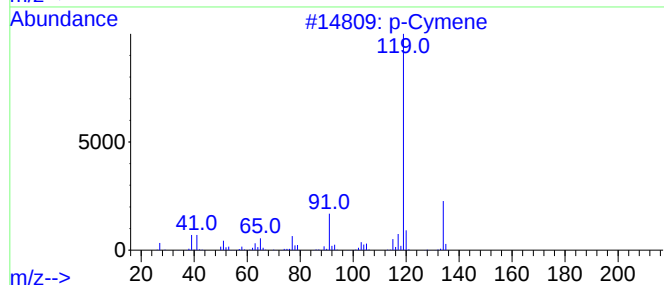
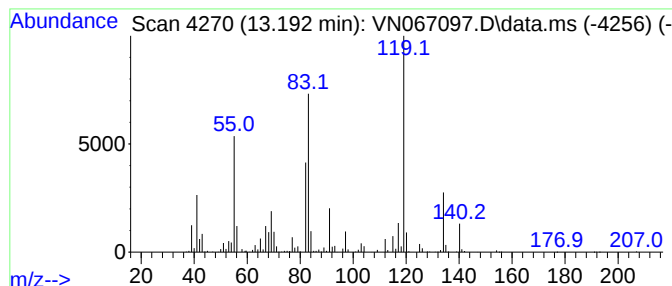
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

Peak Number 2 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	28.17 ug/l	1244740	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	86
2			o-Cymene	134	C10H14	000527-84-4	86
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	83
4			Cyclohexane, butyl-	140	C10H20	001678-93-9	50
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	46



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Instrument :
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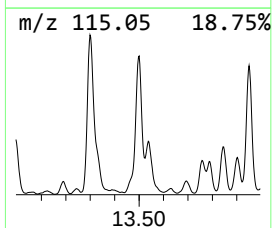
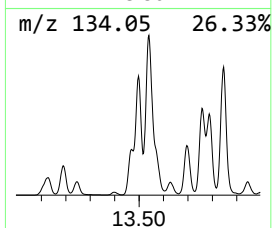
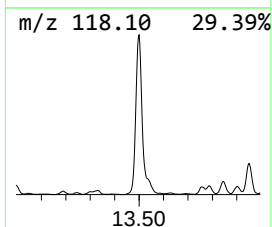
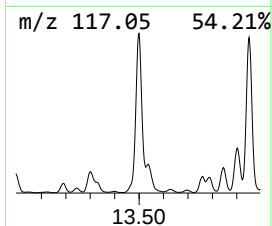
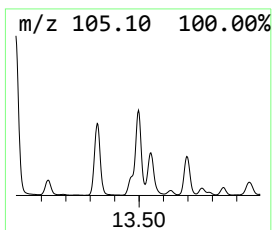
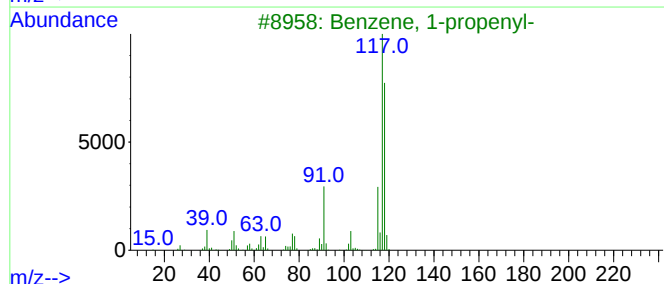
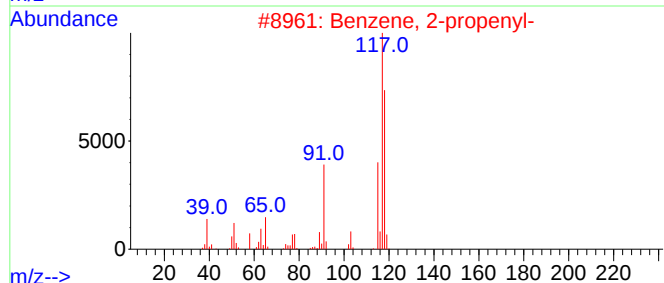
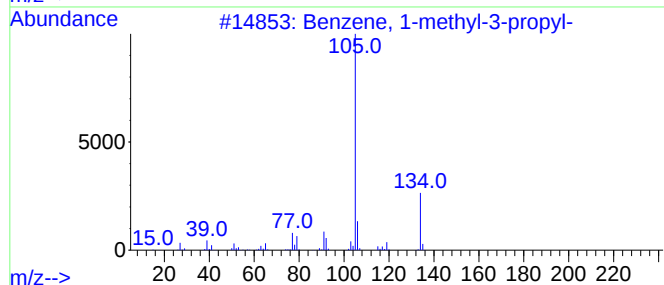
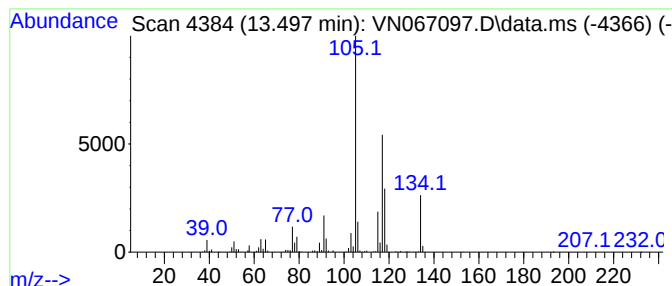
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-methyl-3-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.497	76.61 ug/l	3385090	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	50
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	50
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	49
4			Delta cyclene	118	C9H10	007785-10-6	49
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	46



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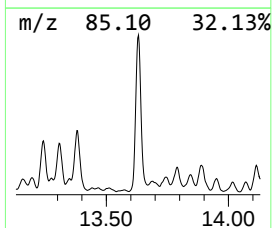
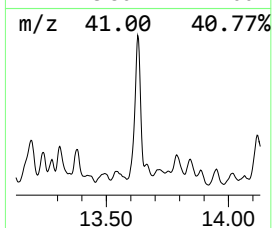
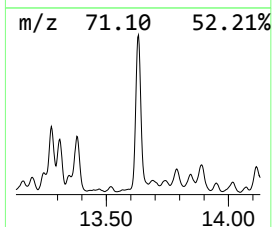
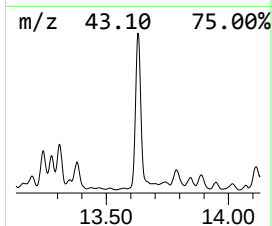
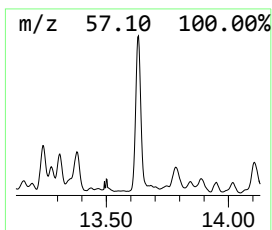
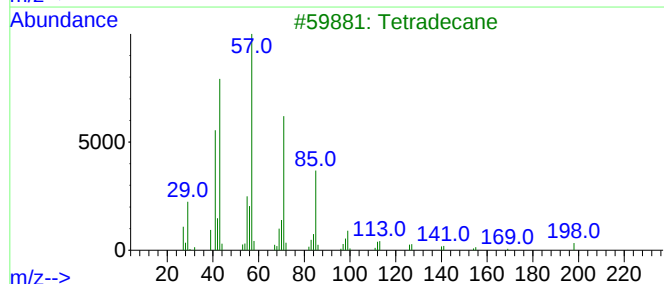
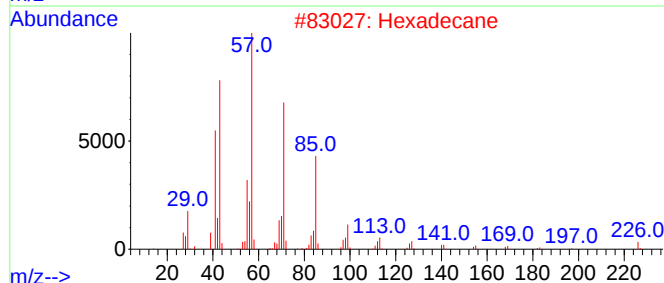
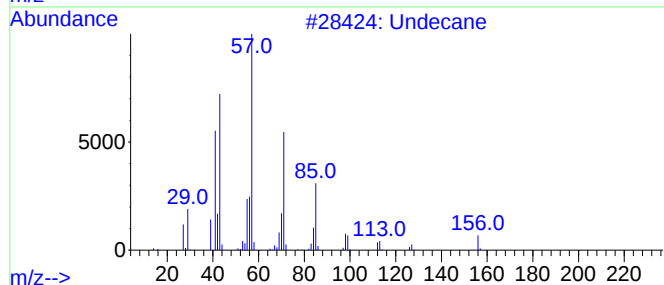
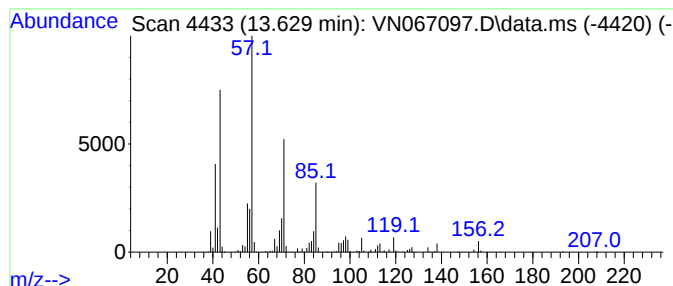
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.629	57.66 ug/l	2547670	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Hexadecane			226	C16H34	000544-76-3	80
3	Tetradecane			198	C14H30	000629-59-4	64
4	Nonadecane			268	C19H40	000629-92-5	59
5	Nonane, 5-(1-methylpropyl)-			184	C13H28	062185-54-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30782

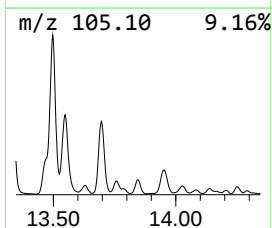
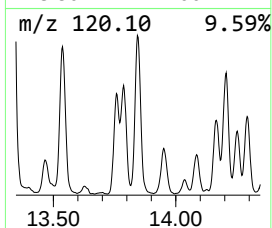
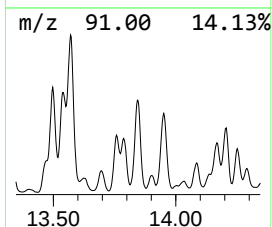
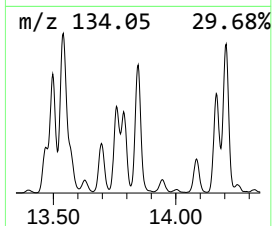
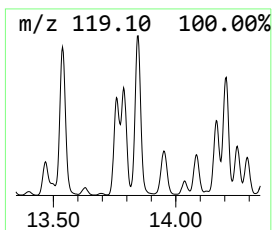
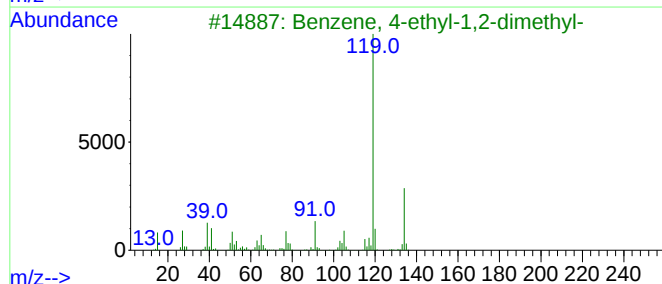
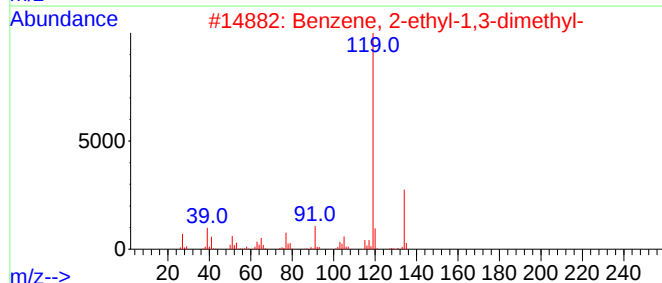
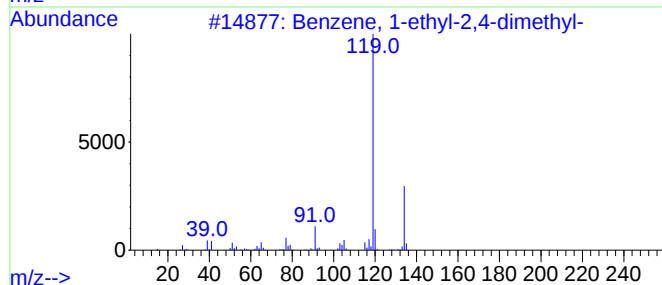
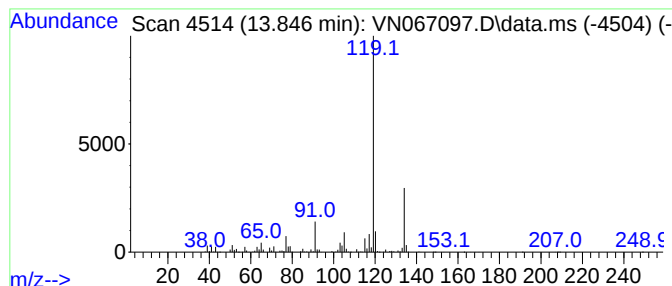
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.846	40.90 ug/l	1807210	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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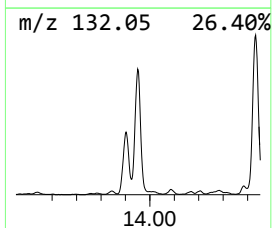
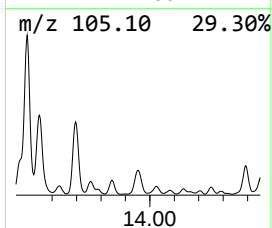
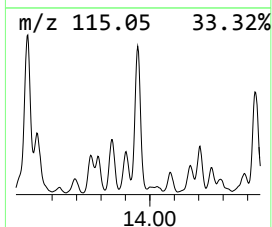
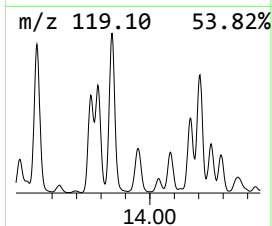
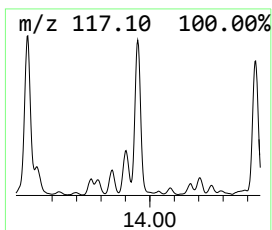
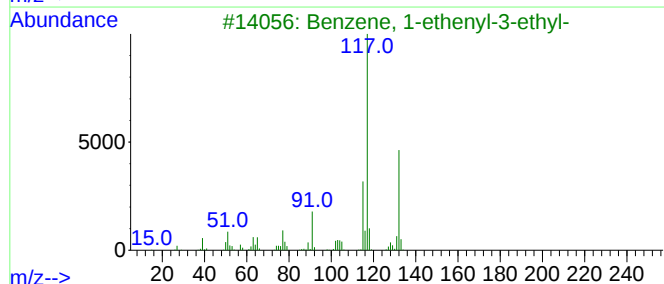
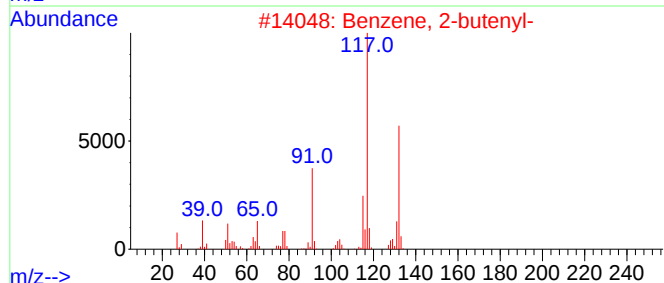
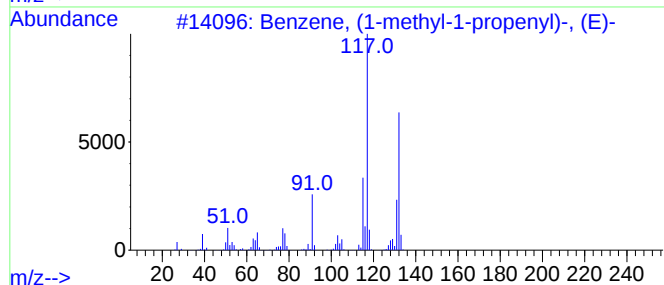
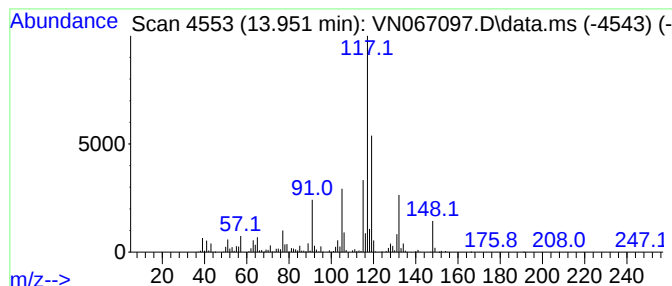
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, (1-methyl-1-propen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	44.08 ug/l	1947800	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	78
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	60
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	60
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	60
5			Indan, 1-methyl-	132	C10H12	000767-58-8	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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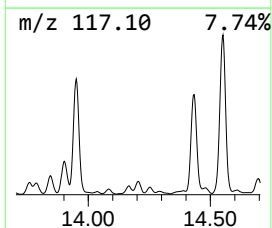
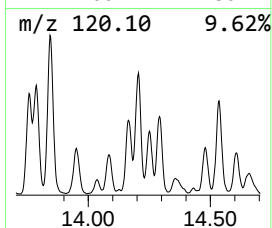
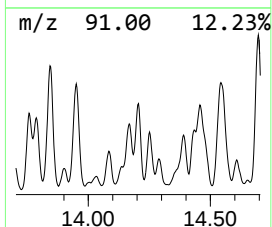
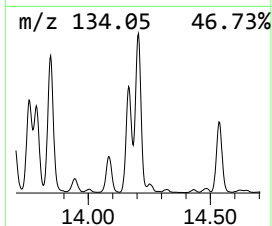
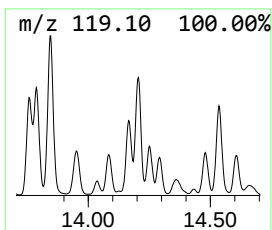
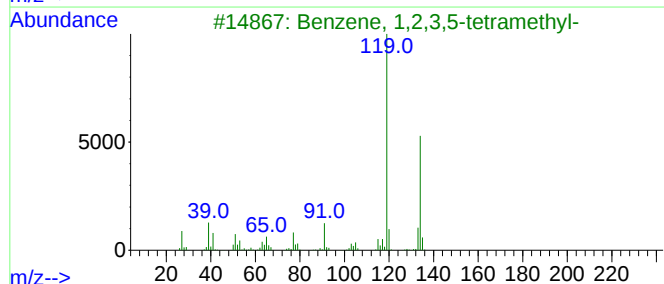
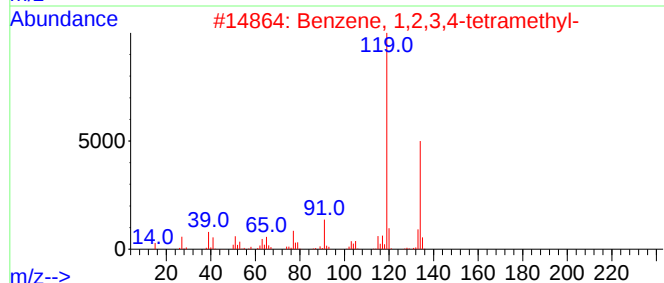
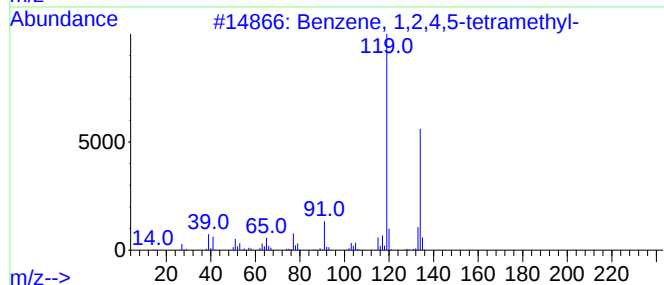
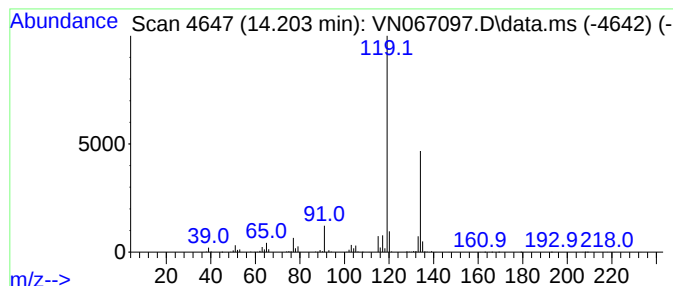
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.203	28.25 ug/l	1248340	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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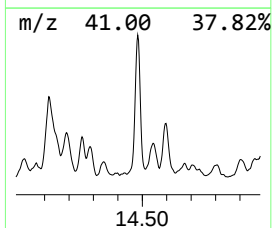
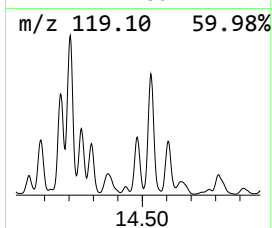
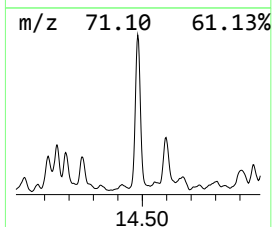
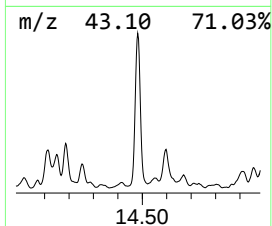
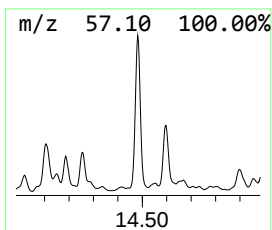
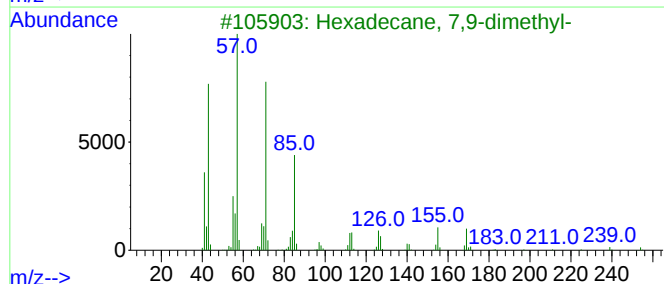
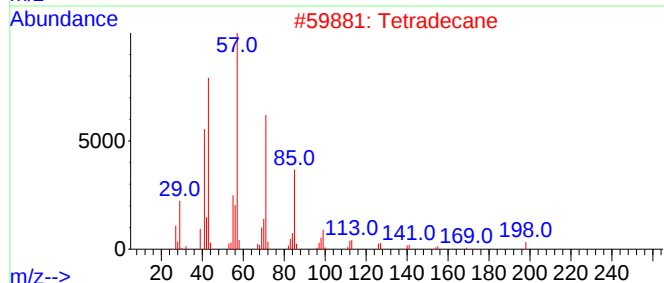
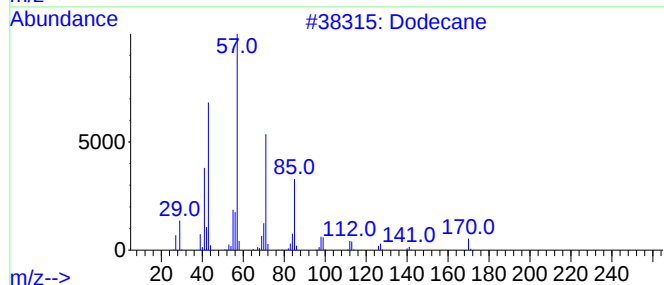
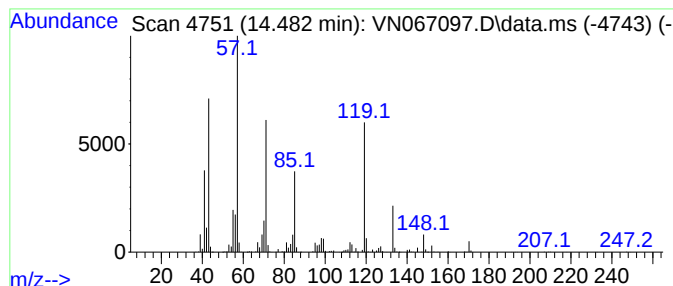
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.482	40.78 ug/l	1801860	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Tetradecane	198	C14H30	000629-59-4	49
3			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	43
4			Nonadecane	268	C19H40	000629-92-5	38
5			Hexadecane	226	C16H34	000544-76-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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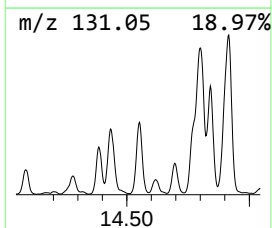
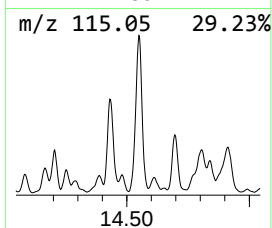
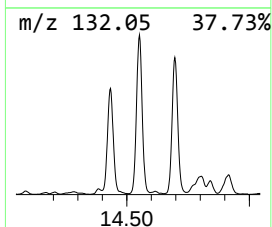
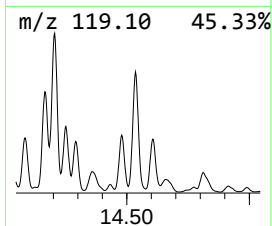
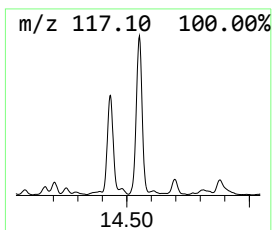
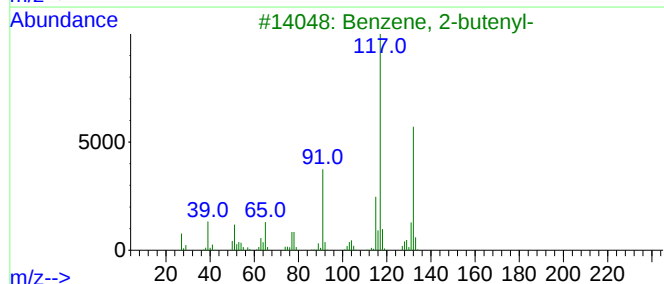
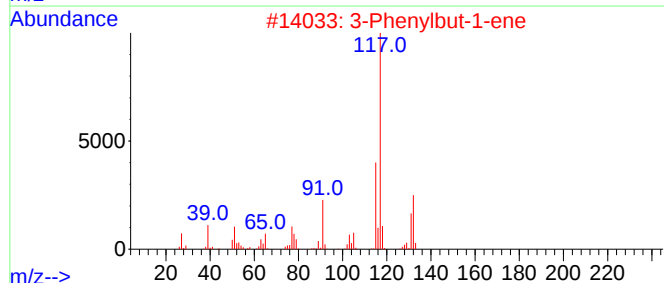
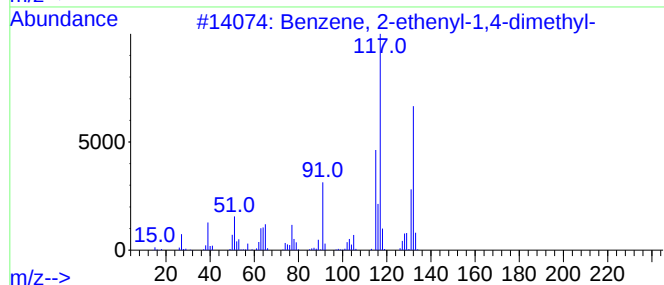
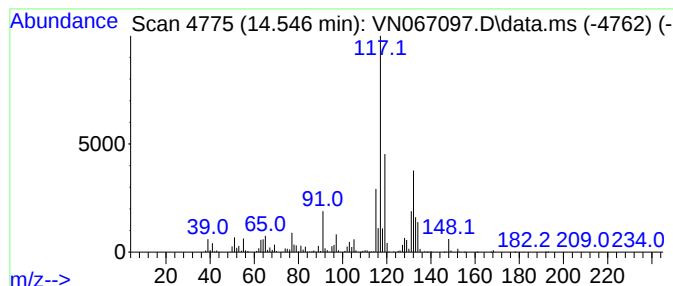
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.546	71.83 ug/l	3173900	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
5			Indan, 1-methyl-	132	C10H12	000767-58-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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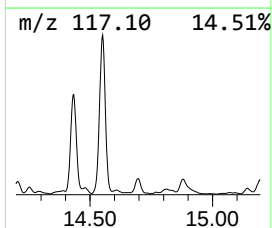
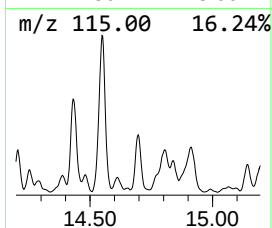
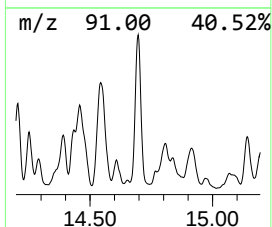
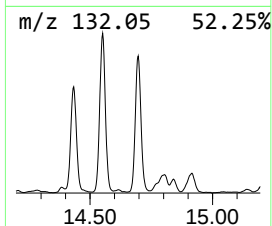
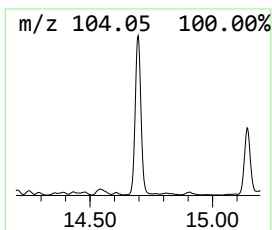
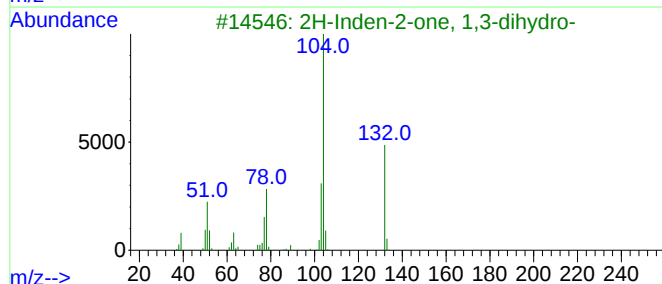
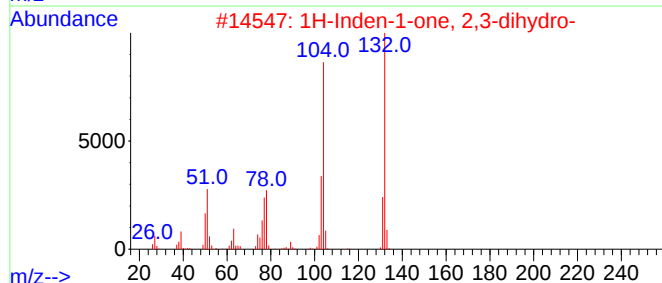
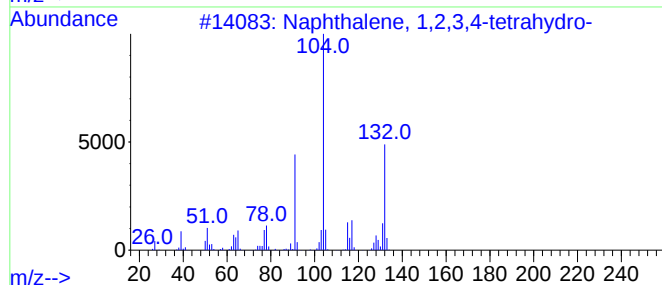
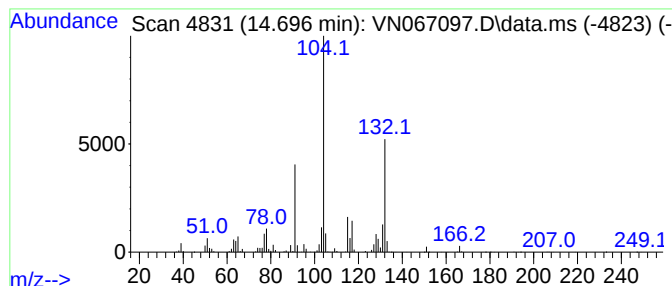
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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.
14.696	33.11 ug/l	1462790	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	97
2			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	59
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	58
4			Indan, epoxide	132	C9H8O	000768-22-9	58
5			Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
Data File : VN067097.D
Acq On : 17 May 2021 13:38
Operator : JC/MD
Sample : M2387-02
Misc : 1.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.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
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o-Cymene	13.192	28.2	ug/l	1244740	4	13.299	2209190	50.0
Benzene, 1-meth...	13.497	76.6	ug/l	3385090	4	13.299	2209190	50.0
Undecane	13.629	57.7	ug/l	2547670	4	13.299	2209190	50.0
Benzene, 1-ethy...	13.846	40.9	ug/l	1807210	4	13.299	2209190	50.0
Benzene, (1-met...	13.951	44.1	ug/l	1947800	4	13.299	2209190	50.0
Benzene, 1,2,4,...	14.203	28.3	ug/l	1248340	4	13.299	2209190	50.0
Dodecane	14.482	40.8	ug/l	1801860	4	13.299	2209190	50.0
Benzene, 2-ethe...	14.546	71.8	ug/l	3173900	4	13.299	2209190	50.0
Naphthalene, 1,...	14.696	33.1	ug/l	1462790	4	13.299	2209190	50.0