

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
 Data File : VN070865.D
 Acq On : 31 Jan 2022 20:47
 Operator : JC/MD
 Sample : N1337-01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SS-1

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\82N011822W.M
 Title : SW846 8260

Signal : TIC: VN070865.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	2254	rBV2	541571	1226346	5.03%	0.257%
2	8.078	2258	2270	2289	rVV2	1464598	3842531	15.77%	0.804%
3	8.166	2290	2303	2327	rVB3	251167	643030	2.64%	0.135%
4	8.287	2327	2348	2367	rBV	807783	1900418	7.80%	0.398%
5	8.432	2384	2402	2429	rBV	669215	1551765	6.37%	0.325%
6	8.609	2429	2468	2490	rBV	1534009	4765794	19.56%	0.998%
7	8.700	2494	2502	2523	rVB3	222635	496184	2.04%	0.104%
8	8.821	2530	2547	2580	rVB	1400321	2954670	12.13%	0.618%
9	8.963	2580	2600	2627	rBV	1747835	3952765	16.22%	0.827%
10	9.268	2697	2714	2733	rVB3	119080	341679	1.40%	0.072%
11	9.454	2748	2783	2794	rBV2	2424883	5801808	23.81%	1.214%
12	9.505	2794	2802	2820	rVB	1237162	2399782	9.85%	0.502%
13	9.633	2840	2850	2863	rVV2	329416	621405	2.55%	0.130%
14	9.727	2863	2885	2902	rVB2	508003	1304123	5.35%	0.273%
15	9.875	2903	2940	2963	rBV3	2237329	4976227	20.43%	1.042%
16	10.014	2964	2992	3003	rVV3	2728326	6126358	25.15%	1.282%
17	10.076	3003	3015	3045	rVB2	4146662	10548328	43.30%	2.208%
18	10.213	3045	3066	3092	rBV	3978478	9452302	38.80%	1.979%
19	10.320	3093	3106	3111	rBV4	284683	512766	2.10%	0.107%
20	10.365	3112	3123	3135	rVV	1697090	3067916	12.59%	0.642%
21	10.435	3135	3149	3176	rVB3	4602982	10442421	42.86%	2.186%
22	10.559	3186	3195	3202	rBV2	364641	575473	2.36%	0.120%
23	10.620	3202	3218	3233	rVB	4851494	9443971	38.76%	1.977%
24	10.682	3234	3241	3249	rBV2	210580	297974	1.22%	0.062%
25	10.730	3252	3259	3267	rBV4	266947	366981	1.51%	0.077%
26	10.778	3267	3277	3294	rVB	1390176	2635048	10.82%	0.552%
27	10.872	3295	3312	3335	rBV6	1463160	4733419	19.43%	0.991%
28	10.961	3336	3345	3357	rVB	1261300	2167026	8.89%	0.454%
29	11.049	3358	3378	3391	rBV	2683523	5066024	20.79%	1.060%
30	11.151	3393	3416	3432	rBV	2195320	5712746	23.45%	1.196%
31	11.221	3433	3442	3448	rBV5	889074	1371354	5.63%	0.287%
32	11.291	3460	3468	3477	rVB	1779482	2506047	10.29%	0.525%
33	11.344	3477	3488	3499	rVB	3215580	5436642	22.31%	1.138%
34	11.452	3517	3528	3537	rBV4	2571279	4381462	17.98%	0.917%
35	11.524	3538	3555	3580	rVB5	7488891	19203357	78.82%	4.020%
36	11.623	3580	3592	3617	rBV	6807799	11956084	49.07%	2.503%

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37	11.744	3626	3637	3649	rBV	2258360	3719102	15.27%	0.778%
38	11.843	3663	3674	3693	rVB	6624568	11419547	46.87%	2.390%
39	11.924	3694	3704	3710	rBV5	1306663	2474747	10.16%	0.518%
40	12.251	3812	3826	3839	rBV4	3955494	8433670	34.62%	1.765%
41	12.363	3860	3868	3879	rVB	4709040	7306497	29.99%	1.529%
42	12.452	3880	3901	3905	rBV5	3516960	7591830	31.16%	1.589%
43	12.763	4012	4017	4027	rVB	3592565	4659897	19.13%	0.975%
44	12.916	4059	4074	4086	rVB	6579806	13621213	55.91%	2.851%
45	13.055	4104	4126	4138	rBV3	10474180	21896121	89.87%	4.583%
46	13.219	4171	4187	4202	rBV4	2365726	7736756	31.76%	1.619%
47	13.281	4203	4210	4227	rVB2	4013628	6521823	26.77%	1.365%
48	13.367	4230	4242	4253	rBV	15274819	24363327	100.00%	5.100%
49	13.603	4325	4330	4338	rVB3	1884451	2078849	8.53%	0.435%
50	13.672	4349	4356	4360	rBV2	2452611	3176861	13.04%	0.665%
51	13.702	4361	4367	4377	rVB	6112627	8473841	34.78%	1.774%
52	13.836	4407	4417	4423	rBV	4638298	7302639	29.97%	1.529%
53	13.871	4425	4430	4436	rVV2	5308791	7740454	31.77%	1.620%
54	13.908	4437	4444	4465	rVB4	10245646	22006976	90.33%	4.607%
55	13.997	4466	4477	4487	rBV3	5759450	9775420	40.12%	2.046%
56	14.128	4519	4526	4532	rBV	3738529	5051991	20.74%	1.057%
57	14.214	4548	4558	4575	rVB	15462369	24007407	98.54%	5.025%
58	14.324	4588	4599	4611	rVB4	7233841	12572830	51.61%	2.632%
59	14.506	4660	4667	4671	rBV6	2942633	4054963	16.64%	0.849%
60	14.536	4674	4678	4686	rVV2	6746261	9043874	37.12%	1.893%
61	14.576	4687	4693	4701	rVB	6077783	7941046	32.59%	1.662%
62	14.619	4702	4709	4717	rVV2	4086727	5092884	20.90%	1.066%
63	14.662	4718	4725	4739	rVB6	3180791	5374161	22.06%	1.125%
64	14.807	4770	4779	4789	rBV3	4759759	8403781	34.49%	1.759%
65	14.922	4807	4822	4834	rBV3	9857411	24192207	99.30%	5.064%
66	15.193	4914	4923	4951	rVB5	4914780	11635573	47.76%	2.436%
67	15.308	4955	4966	4980	rVB4	3727849	8223925	33.76%	1.721%
68	15.464	5015	5024	5028	rBV5	1497210	2219202	9.11%	0.465%
69	15.499	5031	5037	5051	rVB	3773018	6237892	25.60%	1.306%
70	15.802	5142	5150	5166	rVB	1846613	3673340	15.08%	0.769%
71	16.609	5439	5451	5485	rVB	2887881	6924541	28.42%	1.449%

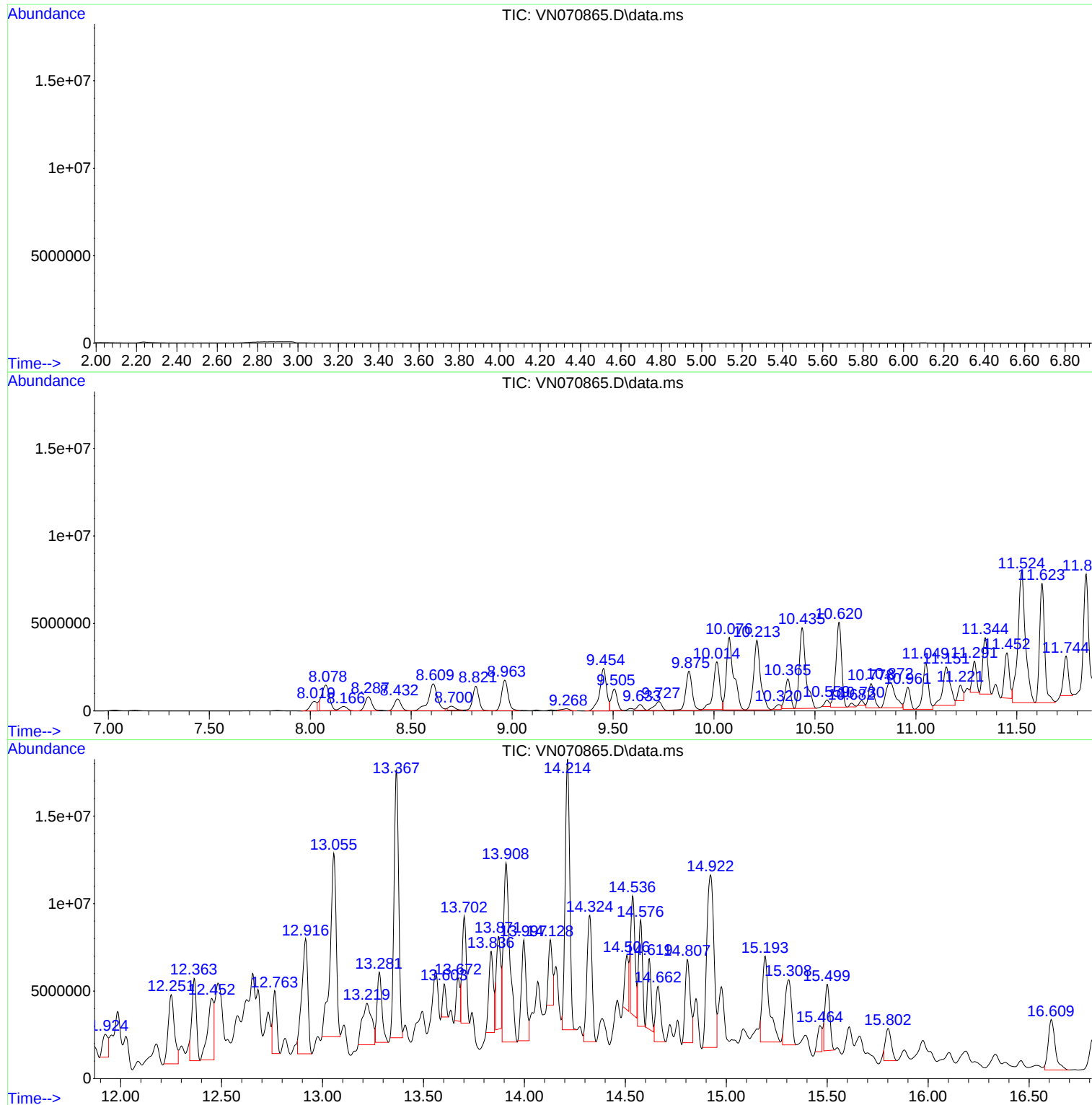
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ClientSampleId :
SS-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.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 :
SS-1

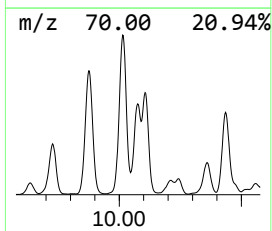
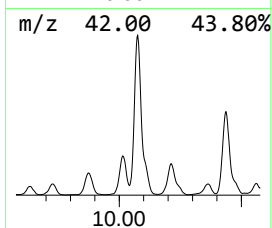
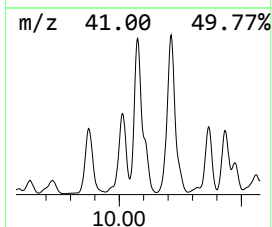
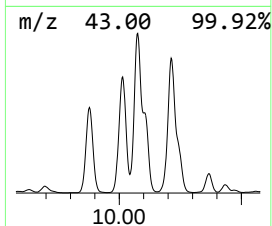
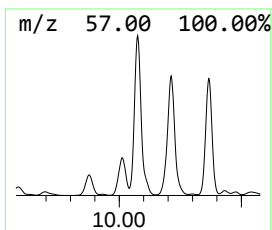
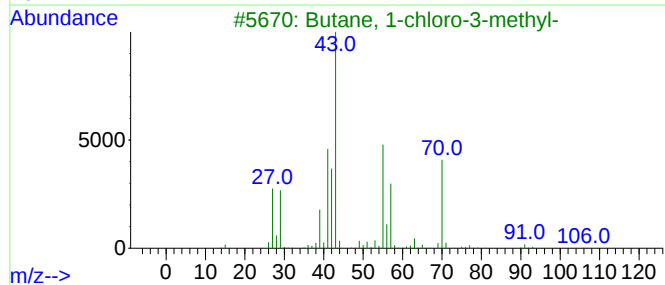
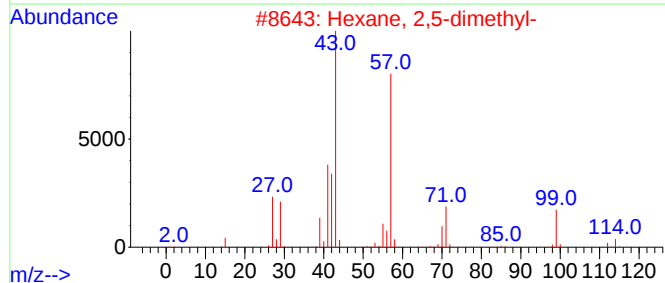
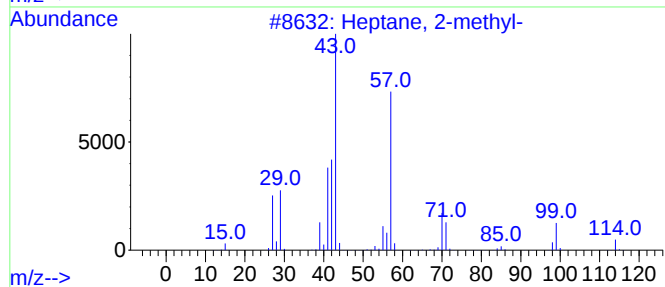
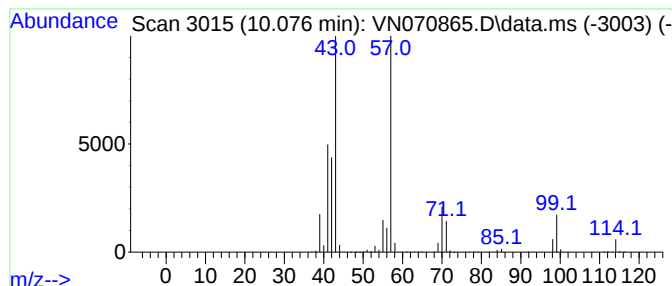
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.076	133.43 ug/l	10548300	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	91
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	80
3			Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	50
4			Heptane, 3-ethyl-	128	C9H20	015869-80-4	38
5			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	38



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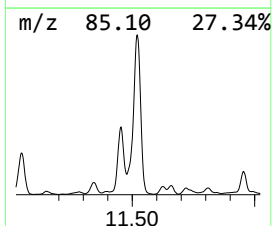
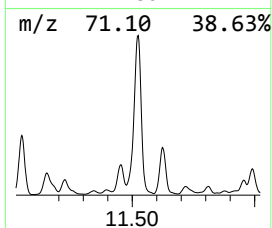
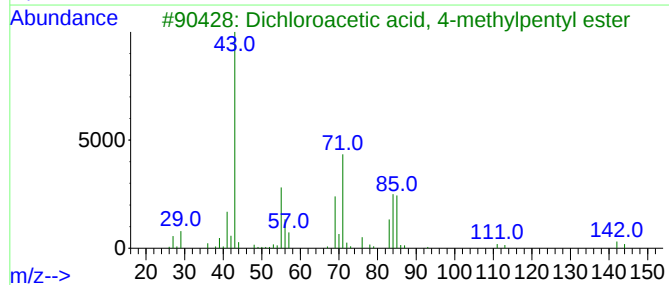
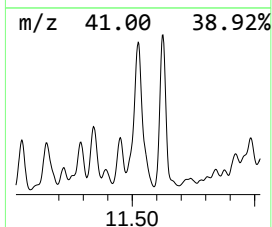
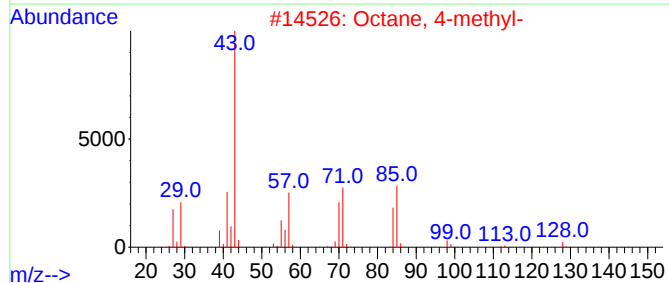
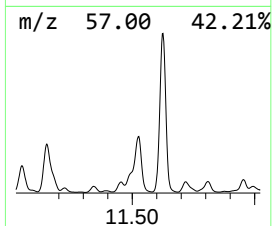
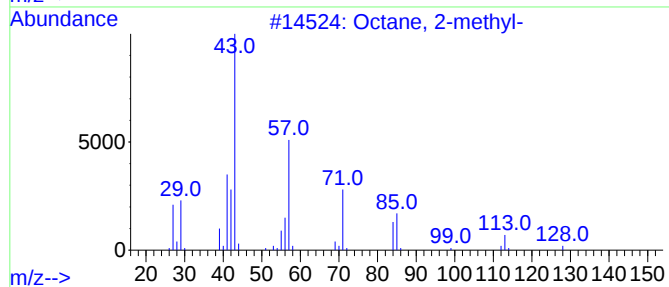
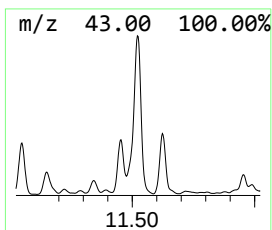
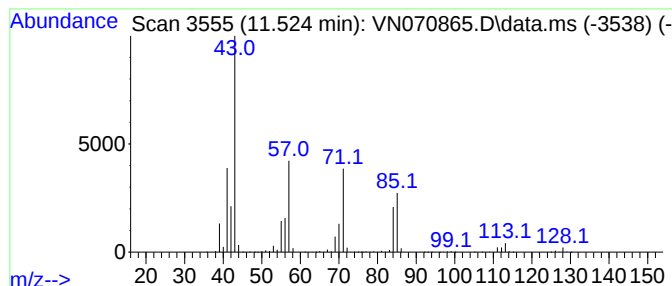
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.524	258.17 ug/l	19203400	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	80
2			Octane, 4-methyl-	128	C9H20	002216-34-4	64
3			Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	59
4			Dodecane, 5-methyl-	184	C13H28	017453-93-9	59
5			Ether, hexyl pentyl	172	C11H24O	032357-83-8	53



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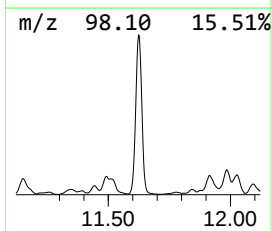
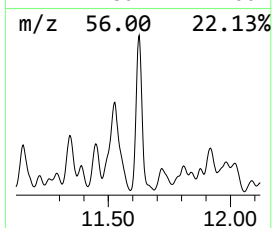
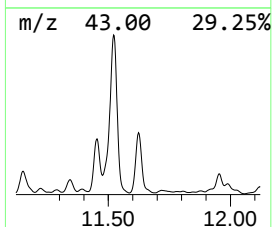
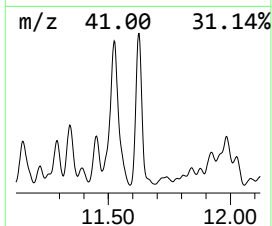
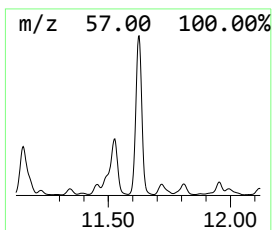
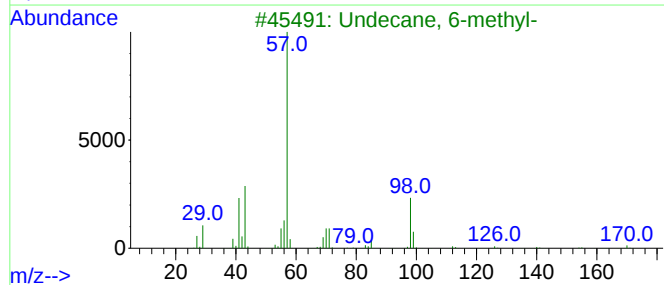
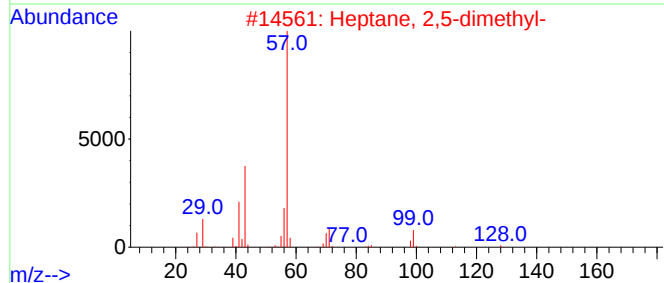
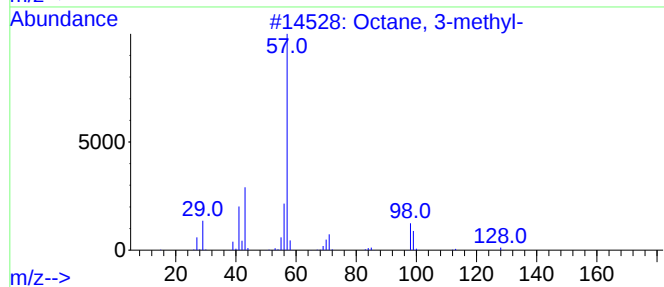
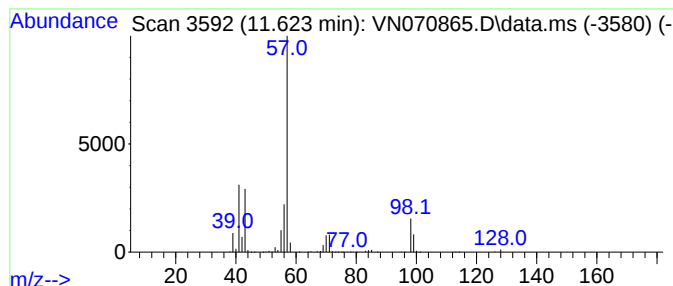
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.623	160.74 ug/l	11956100	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	91
2			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	72
3			Undecane, 6-methyl-	170	C12H26	017302-33-9	64
4			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	64
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	52



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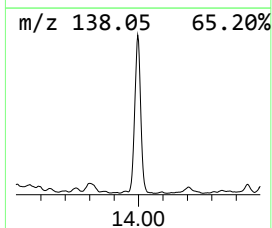
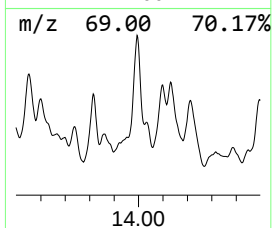
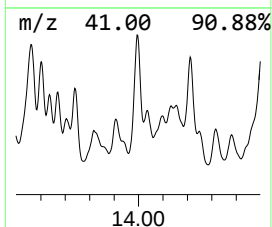
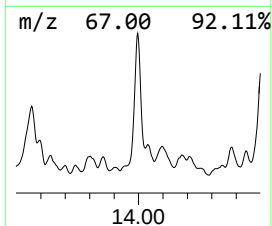
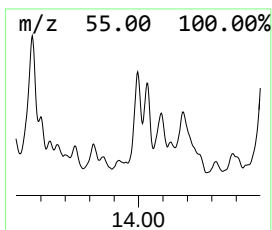
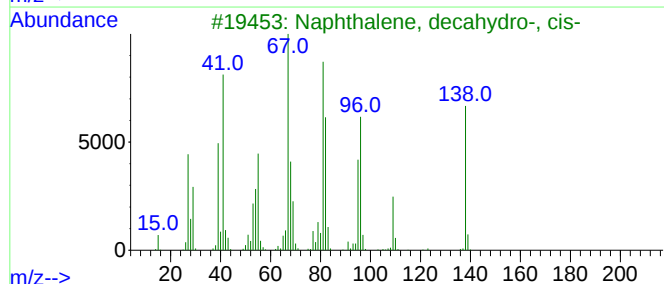
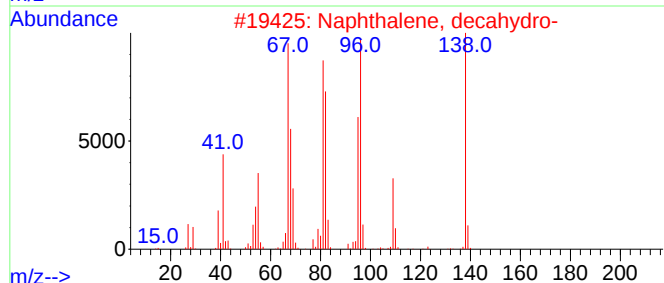
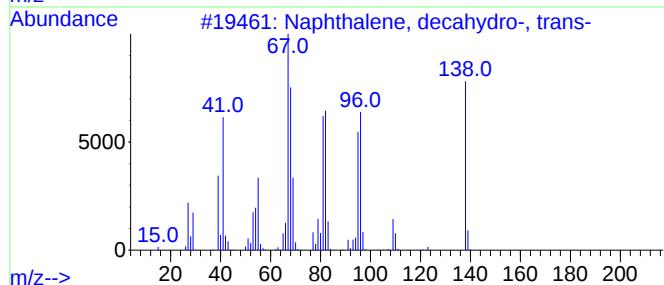
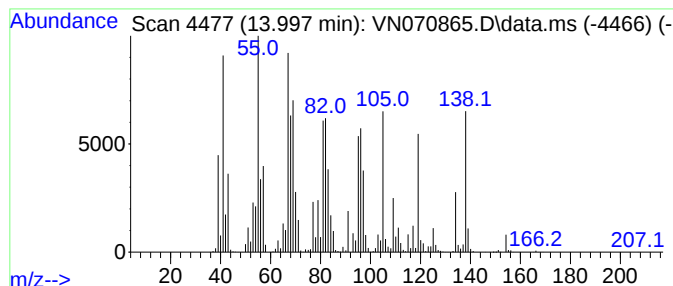
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, decahydro-, tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	153.85 ug/l	9775420	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2			Naphthalene, decahydro-	138	C10H18	000091-17-8	93
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	92
4			Spiro[4.5]decane	138	C10H18	000176-63-6	70
5			4-Isopropenylcyclohexanone	138	C9H14O	022460-53-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

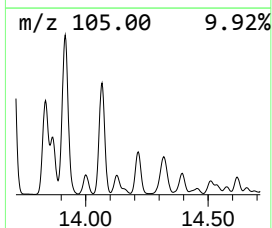
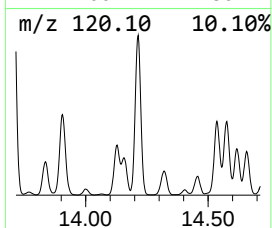
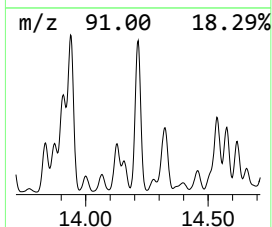
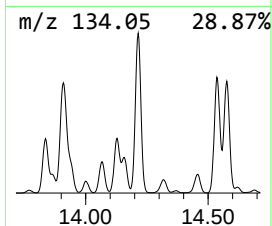
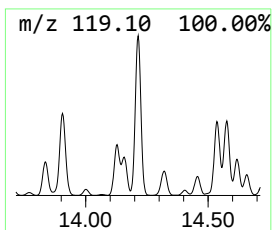
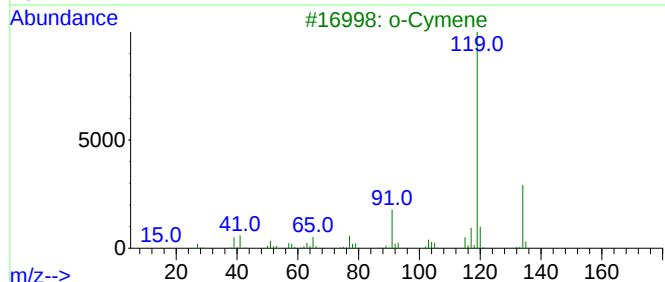
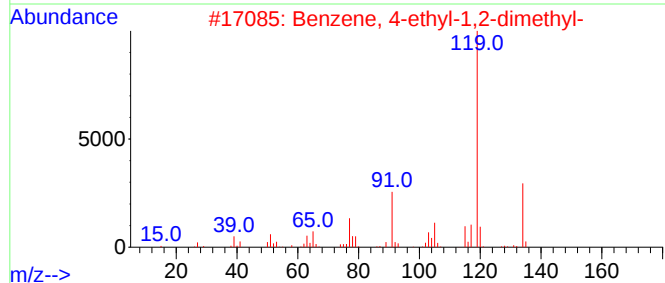
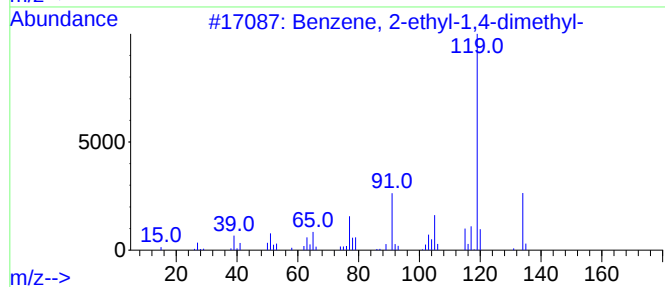
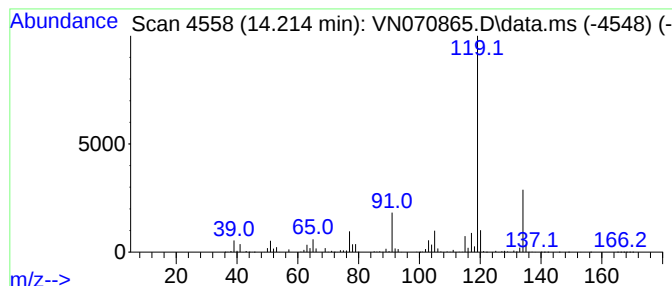
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	377.85 ug/l	24007400	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

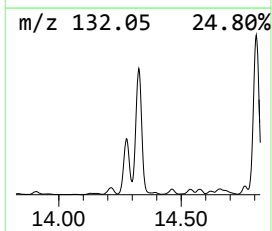
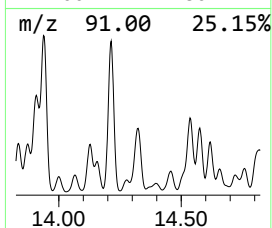
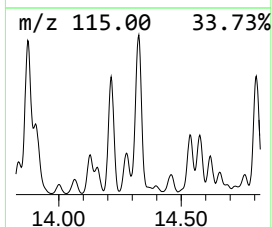
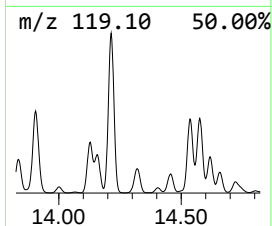
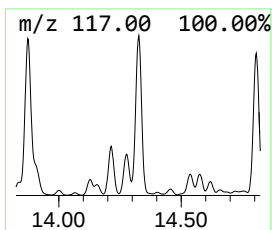
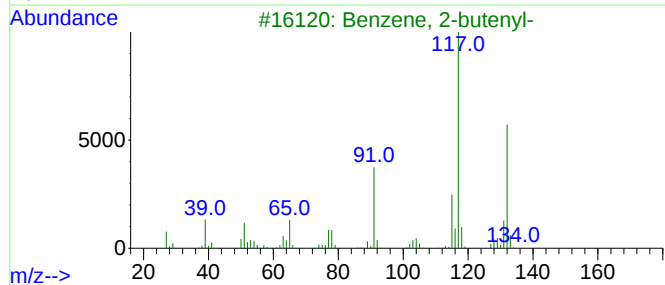
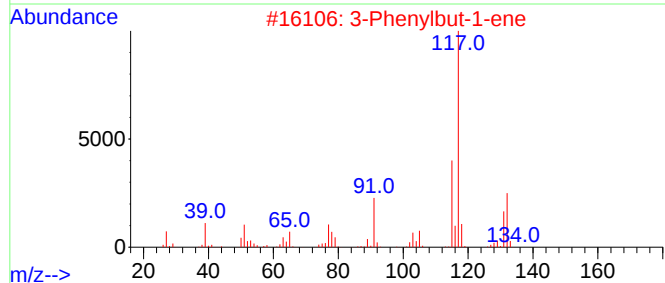
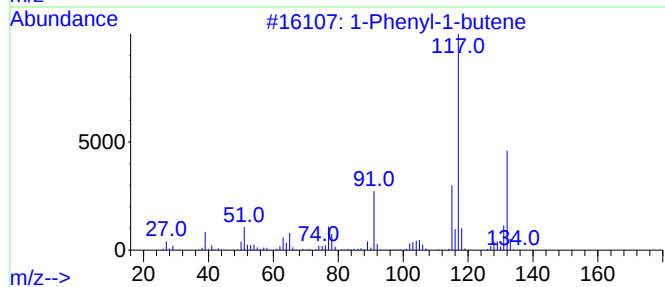
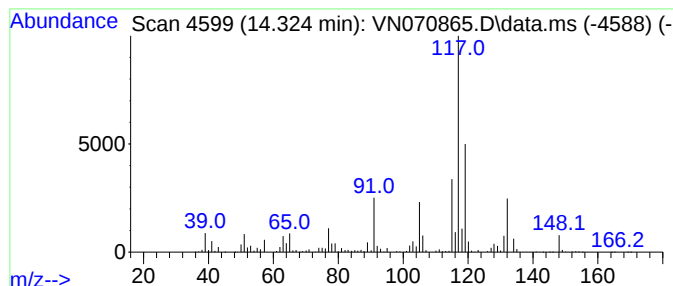
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Quant Title : SW846 8260

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

Peak Number 6 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.324	197.88 ug/l	12572800	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	83
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

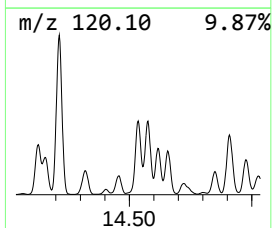
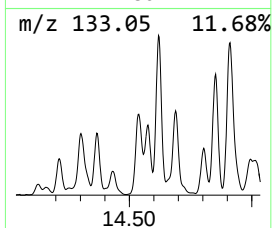
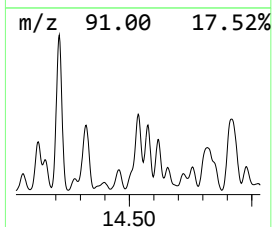
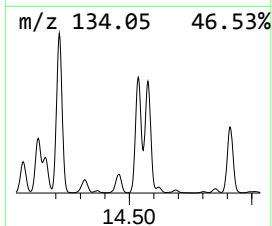
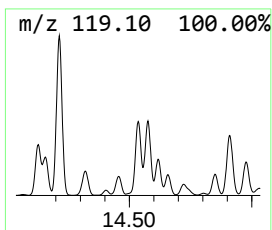
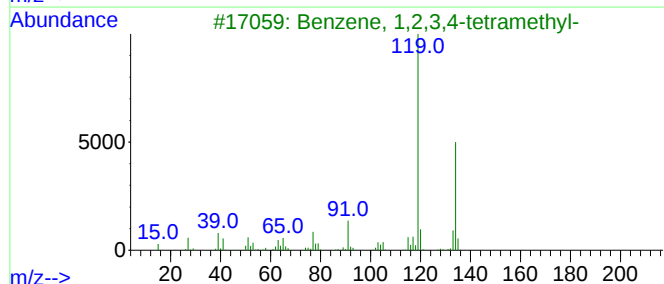
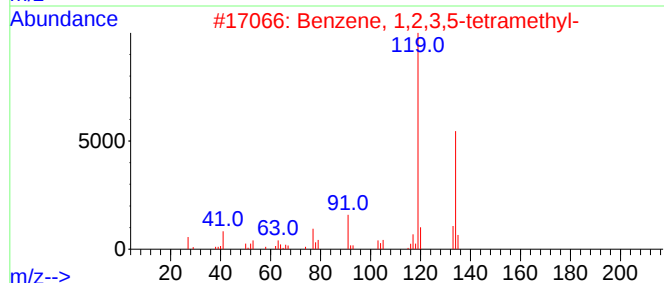
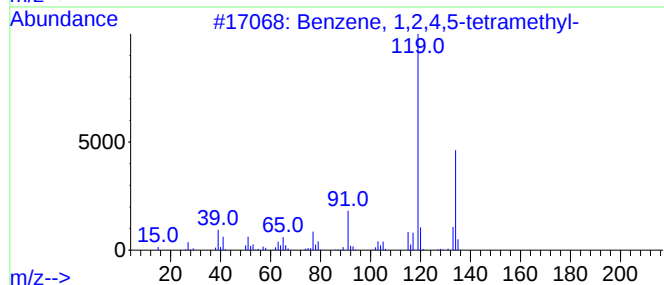
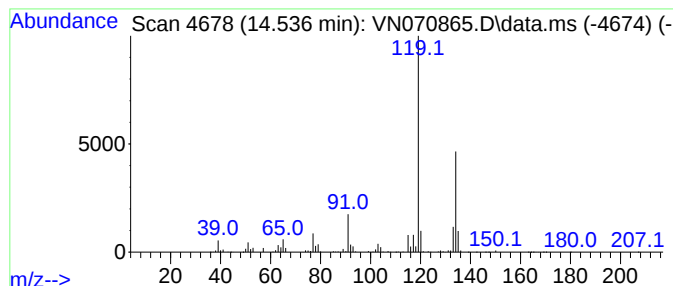
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.536	142.34 ug/l	9043870	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4			p-Cymene	134	C10H14	000099-87-6	91
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

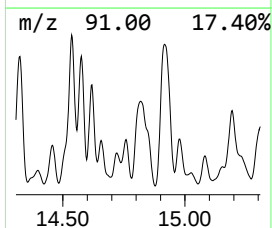
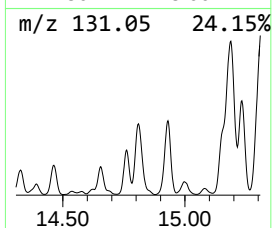
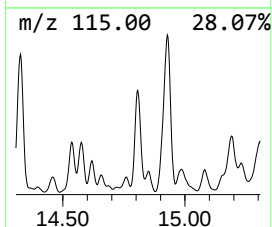
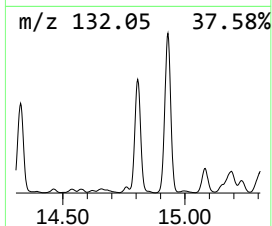
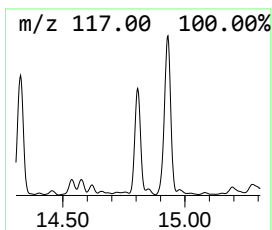
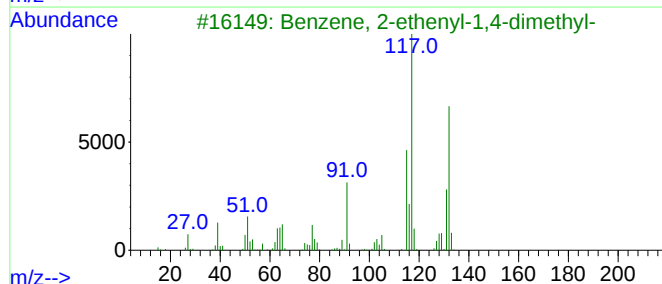
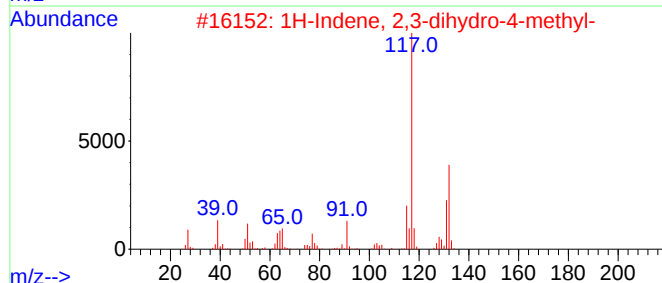
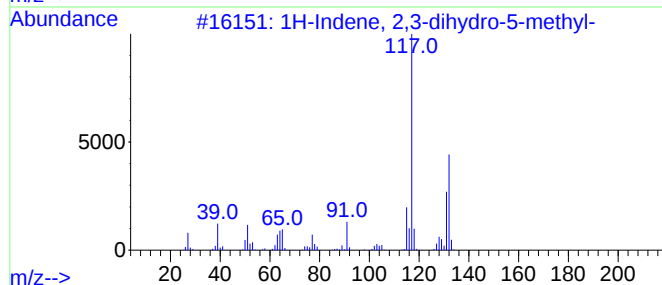
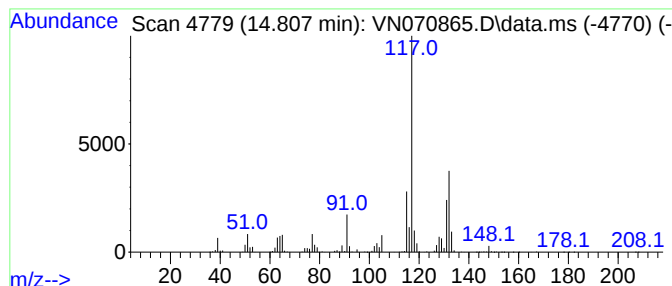
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.807	132.26 ug/l	8403780	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

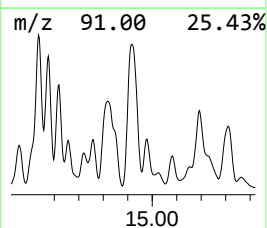
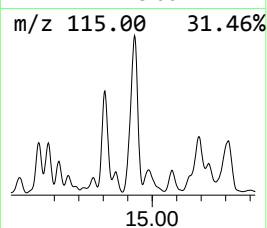
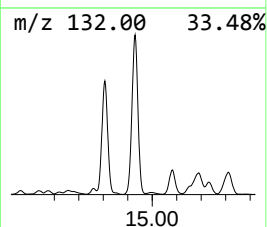
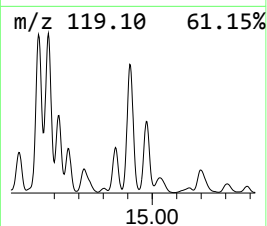
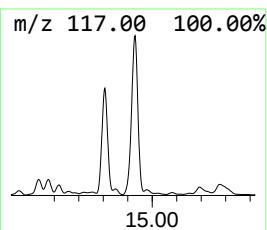
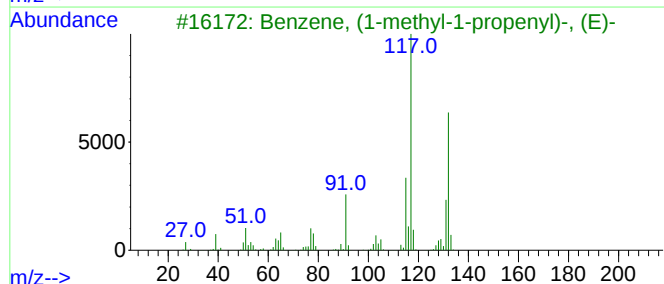
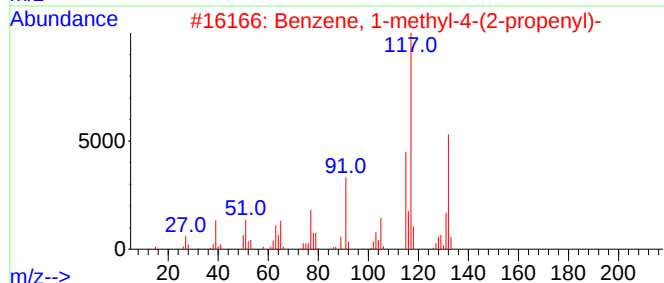
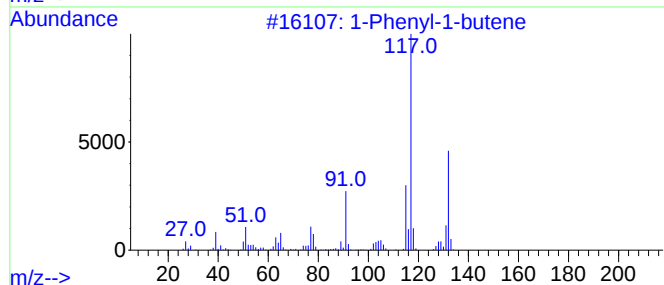
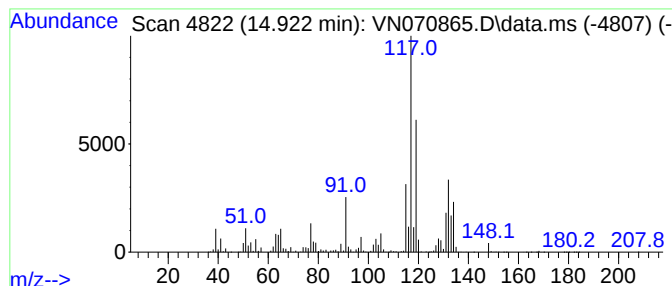
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-methyl-4-(2-prop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	380.76 ug/l	24192200	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
2			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	64
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

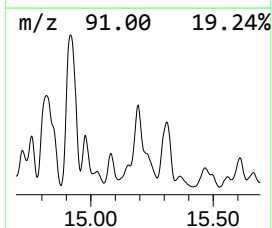
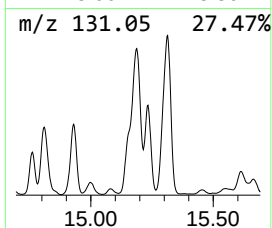
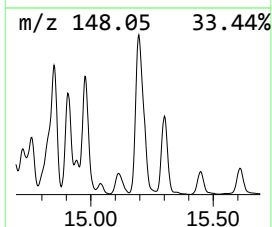
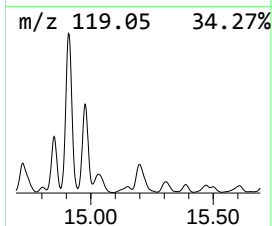
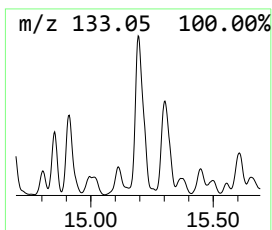
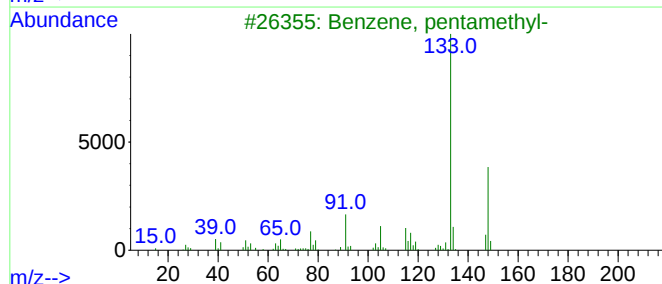
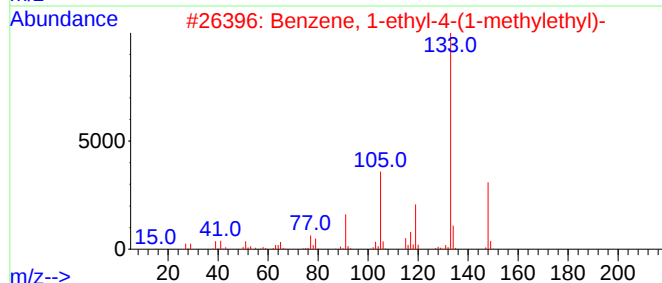
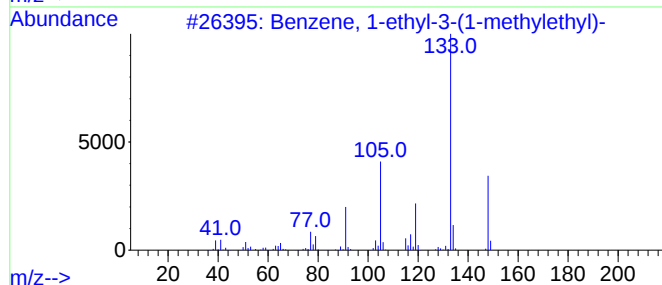
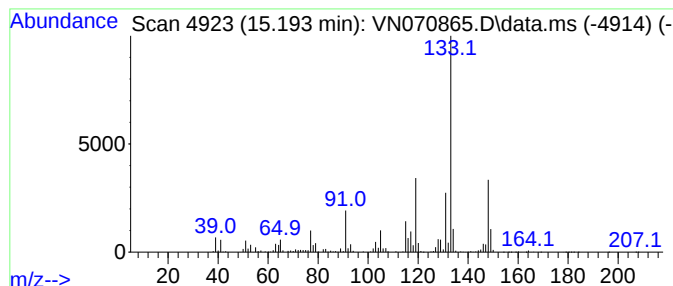
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-3-(1-methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.193	183.13 ug/l	11635600	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	72
2			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	72
3			Benzene, pentamethyl-	148	C11H16	000700-12-9	70
4			1,5,6,7-Tetramethylbicyclo[3.2.0]...	148	C11H16	134329-46-7	64
5			3,4-Dimethylcumene	148	C11H16	1000370-34-1	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
Data File : VN070865.D
Acq On : 31 Jan 2022 20:47
Operator : JC/MD
Sample : N1337-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.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
Heptane, 2-methyl-	10.076	133.4	ug/l	10548300	2	8.965	3952770	50.0
Octane, 2-methyl-	11.524	258.2	ug/l	19203400	3	11.744	3719100	50.0
Octane, 3-methyl-	11.623	160.7	ug/l	11956100	3	11.744	3719100	50.0
Naphthalene, de...	13.997	153.8	ug/l	9775420	4	13.672	3176860	50.0
Benzene, 2-ethy...	14.214	377.9	ug/l	24007400	4	13.672	3176860	50.0
1-Phenyl-1-butene	14.324	197.9	ug/l	12572800	4	13.672	3176860	50.0
Benzene, 1,2,4,...	14.536	142.3	ug/l	9043870	4	13.672	3176860	50.0
1H-Indene, 2,3-...	14.807	132.3	ug/l	8403780	4	13.672	3176860	50.0
Benzene, 1-meth...	14.922	380.8	ug/l	24192200	4	13.672	3176860	50.0
Benzene, 1-ethy...	15.193	183.1	ug/l	11635600	4	13.672	3176860	50.0