

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN051820\
 Data File : VN061465.D
 Acq On : 19 May 2020 7:19
 Operator : JC/MD
 Sample : L2645-02
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N051820W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.153	114	118	135	rVB	336713	470717	2.01%	0.264%
2	2.352	173	180	190	rVB	183285	283128	1.21%	0.159%
3	2.770	295	310	332	rBV	1232531	2494122	10.63%	1.397%
4	3.101	399	413	434	rVB2	124444	287333	1.22%	0.161%
5	3.761	596	618	641	rBV4	74448	242963	1.04%	0.136%
6	4.487	823	844	847	rBV2	278636	686912	2.93%	0.385%
7	4.998	974	1003	1037	rBV3	686310	2560407	10.91%	1.434%
8	5.519	1141	1165	1193	rBV2	106166	338817	1.44%	0.190%
9	5.879	1237	1277	1299	rBV2	137064	461390	1.97%	0.258%
10	6.021	1300	1321	1339	rBV3	77411	248141	1.06%	0.139%
11	6.326	1394	1416	1439	rBV4	72072	240214	1.02%	0.135%
12	6.580	1474	1495	1516	rBV	926584	2881343	12.28%	1.614%
13	7.330	1694	1728	1752	rBV	698710	2017827	8.60%	1.130%
14	7.548	1777	1796	1803	rBV2	181887	442347	1.89%	0.248%
15	7.619	1804	1818	1834	rVV4	737989	2111215	9.00%	1.183%
16	7.706	1835	1845	1869	rVB3	168259	479727	2.04%	0.269%
17	7.838	1869	1886	1897	rBV2	120265	298835	1.27%	0.167%
18	7.998	1918	1936	1955	rBV3	554161	1488168	6.34%	0.834%
19	8.124	1957	1975	1986	rVV6	293595	885060	3.77%	0.496%
20	8.194	1990	1997	2009	rVV5	252393	590282	2.52%	0.331%
21	8.265	2009	2019	2040	rVB	184555	441665	1.88%	0.247%
22	8.551	2087	2108	2130	rBV2	691571	1610306	6.86%	0.902%
23	9.047	2230	2262	2277	rBV3	604629	1795175	7.65%	1.006%
24	9.236	2310	2321	2336	rVB	144122	285947	1.22%	0.160%
25	9.583	2416	2429	2436	rBV2	188964	378240	1.61%	0.212%
26	9.940	2528	2540	2550	rBV3	131093	282667	1.20%	0.158%
27	10.059	2564	2577	2590	rBV	968304	1815458	7.74%	1.017%
28	11.381	2973	2988	3004	rBV	983290	1882991	8.03%	1.055%
29	11.487	3005	3021	3038	rBV	12651498	23004294	98.05%	12.888%
30	11.603	3043	3057	3079	rVB	10859532	18960659	80.82%	10.623%
31	11.921	3148	3156	3169	rVV	162115	288778	1.23%	0.162%
32	12.127	3202	3220	3238	rBV8	112543	404865	1.73%	0.227%
33	12.223	3239	3250	3261	rBV	1311583	2114381	9.01%	1.185%
34	12.378	3282	3298	3319	rVB	835682	1489200	6.35%	0.834%

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ALS Vial : 45 Sample Multiplier: 1

Instrument :
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Integration Parameters: RTEINT.P

Integrator: RTE
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	12.564	3344	3356	3368	rBV	3427126	5601723	23.88%	3.138%
36	12.664	3368	3387	3394	rVV	3536561	6735986	28.71%	3.774%
37	12.709	3394	3401	3414	rVB	2757261	4245779	18.10%	2.379%
38	12.866	3437	3450	3465	rBV	2631165	4341718	18.51%	2.432%
39	13.014	3482	3496	3511	rBV	13922096	23461182	100.00%	13.144%
40	13.143	3524	3536	3546	rVB2	269176	618846	2.64%	0.347%
41	13.207	3547	3556	3565	rBV	160113	258960	1.10%	0.145%
42	13.349	3580	3600	3616	rBV2	4571077	9100154	38.79%	5.098%
43	13.519	3633	3653	3661	rBV2	6609891	12801017	54.56%	7.172%
44	13.561	3661	3666	3684	rVB4	1316004	2497282	10.64%	1.399%
45	13.648	3684	3693	3702	rBV	274316	435423	1.86%	0.244%
46	13.715	3702	3714	3723	rVB	593354	991137	4.22%	0.555%
47	13.776	3723	3733	3739	rBV	1192773	1998249	8.52%	1.120%
48	13.863	3751	3760	3770	rVV	2576634	3923916	16.73%	2.198%
49	13.921	3770	3778	3784	rVV	480611	711064	3.03%	0.398%
50	13.969	3784	3793	3806	rVB2	1840050	2962928	12.63%	1.660%
51	14.101	3823	3834	3846	rBV	461051	776006	3.31%	0.435%
52	14.185	3847	3860	3866	rBV	1488821	2419350	10.31%	1.355%
53	14.223	3866	3872	3882	rVB	1631274	2443902	10.42%	1.369%
54	14.451	3933	3943	3953	rBV	1643004	2556854	10.90%	1.432%
55	14.570	3965	3980	3991	rBV3	3217477	6106867	26.03%	3.421%
56	14.632	3991	3999	4012	rVB4	211419	372277	1.59%	0.209%
57	14.715	4015	4025	4041	rBV	436408	726728	3.10%	0.407%
58	14.824	4050	4059	4067	rBV5	232364	448755	1.91%	0.251%
59	14.931	4081	4092	4110	rVB2	255072	597783	2.55%	0.335%
60	15.104	4134	4146	4161	rVB	3149107	5450394	23.23%	3.054%
61	15.204	4168	4177	4187	rBV3	122456	235998	1.01%	0.132%
62	16.123	4451	4463	4489	rVB	378936	789501	3.37%	0.442%
63	16.313	4509	4522	4537	rVB	289697	620407	2.64%	0.348%

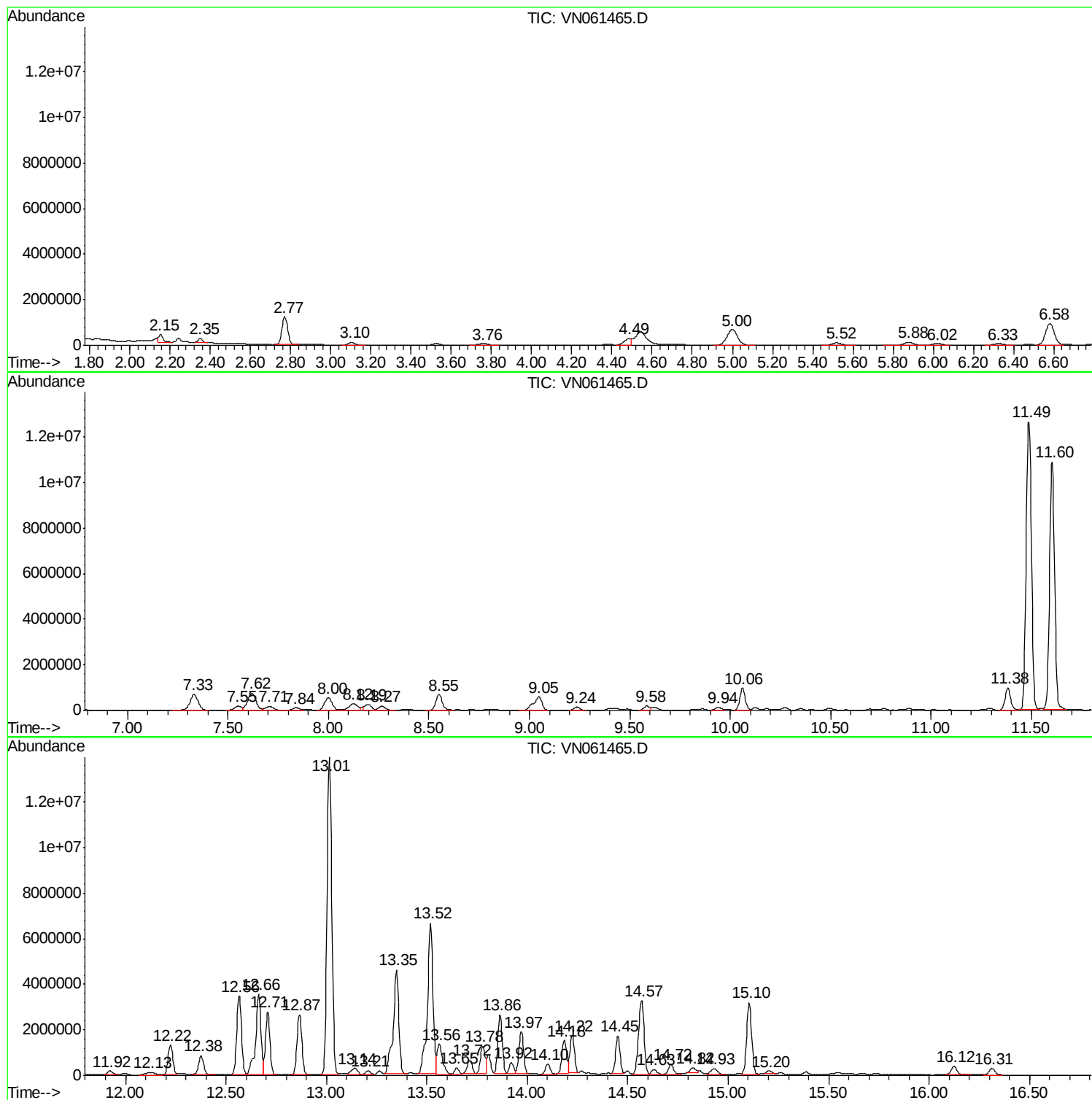
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051820W.M
Quant Title : SW846 8260

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



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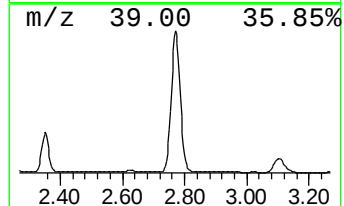
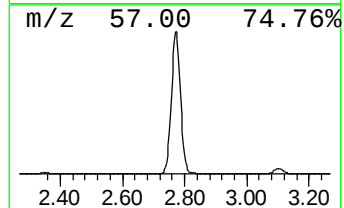
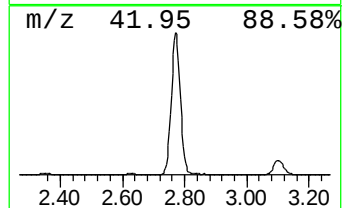
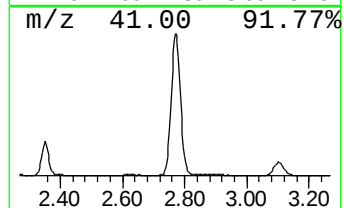
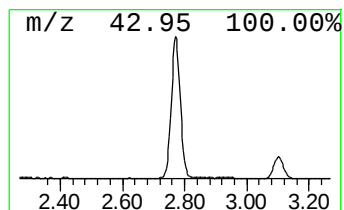
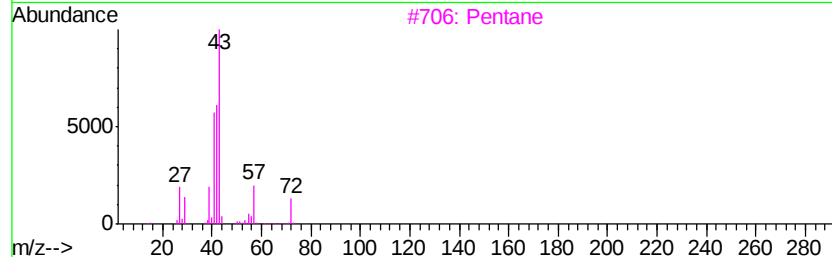
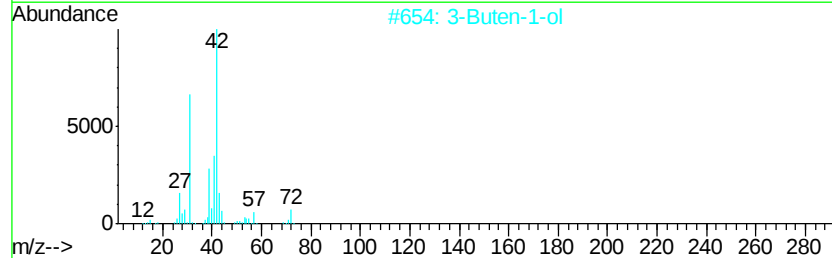
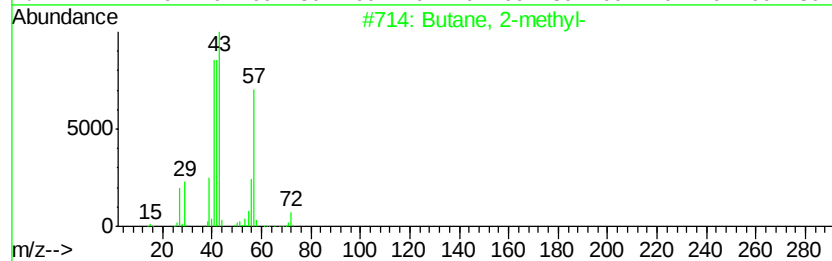
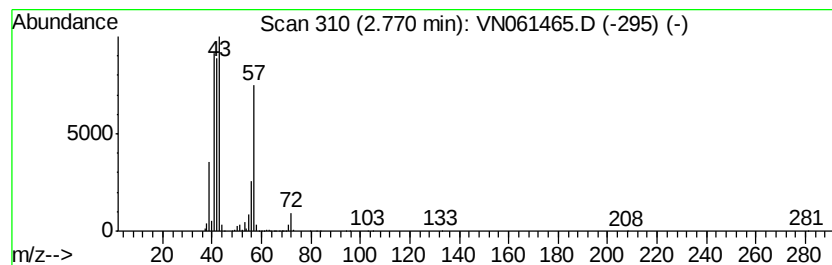
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051820W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.77	59.07 ug/l	2494120	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	43
3		Pentane	72	C5H12	000109-66-0	28
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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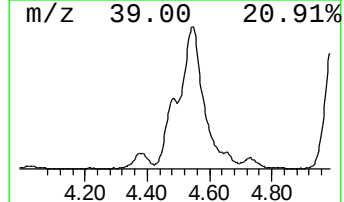
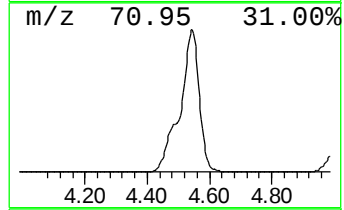
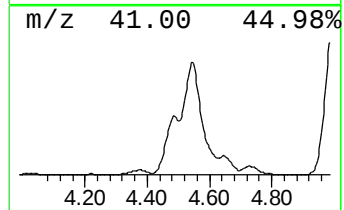
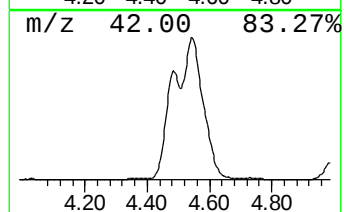
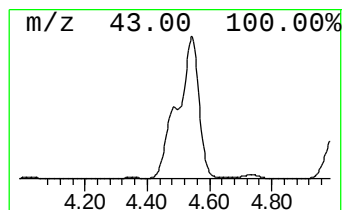
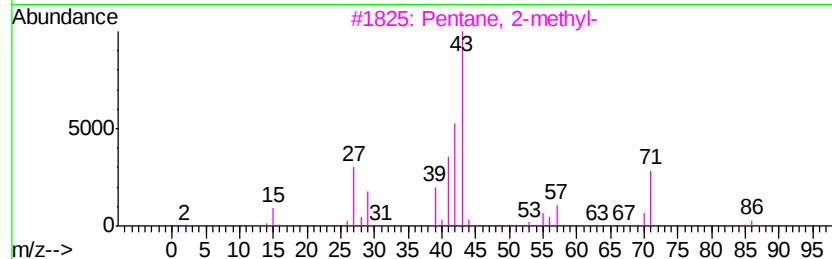
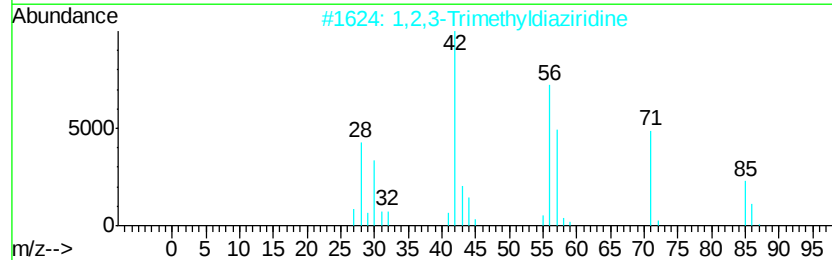
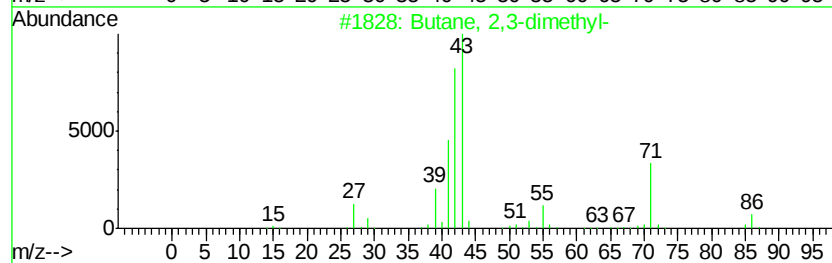
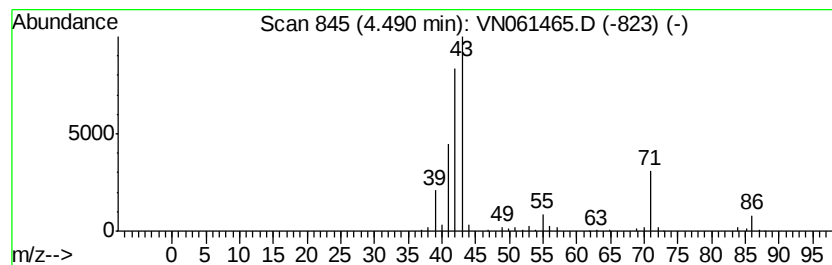
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Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	16.27 ug/l	686912	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	38
3		Pentane, 2-methyl-	86	C6H14	000107-83-5	28
4		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	14
5		C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	12



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Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 45 Sample Multiplier: 1

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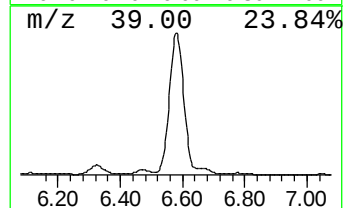
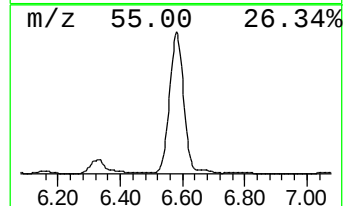
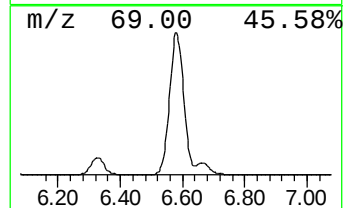
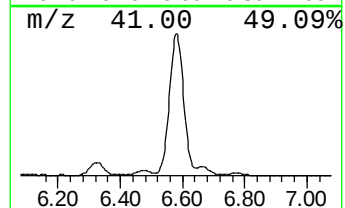
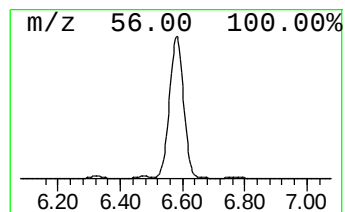
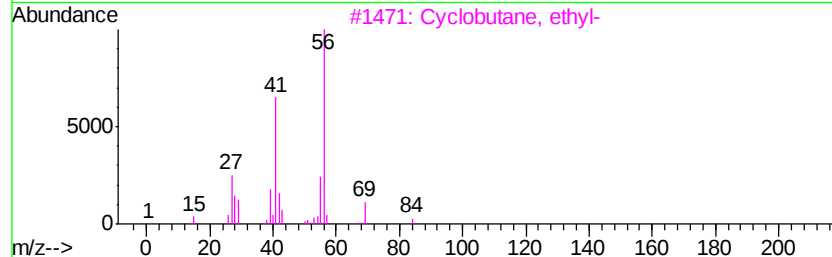
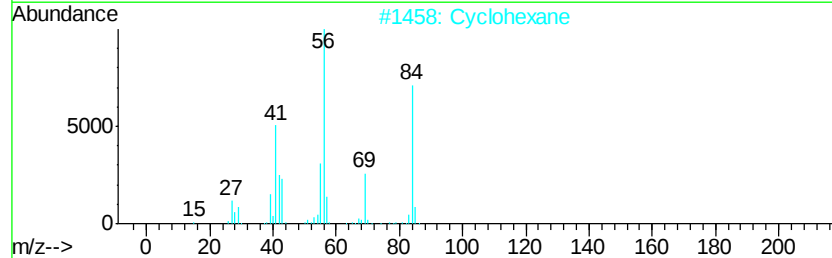
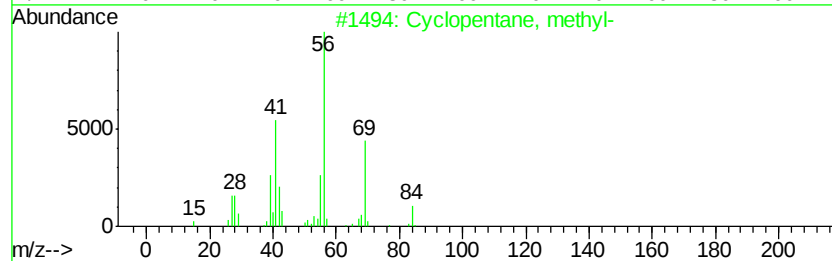
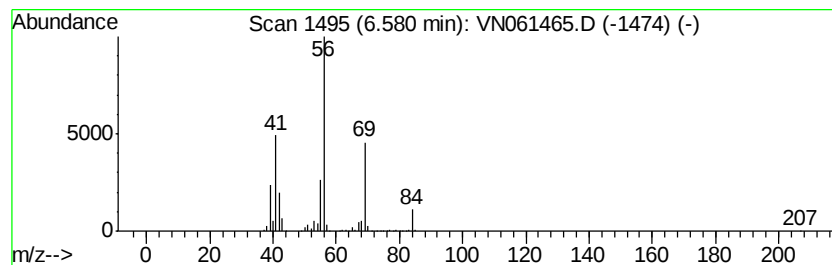
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	68.24 ug/l	2881340	Pentafluorobenzene	7.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclohexane	84	C6H12	000110-82-7	78
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



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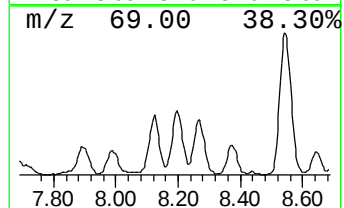
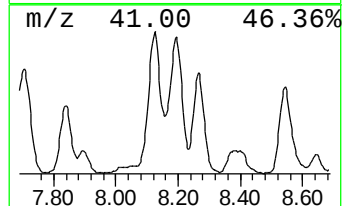
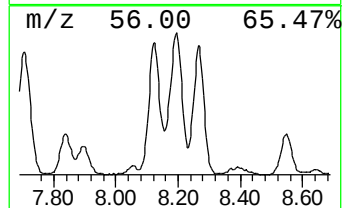
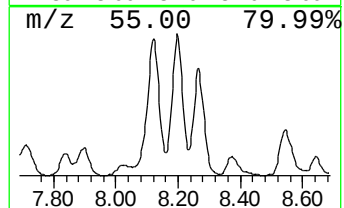
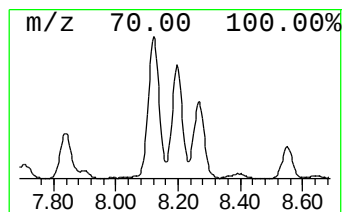
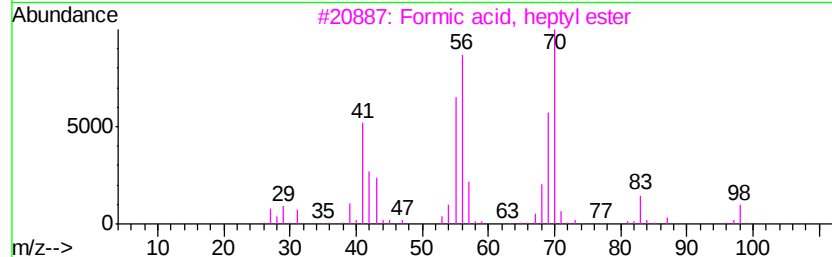
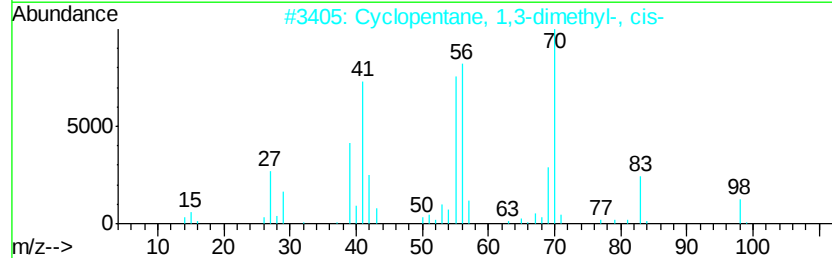
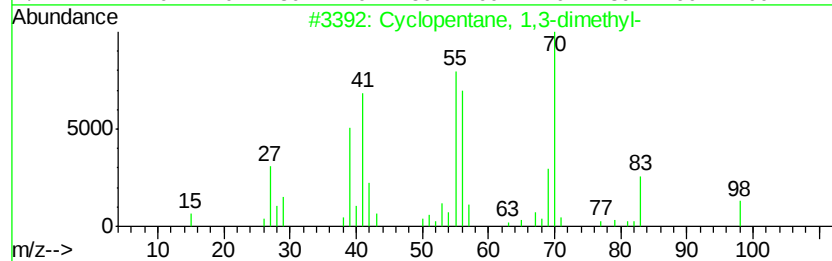
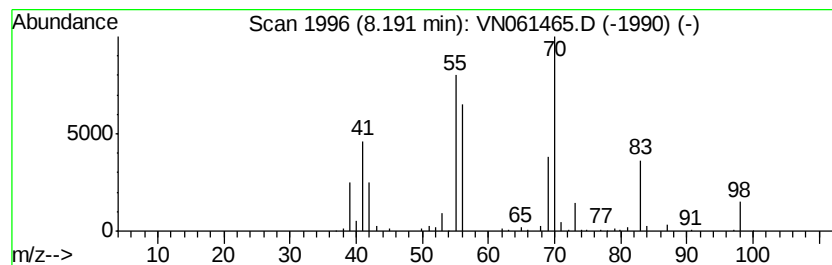
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.19	18.33 ug/l	590282	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	80
2		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	52
3		Formic acid, heptyl ester	144	C8H16O2	000112-23-2	50
4		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	50
5		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	46



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ClientSampled :
MW-3

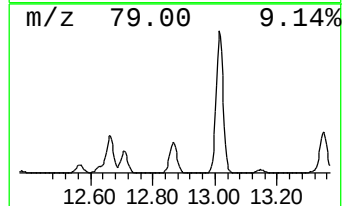
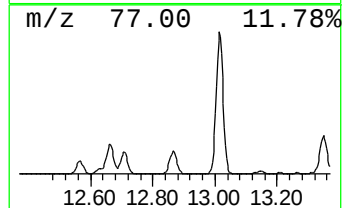
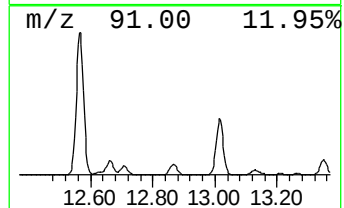
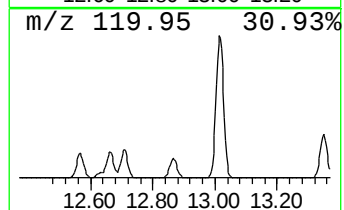
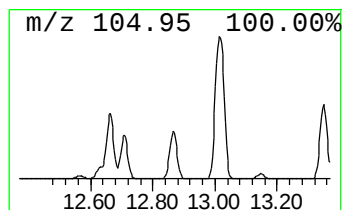
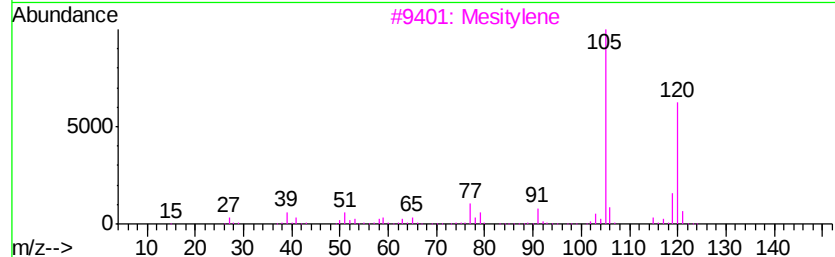
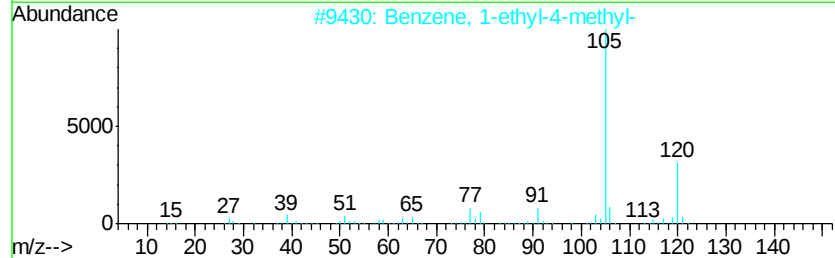
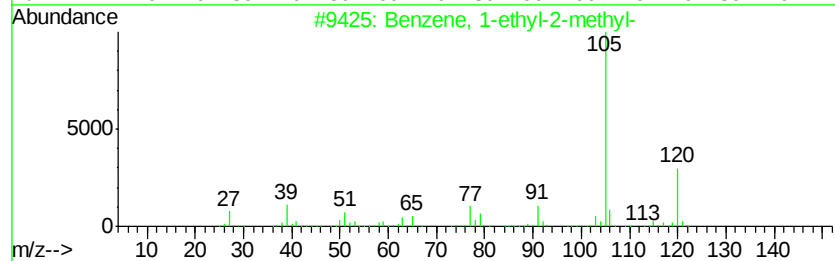
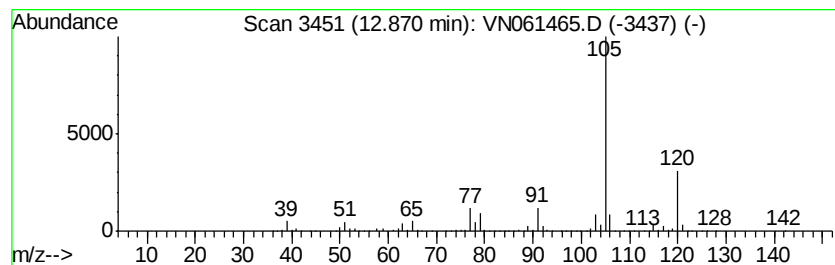
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	23.86 ug/l	4341720	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051820\
Data File : VN061465.D
Acq On : 19 May 2020 7:19
Operator : JC/MD
Sample : L2645-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

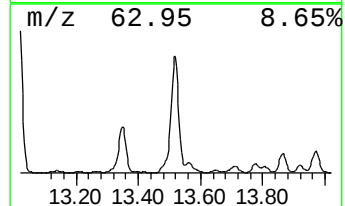
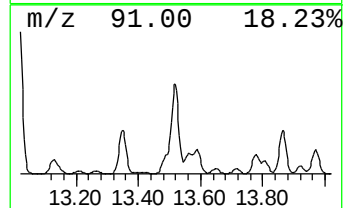
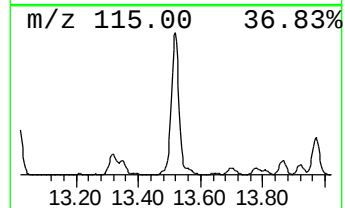
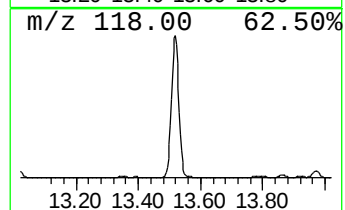
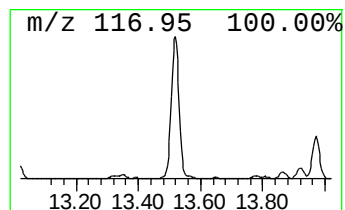
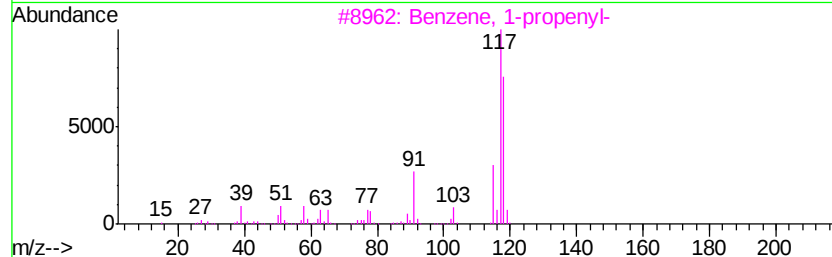
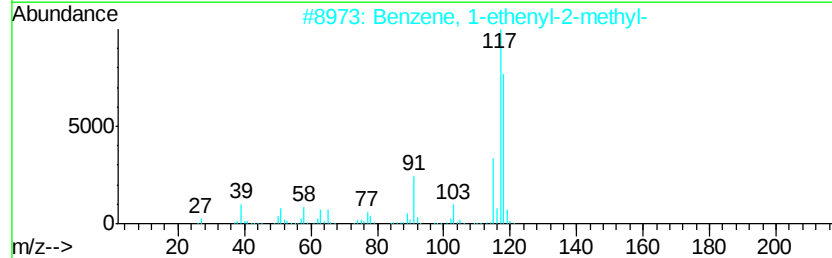
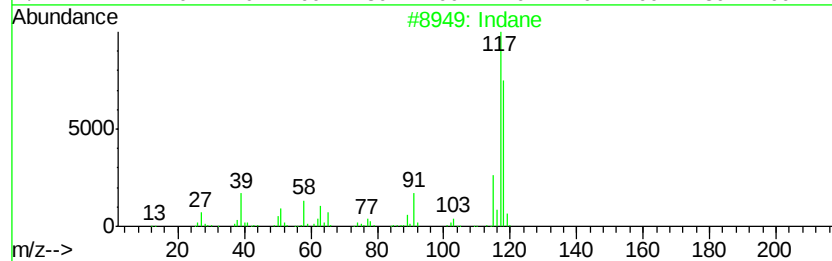
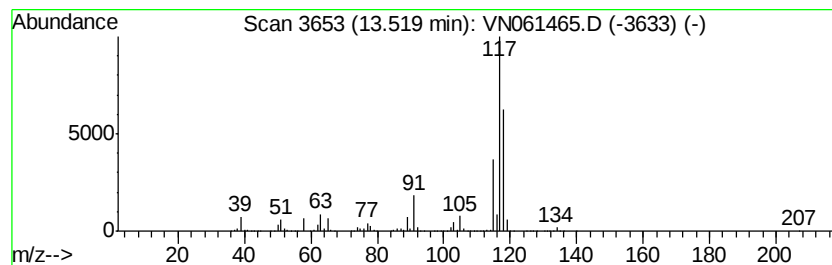
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	70.33 ug/l	12801000	1,4-Dichlorobenzene-d4	13.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	91
2	Benzene, 1-ethenyl-2-methyl-		118	C9H10	000611-15-4	81
3	Benzene, 1-propenyl-		118	C9H10	000637-50-3	74
4	Benzene, cyclopropyl-		118	C9H10	000873-49-4	74
5	Benzene, 2-propenyl-		118	C9H10	000300-57-2	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051820\
Data File : VN061465.D
Acq On : 19 May 2020 7:19
Operator : JC/MD
Sample : L2645-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
MW-3

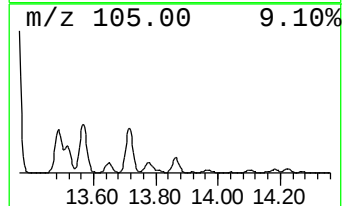
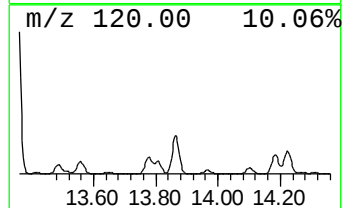
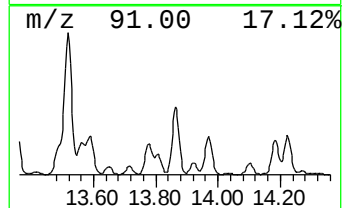
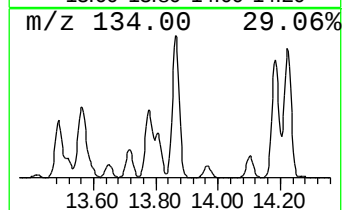
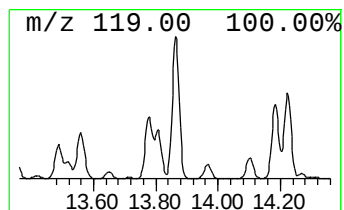
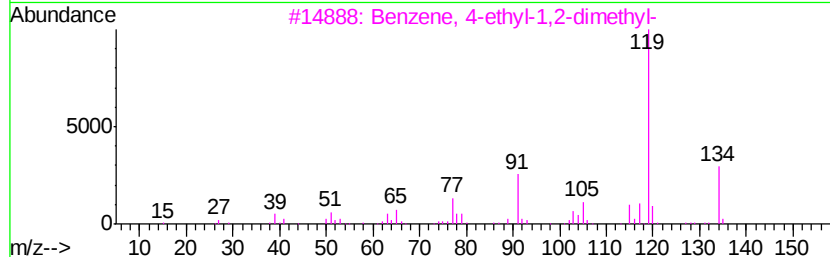
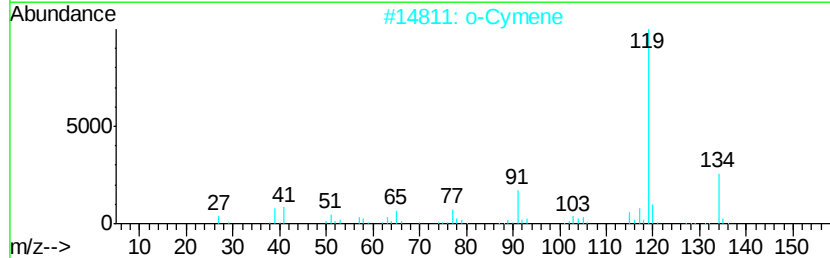
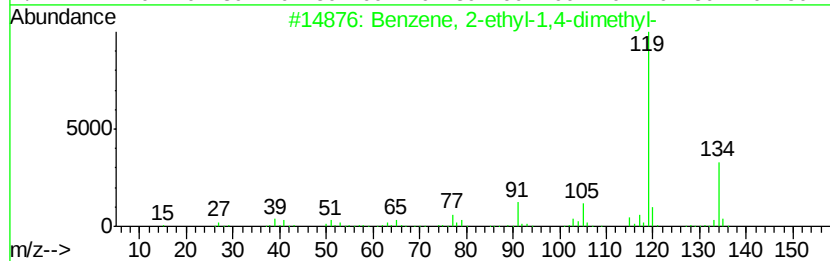
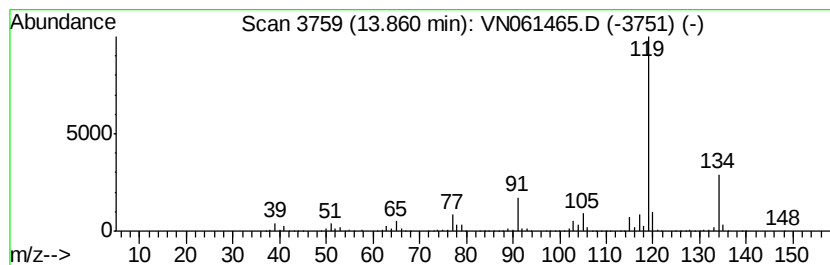
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	21.56 ug/l	3923920	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2		o-Cymene	134	C10H14	000527-84-4	95
3		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051820\
Data File : VN061465.D
Acq On : 19 May 2020 7:19
Operator : JC/MD
Sample : L2645-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
MW-3

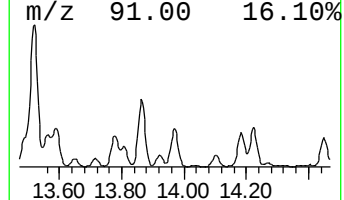
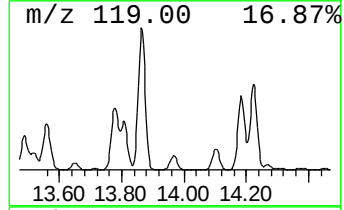
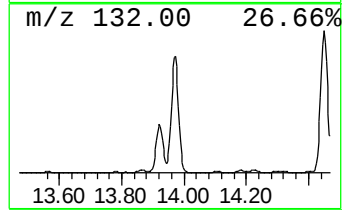
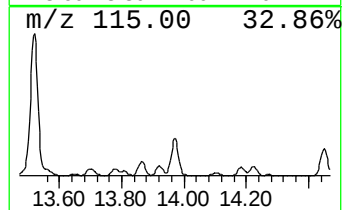
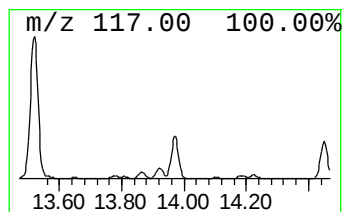
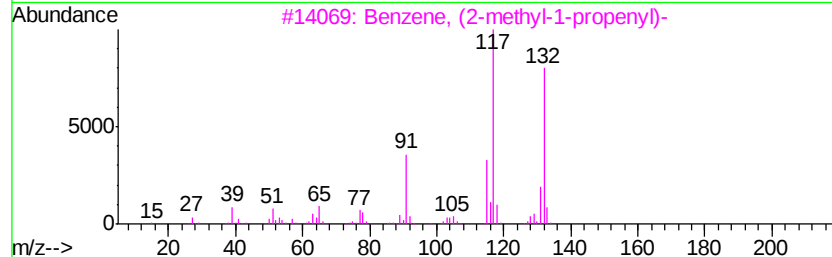
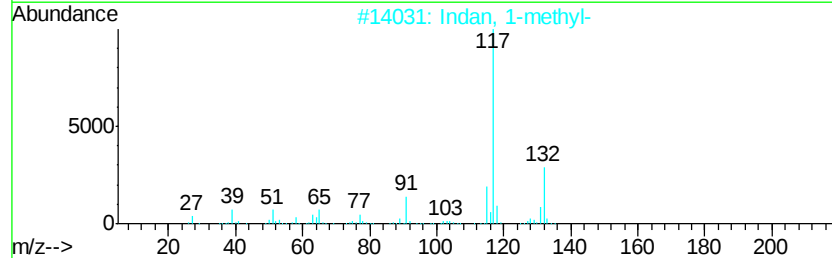
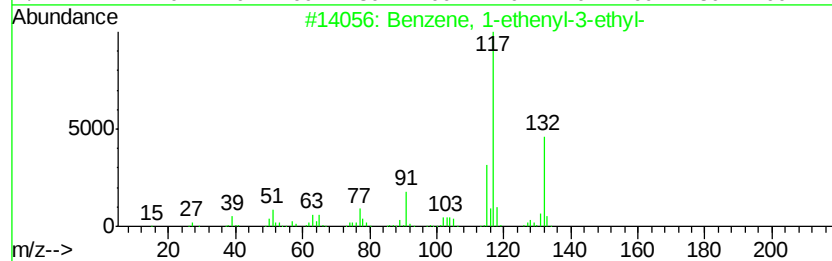
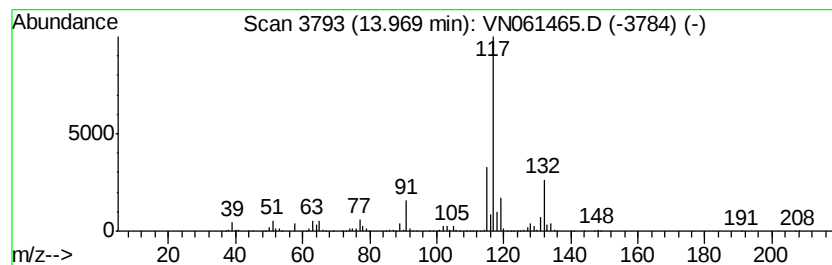
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	16.28 ug/l	2962930	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2		Indan, 1-methyl-	132	C10H12	000767-58-8	81
3		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051820\
Data File : VN061465.D
Acq On : 19 May 2020 7:19
Operator : JC/MD
Sample : L2645-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

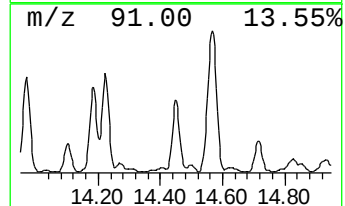
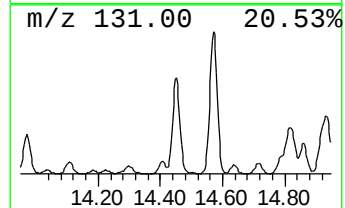
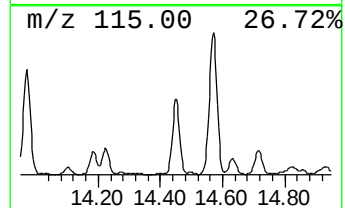
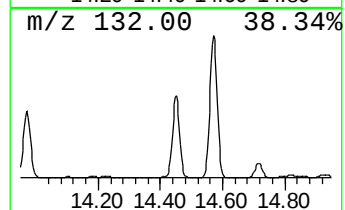
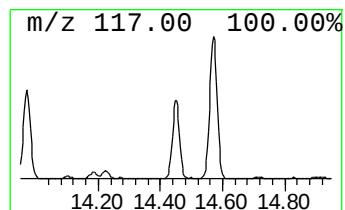
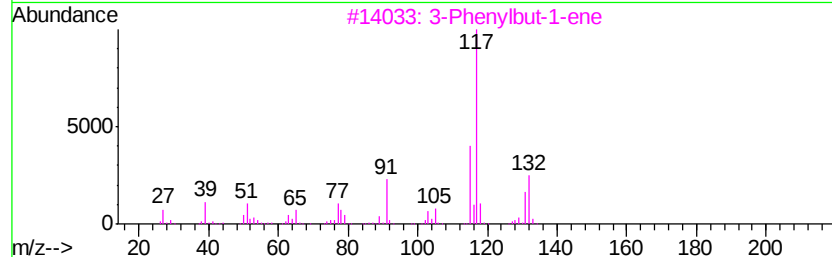
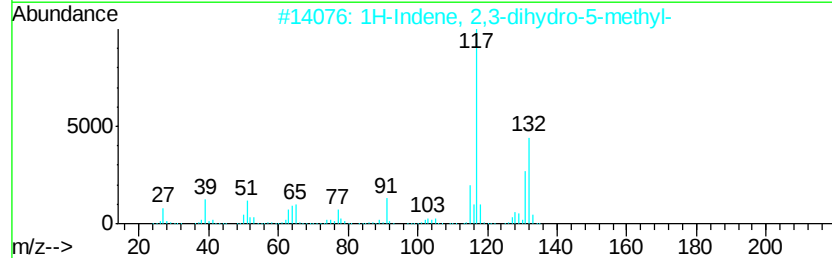
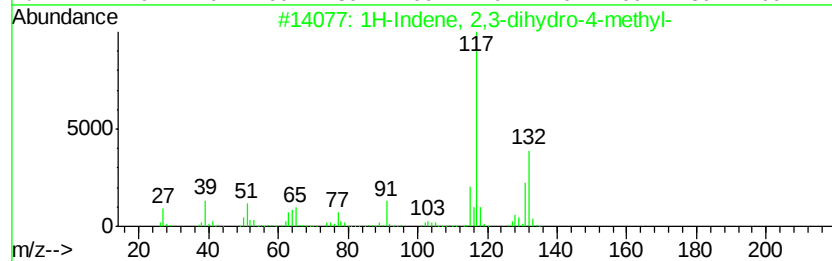
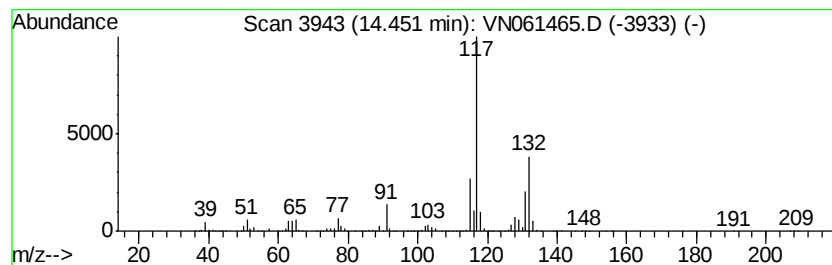
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	14.05 ug/l	2556850	1,4-Dichlorobenzene-d4	13.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4		1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5		Indan, 1-methyl-	132	C10H12	000767-58-8	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051820\
Data File : VN061465.D
Acq On : 19 May 2020 7:19
Operator : JC/MD
Sample : L2645-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

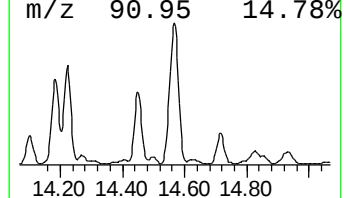
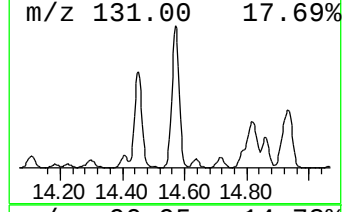
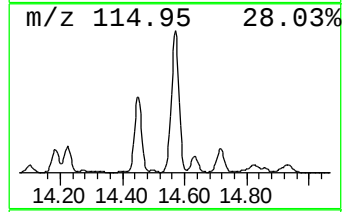
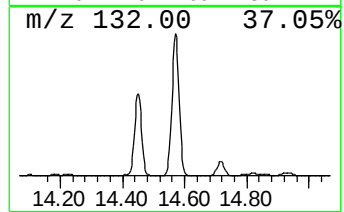
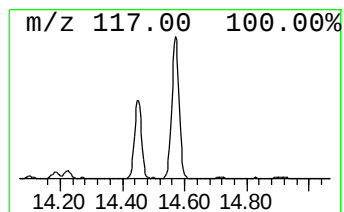
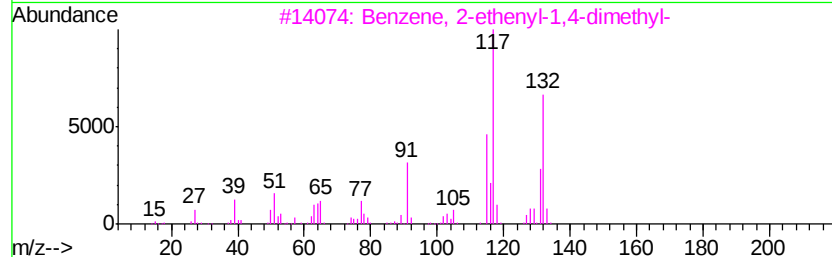
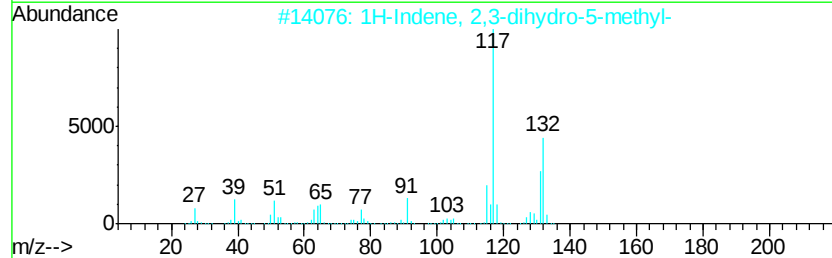
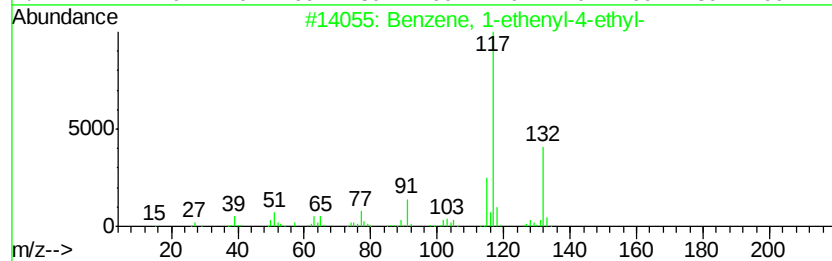
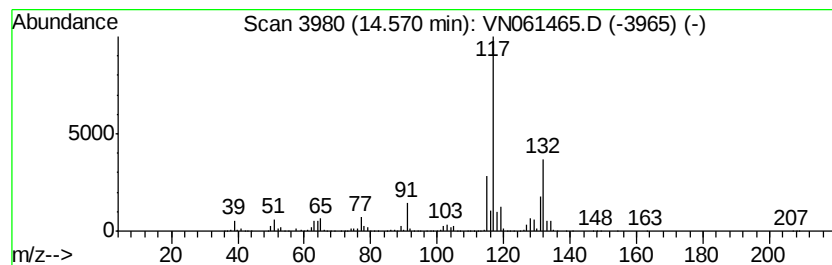
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	33.55 ug/l	6106870	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN051820\
 Data File : VN061465.D
 Acq On : 19 May 2020 7:19
 Operator : JC/MD
 Sample : L2645-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N051820W.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
Butane, 2-methyl-	2.77	59.1	ug/l	2494120	1	7.63	2111220	50.0
Butane, 2,3-dimet...	4.49	16.3	ug/l	686912	1	7.63	2111220	50.0
Cyclopentane, met...	6.58	68.2	ug/l	2881340	1	7.63	2111220	50.0
Cyclopentane, 1,3...	8.19	18.3	ug/l	590282	2	8.55	1610310	50.0
Benzene, 1-ethyl-...	12.87	23.9	ug/l	4341720	4	13.32	9100150	50.0
Indane	13.52	70.3	ug/l	12801000	4	13.32	9100150	50.0
Benzene, 2-ethyl-...	13.86	21.6	ug/l	3923920	4	13.32	9100150	50.0
Benzene, 1-etheny...	13.97	16.3	ug/l	2962930	4	13.32	9100150	50.0
1H-Indene, 2,3-di...	14.45	14.1	ug/l	2556850	4	13.32	9100150	50.0
Benzene, 1-etheny...	14.57	33.5	ug/l	6106870	4	13.32	9100150	50.0