

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
 Data File : VN067581.D
 Acq On : 30 Jun 2021 18:55
 Operator : JC/MD
 Sample : M2896-03 40X
 Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FS-02

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\82N062821W.M
 Title : SW846 8260

Signal : TIC: VN067581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.337	1971	1994	2020	rBV3	17513	52379	1.54%	0.119%
2	8.024	2225	2250	2261	rBV	224203	530958	15.63%	1.205%
3	8.086	2261	2273	2300	rVB	407301	915940	26.96%	2.078%
4	8.440	2385	2405	2436	rBV2	281703	704366	20.73%	1.598%
5	8.845	2537	2556	2574	rBV3	41628	92744	2.73%	0.210%
6	8.968	2581	2602	2645	rVB	634339	1309162	38.53%	2.971%
7	9.271	2697	2715	2752	rBV	228263	449505	13.23%	1.020%
8	9.413	2752	2768	2786	rBV2	55849	110859	3.26%	0.252%
9	9.765	2886	2899	2919	rBV3	26604	50292	1.48%	0.114%
10	10.443	3133	3152	3165	rBV	1117840	2103119	61.90%	4.772%
11	10.507	3165	3176	3206	rVB	735038	1440599	42.40%	3.269%
12	10.647	3216	3228	3241	rVB6	32677	66188	1.95%	0.150%
13	10.819	3275	3292	3316	rBV	227207	396347	11.67%	0.899%
14	10.980	3338	3352	3366	rBV2	47692	78870	2.32%	0.179%
15	11.063	3369	3383	3407	rVB2	75650	207643	6.11%	0.471%
16	11.312	3465	3476	3498	rVB5	34917	69853	2.06%	0.159%
17	11.521	3543	3554	3570	rVB	36736	65959	1.94%	0.150%
18	11.655	3590	3604	3615	rBV5	17170	34424	1.01%	0.078%
19	11.747	3615	3638	3661	rBV	1049888	1957401	57.61%	4.442%
20	11.846	3662	3675	3690	rVV	405401	710370	20.91%	1.612%
21	11.953	3690	3715	3742	rVB2	1196721	2433934	71.64%	5.523%
22	12.063	3744	3756	3762	rBV7	20925	37157	1.09%	0.084%
23	12.103	3763	3771	3780	rVB4	43615	62631	1.84%	0.142%
24	12.178	3791	3799	3813	rVB	67176	107589	3.17%	0.244%
25	12.283	3814	3838	3855	rBV2	623371	1166789	34.34%	2.648%
26	12.353	3856	3864	3874	rBV	45491	69857	2.06%	0.159%
27	12.487	3903	3914	3916	rBV4	34532	45500	1.34%	0.103%
28	12.581	3940	3949	3959	rVB2	43361	66815	1.97%	0.152%
29	12.637	3959	3970	3985	rVB3	83054	144580	4.26%	0.328%
30	12.734	3986	4006	4026	rBV	960514	1691119	49.78%	3.837%
31	12.876	4043	4059	4067	rBV5	76398	160965	4.74%	0.365%
32	12.924	4067	4077	4089	rVB	192670	297321	8.75%	0.675%
33	12.986	4089	4100	4107	rBV	387667	657122	19.34%	1.491%
34	13.224	4166	4189	4206	rBV	283545	550445	16.20%	1.249%
35	13.372	4219	4244	4255	rBV	694844	1238059	36.44%	2.809%
36	13.417	4255	4261	4273	rVB4	109679	169402	4.99%	0.384%

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37	13.535	4292	4305	4314	rBV4	101618	206435	6.08%	0.468%
38	13.594	4316	4327	4343	rVB	536761	976114	28.73%	2.215%
39	13.678	4344	4358	4379	rBV3	1315459	3397501	100.00%	7.709%
40	13.876	4412	4432	4442	rBV4	461410	990614	29.16%	2.248%
41	13.999	4472	4478	4488	rVB4	63903	88576	2.61%	0.201%
42	14.061	4489	4501	4516	rVB2	416775	770575	22.68%	1.749%
43	14.133	4518	4528	4532	rBV	98927	143107	4.21%	0.325%
44	14.163	4534	4539	4548	rVB	116876	152460	4.49%	0.346%
45	14.217	4549	4559	4570	rVB2	207368	340229	10.01%	0.772%
46	14.278	4574	4582	4590	rBV	56985	82362	2.42%	0.187%
47	14.329	4591	4601	4627	rVB5	209866	492384	14.49%	1.117%
48	14.439	4628	4642	4658	rVB5	269201	616167	18.14%	1.398%
49	14.517	4659	4671	4680	rBV3	447622	771516	22.71%	1.751%
50	14.635	4691	4715	4727	rBV2	1311114	3322071	97.78%	7.538%
51	14.815	4771	4782	4808	rVB5	309357	805615	23.71%	1.828%
52	14.933	4810	4826	4840	rBV5	351955	936757	27.57%	2.126%
53	15.000	4842	4851	4870	rVB	571960	980558	28.86%	2.225%
54	15.086	4871	4883	4901	rBV	513393	977662	28.78%	2.218%
55	15.161	4904	4911	4913	rVV4	56287	68597	2.02%	0.156%
56	15.198	4916	4925	4949	rVB10	172029	519579	15.29%	1.179%
57	15.456	5000	5021	5030	rBV2	726957	1812512	53.35%	4.113%
58	15.590	5059	5071	5084	rBV	1237540	2217698	65.27%	5.032%
59	15.676	5095	5103	5113	rVB	270055	401594	11.82%	0.911%
60	15.804	5139	5151	5170	rBV9	88900	241900	7.12%	0.549%
61	16.443	5380	5389	5404	rVB2	195067	419121	12.34%	0.951%
62	16.520	5408	5418	5433	rVB	200486	415458	12.23%	0.943%
63	16.617	5444	5454	5472	rVB2	565909	1297391	38.19%	2.944%
64	16.765	5496	5509	5517	rBV3	179133	378571	11.14%	0.859%

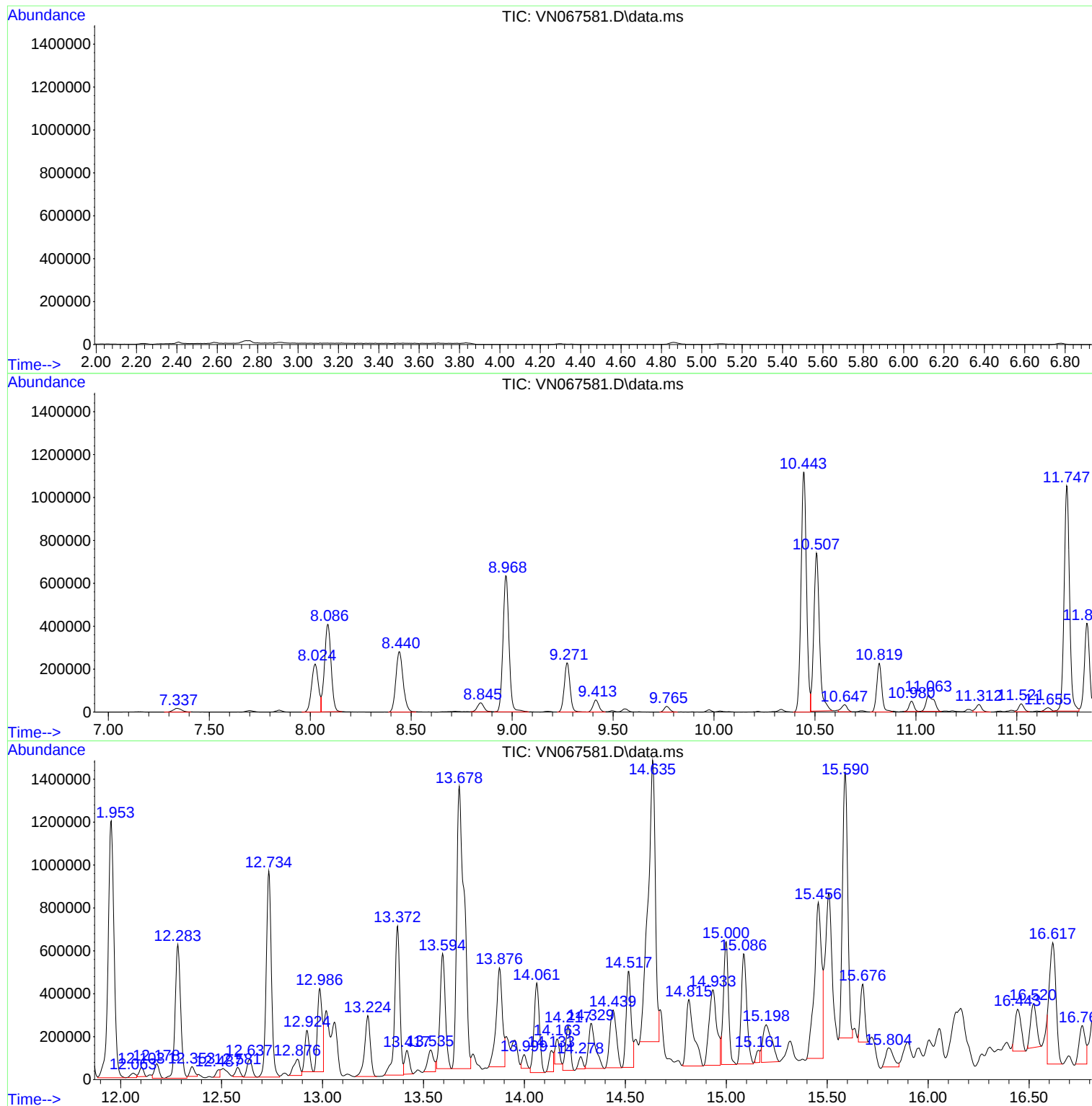
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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



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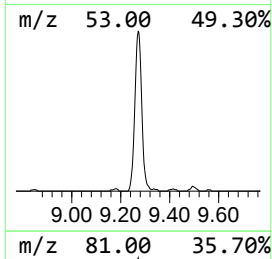
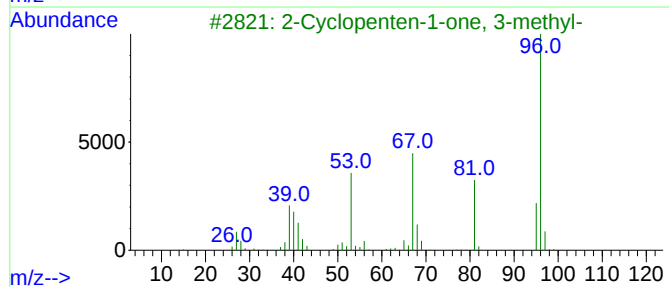
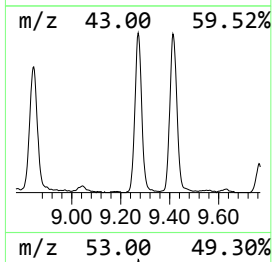
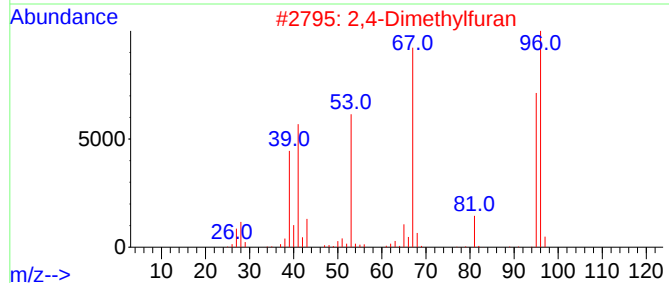
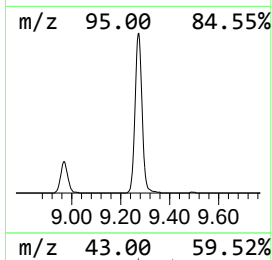
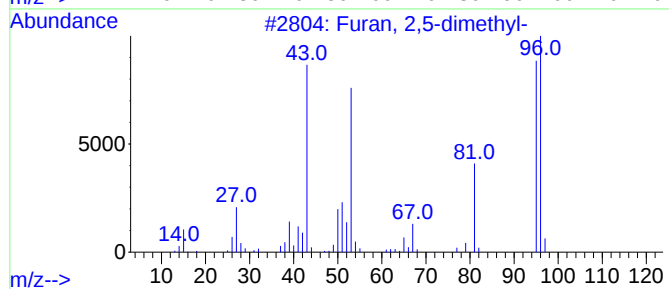
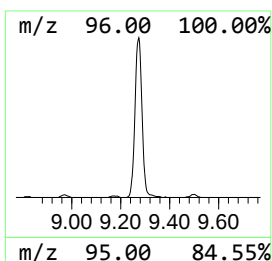
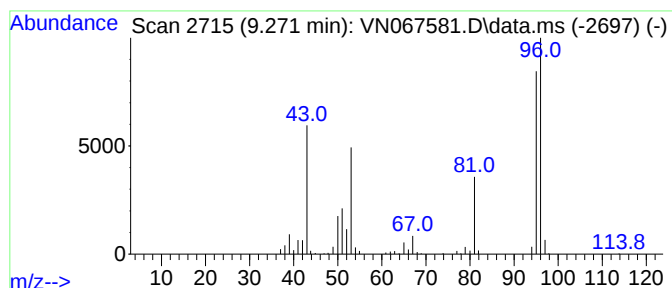
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Furan, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	17.17 ug/l	449505	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	91
2			2,4-Dimethylfuran	96	C6H8O	003710-43-8	72
3			2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	53
4			1H-Imidazole, 4,5-dimethyl-	96	C5H8N2	002302-39-8	43
5			1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	000694-48-4	38



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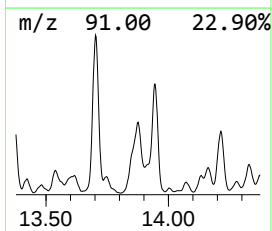
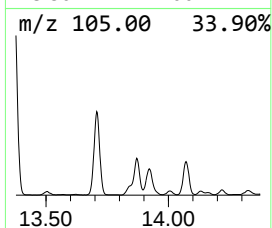
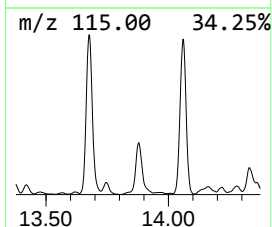
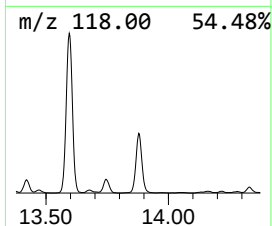
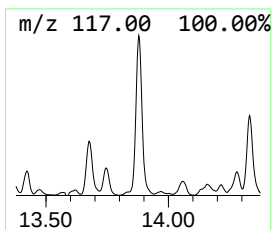
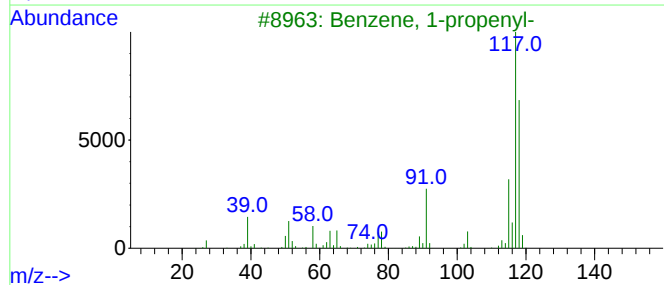
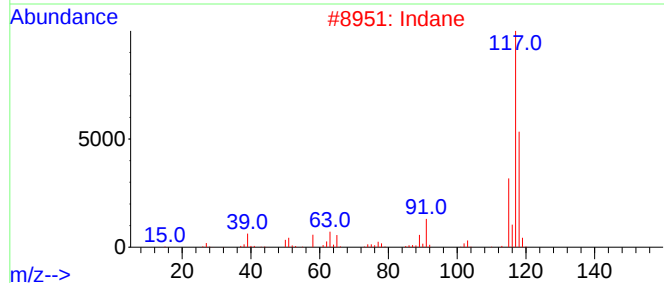
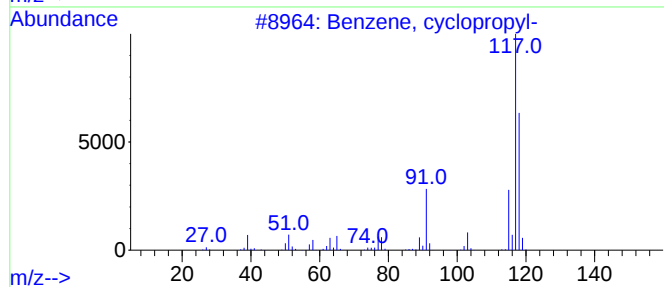
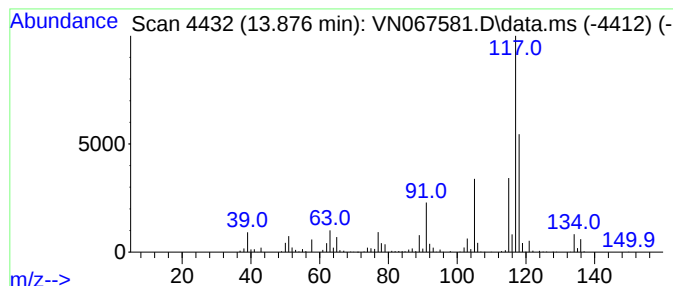
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, cyclopropyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	14.58 ug/l	990614	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	92
2			Indane	118	C9H10	000496-11-7	64
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	58
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	52
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	52



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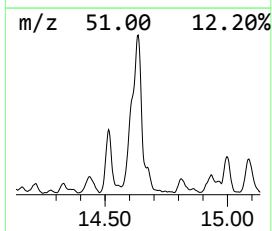
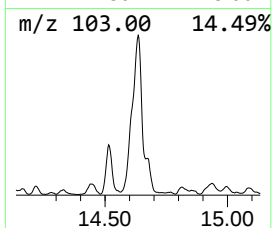
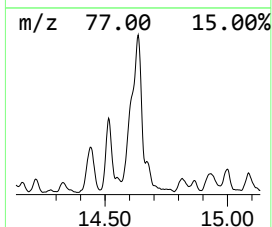
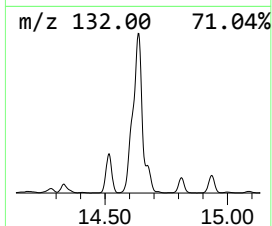
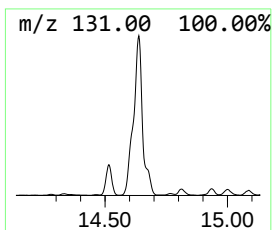
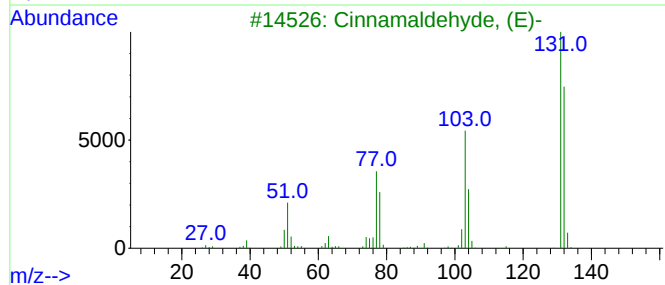
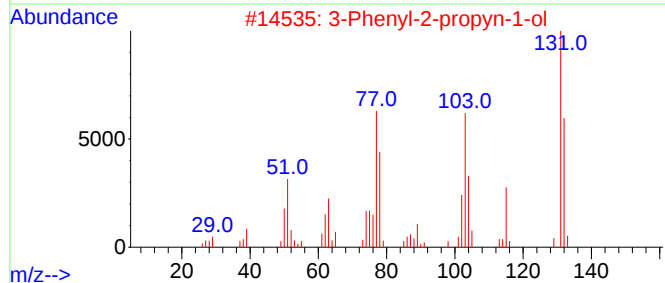
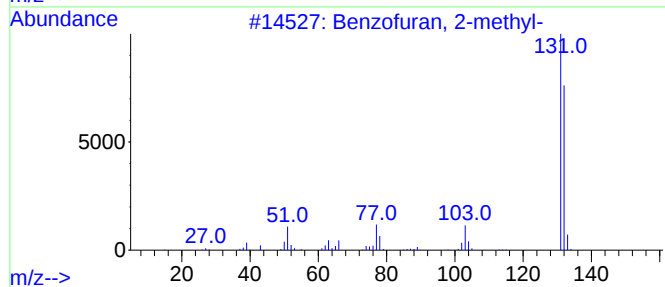
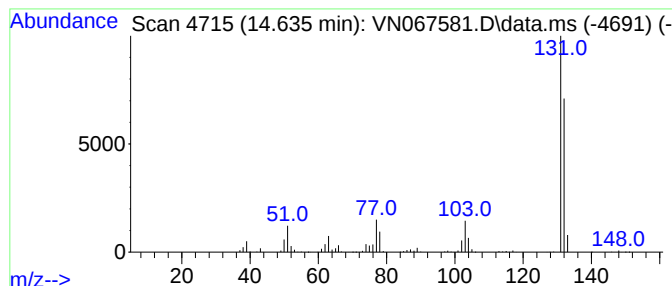
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Benzofuran, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	48.89 ug/l	3322070	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2			3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	83
3			Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	80
4			4-Aminobenzyl cyanide	132	C8H8N2	003544-25-0	80
5			Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	68



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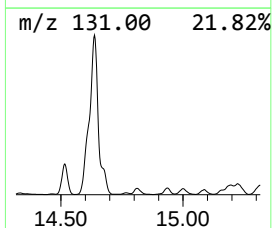
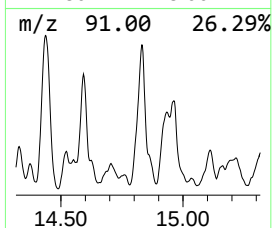
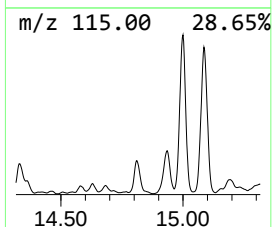
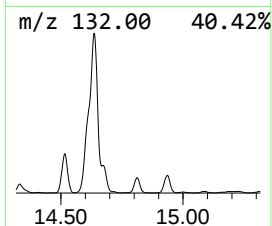
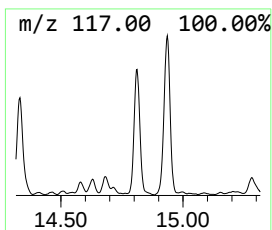
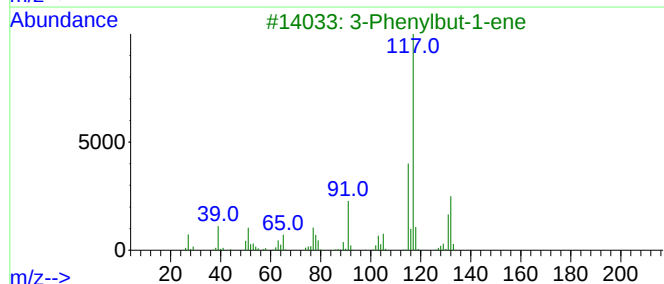
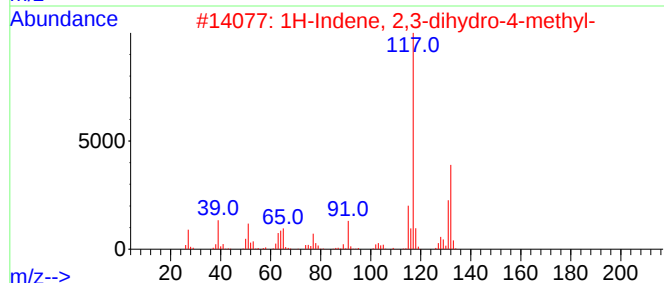
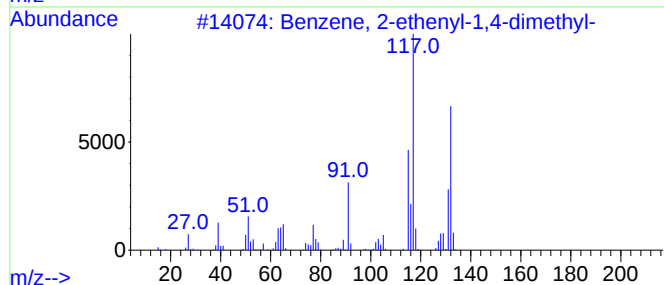
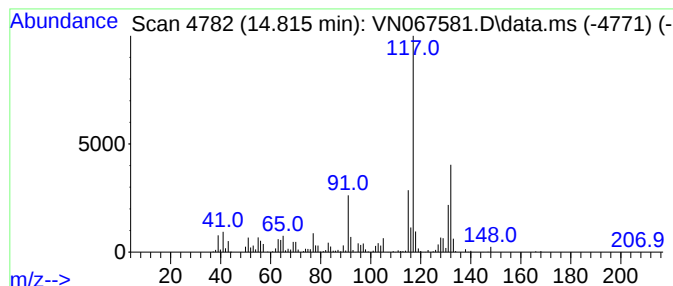
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	11.86 ug/l	805615	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	90



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Data File : VN067581.D
Acq On : 30 Jun 2021 18:55
Operator : JC/MD
Sample : M2896-03 40X
Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FS-02

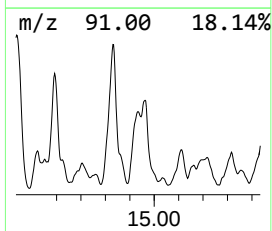
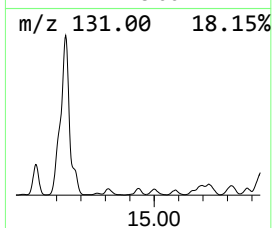
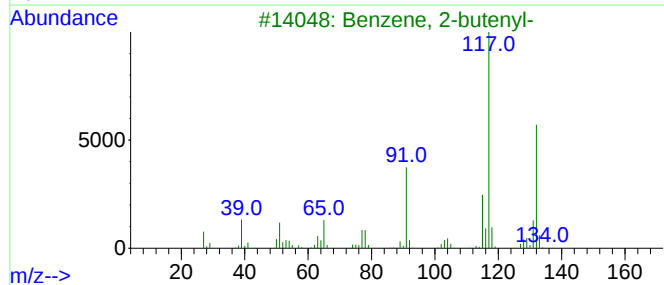
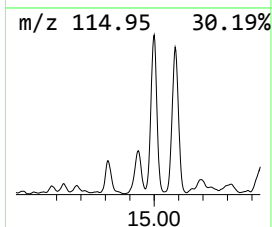
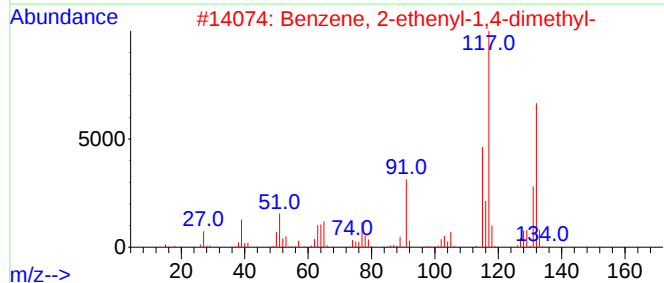
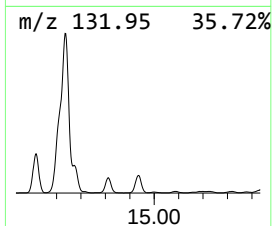
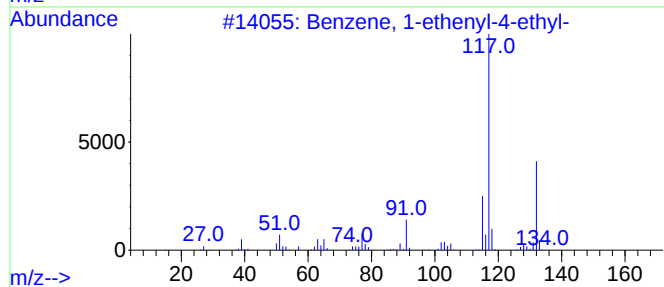
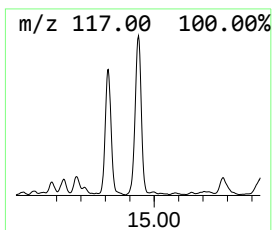
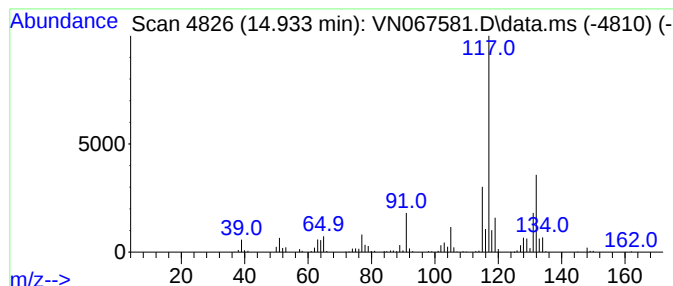
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	13.79 ug/l	936757	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067581.D
Acq On : 30 Jun 2021 18:55
Operator : JC/MD
Sample : M2896-03 40X
Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FS-02

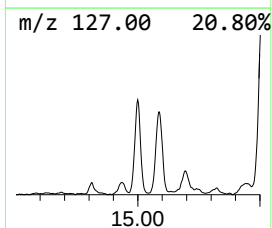
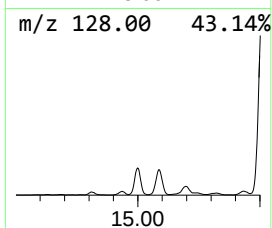
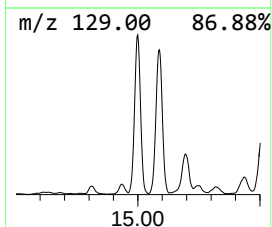
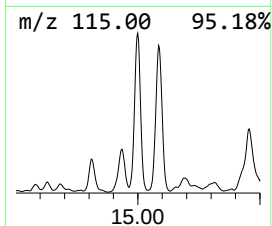
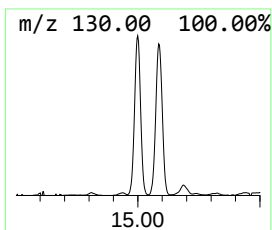
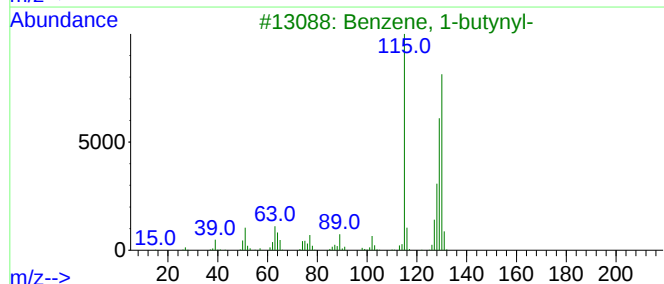
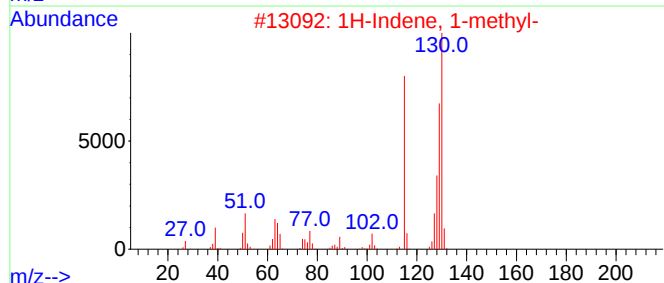
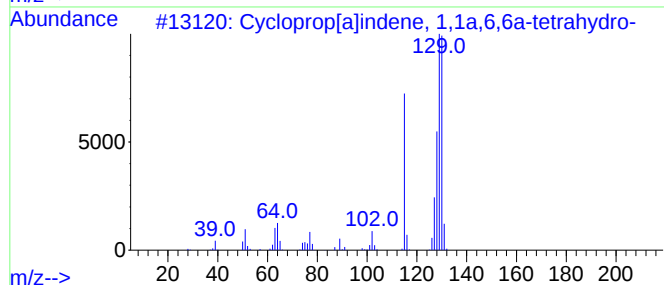
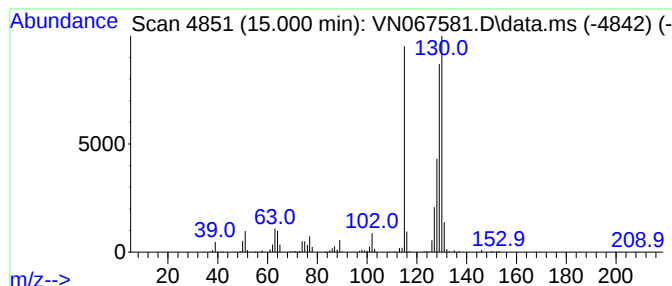
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Quant Title : SW846 8260

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

Peak Number 6 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.000	14.43 ug/l	980558	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
3			Benzene, 1-butynyl-	130	C10H10	000622-76-4	93
4			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	91
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067581.D
Acq On : 30 Jun 2021 18:55
Operator : JC/MD
Sample : M2896-03 40X
Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FS-02

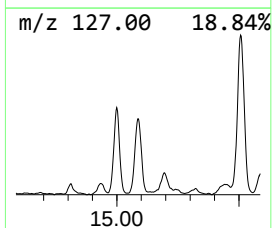
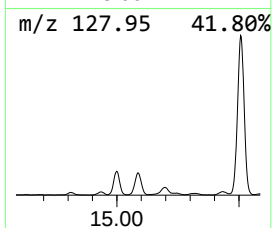
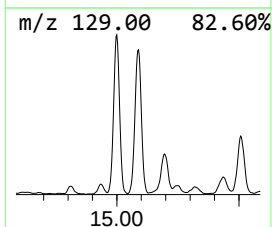
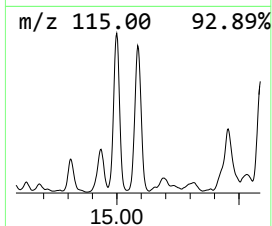
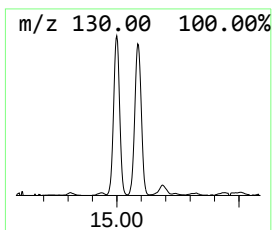
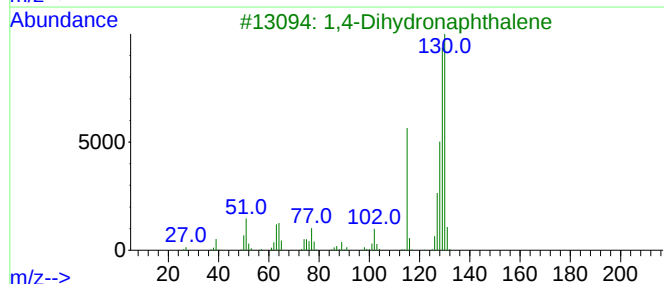
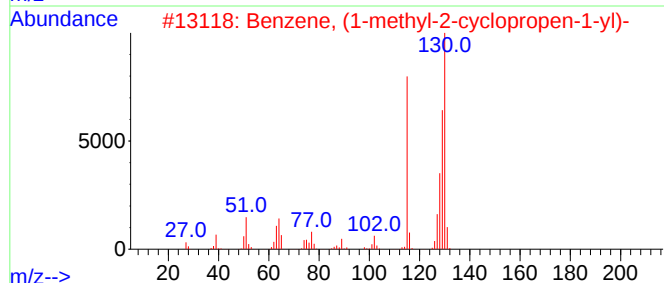
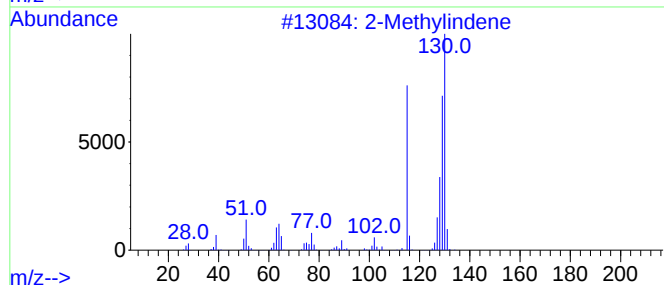
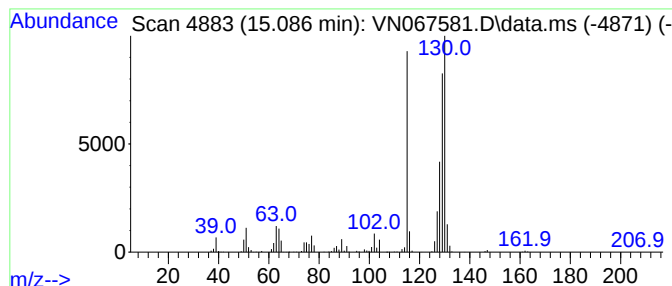
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Quant Title : SW846 8260

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

Peak Number 7 2-Methylindene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	14.39 ug/l	977662	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	95
2			Benzene, (1-methyl-2-cyclopropen-1-yl)-	130	C10H10	065051-83-4	95
3			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
4			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
5			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067581.D
Acq On : 30 Jun 2021 18:55
Operator : JC/MD
Sample : M2896-03 40X
Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FS-02

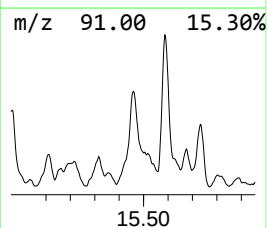
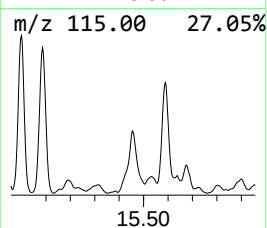
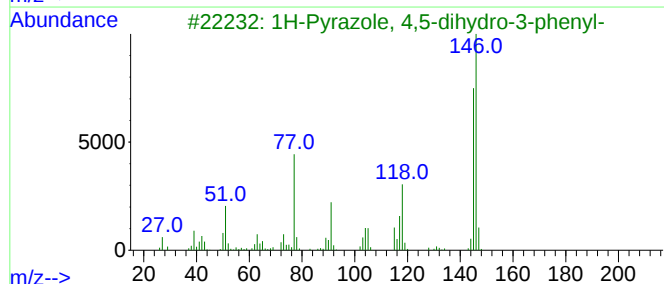
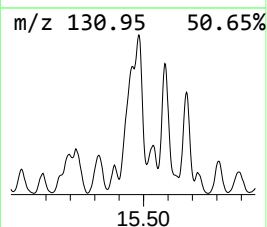
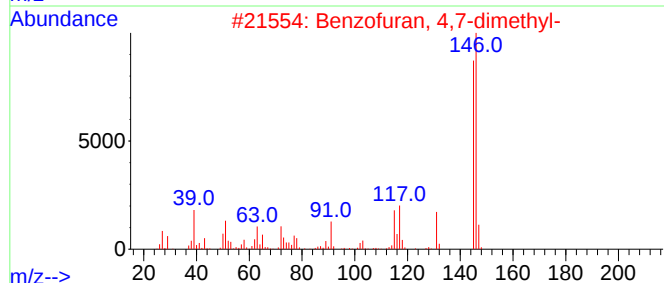
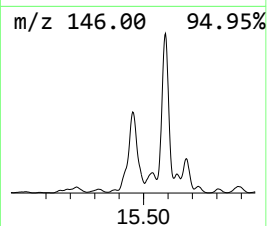
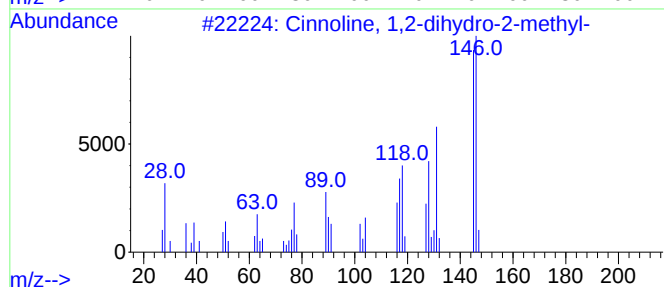
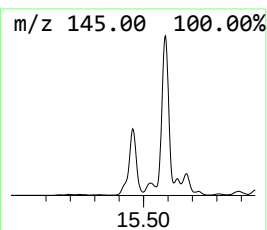
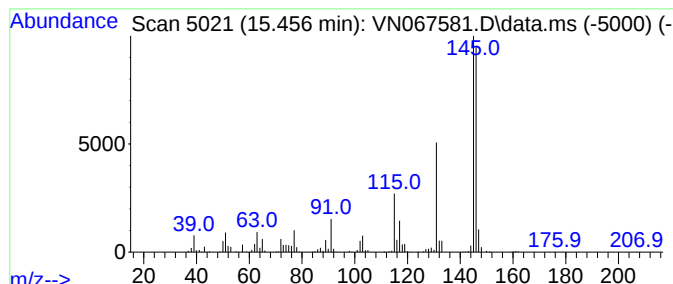
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Quant Title : SW846 8260

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

Peak Number 8 Cinnoline, 1,2-dihydro-2-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.456	26.67 ug/l	1812510	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	87
2			Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	72
3			1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	64
4			2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	59
5			1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067581.D
Acq On : 30 Jun 2021 18:55
Operator : JC/MD
Sample : M2896-03 40X
Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FS-02

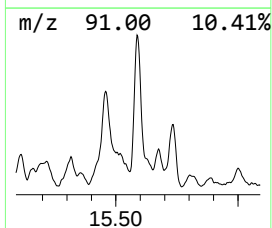
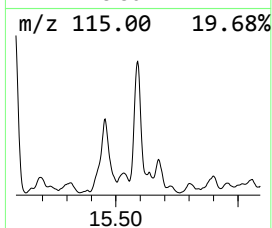
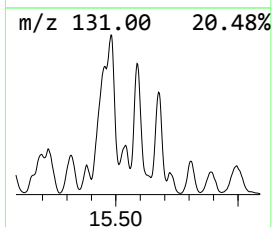
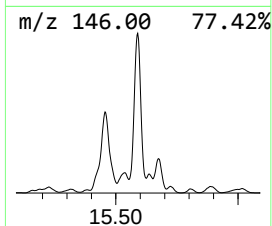
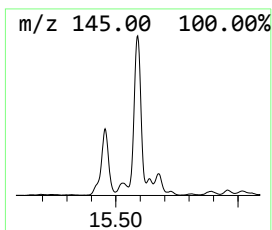
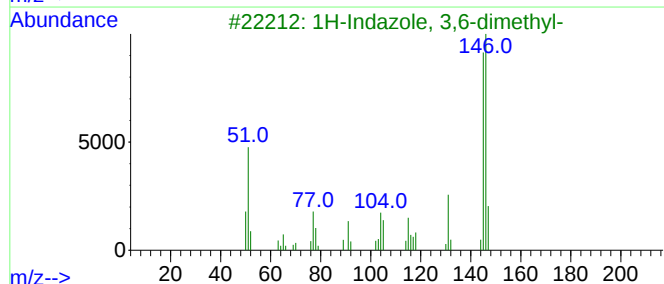
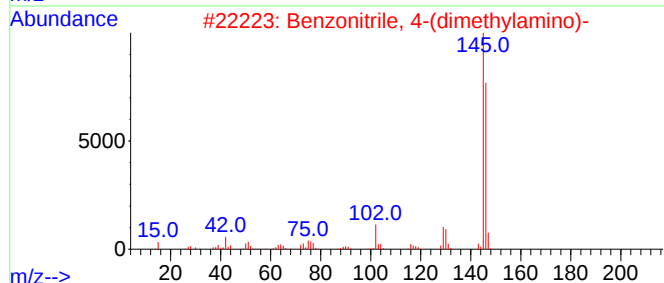
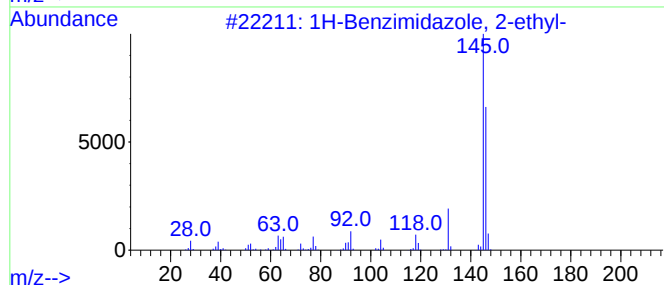
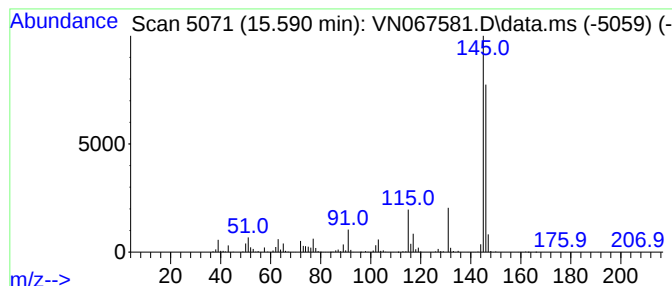
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Quant Title : SW846 8260

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

Peak Number 9 1H-Benzimidazole, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.590	32.64 ug/l	2217700	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	72
2			Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	59
3			1H-Indazole, 3,6-dimethyl-	146	C9H10N2	007746-28-3	56
4			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	50
5			2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067581.D
Acq On : 30 Jun 2021 18:55
Operator : JC/MD
Sample : M2896-03 40X
Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FS-02

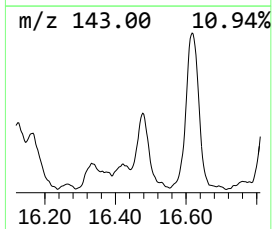
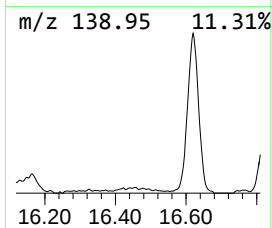
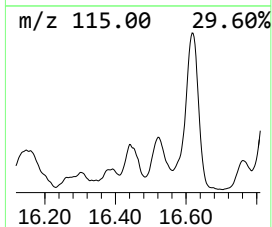
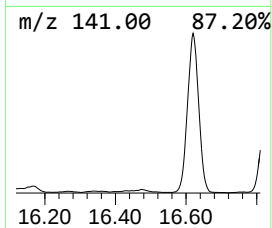
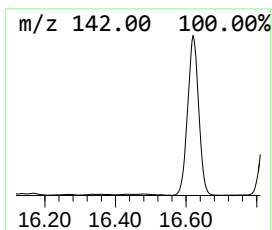
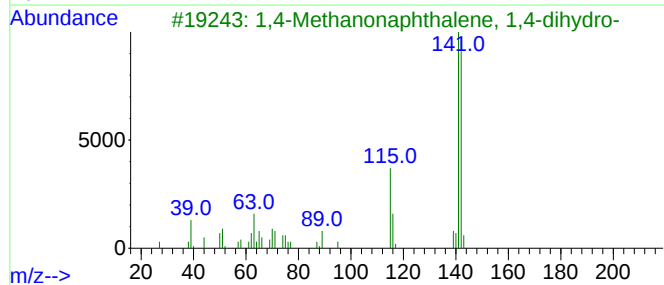
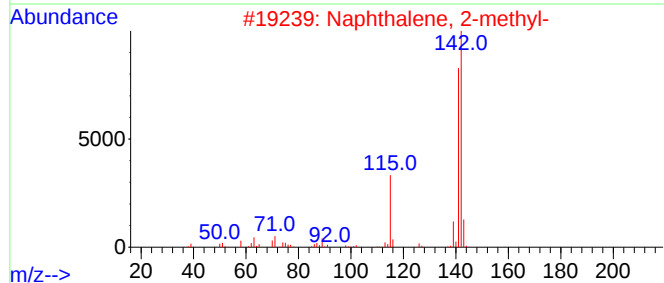
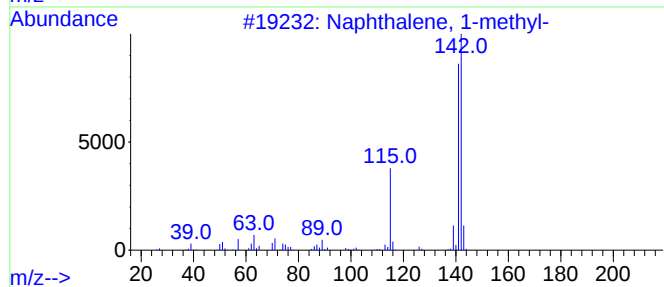
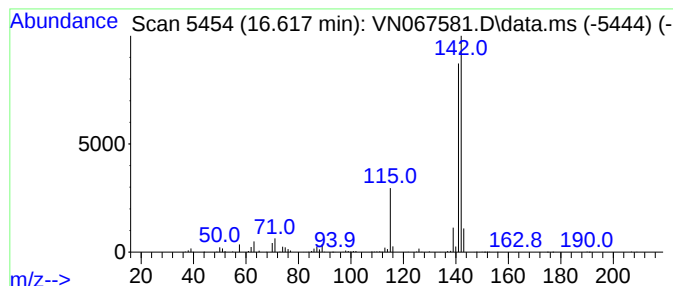
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.617	19.09 ug/l	1297390	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86
5			Benzocycloheptatriene	142	C11H10	000264-09-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
 Data File : VN067581.D
 Acq On : 30 Jun 2021 18:55
 Operator : JC/MD
 Sample : M2896-03 40X
 Misc : 8.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FS-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.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
Furan, 2,5-dime...	9.271	17.2	ug/l	449505	2	8.971	1309160	50.0
Benzene, cyclop...	13.876	14.6	ug/l	990614	4	13.678	3397500	50.0
Benzofuran, 2-m...	14.635	48.9	ug/l	3322070	4	13.678	3397500	50.0
Benzene, 2-ethe...	14.815	11.9	ug/l	805615	4	13.678	3397500	50.0
Benzene, 1-ethe...	14.933	13.8	ug/l	936757	4	13.678	3397500	50.0
Cycloprop[a]ind...	15.000	14.4	ug/l	980558	4	13.678	3397500	50.0
2-Methylindene	15.086	14.4	ug/l	977662	4	13.678	3397500	50.0
Cinnoline, 1,2-...	15.456	26.7	ug/l	1812510	4	13.678	3397500	50.0
1H-Benzimidazol...	15.590	32.6	ug/l	2217700	4	13.678	3397500	50.0
Naphthalene, 1-...	16.617	19.1	ug/l	1297390	4	13.678	3397500	50.0