

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100720\
 Data File : VN063948.D
 Acq On : 7 Oct 2020 17:19
 Operator : JC/MD
 Sample : L4250-02
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-06

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\82N093020W.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	4.020	697	709	720	rBV3	7875	18150	1.13%	0.096%
2	4.489	834	855	869	rBV5	20513	75663	4.71%	0.400%
3	5.007	990	1016	1036	rBV5	14907	53516	3.33%	0.283%
4	6.479	1451	1474	1491	rBV3	32331	109779	6.84%	0.580%
5	6.579	1492	1505	1526	rVB6	28095	85047	5.30%	0.449%
6	7.347	1728	1744	1762	rVB7	9706	29505	1.84%	0.156%
7	7.550	1785	1807	1818	rBV	202578	511782	31.87%	2.703%
8	7.627	1819	1831	1844	rVV	339319	826653	51.48%	4.367%
9	7.708	1844	1856	1874	rVB	149611	385931	24.03%	2.039%
10	7.836	1883	1896	1909	rBV6	10305	26802	1.67%	0.142%
11	7.990	1925	1944	1966	rBV3	262180	662564	41.26%	3.500%
12	8.174	1970	2001	2021	rVV	520861	1366652	85.10%	7.219%
13	8.264	2022	2029	2047	rVB7	11845	29248	1.82%	0.154%
14	8.550	2101	2118	2137	rBV	547665	1158959	72.17%	6.122%
15	8.791	2181	2193	2201	rBV10	7666	16752	1.04%	0.088%
16	9.019	2247	2264	2266	rBV4	28090	53083	3.31%	0.280%
17	9.055	2267	2275	2284	rVV3	74359	148255	9.23%	0.783%
18	9.109	2284	2292	2304	rVB3	70565	131770	8.21%	0.696%
19	9.190	2304	2317	2327	rBV3	35317	71027	4.42%	0.375%
20	9.328	2357	2360	2372	rVB5	11959	19019	1.18%	0.100%
21	9.489	2396	2410	2429	rVB	390227	783876	48.81%	4.141%
22	9.621	2429	2451	2469	rBV2	483066	1071088	66.70%	5.658%
23	9.730	2478	2485	2496	rVB6	12401	23526	1.46%	0.124%
24	9.817	2497	2512	2524	rBV6	28745	77171	4.81%	0.408%
25	9.994	2555	2567	2576	rVV	88292	160651	10.00%	0.849%
26	10.061	2576	2588	2605	rVB	880773	1605921	100.00%	8.483%
27	10.251	2632	2647	2667	rVB	11817	43785	2.73%	0.231%
28	10.492	2714	2722	2746	rVV10	31763	94361	5.88%	0.498%
29	10.598	2748	2755	2766	rVB7	9743	17024	1.06%	0.090%
30	10.691	2774	2784	2793	rBV6	9080	16588	1.03%	0.088%
31	10.794	2810	2816	2830	rVB2	15460	30870	1.92%	0.163%
32	10.894	2838	2847	2863	rVB10	11663	21603	1.35%	0.114%
33	10.974	2863	2872	2883	rVB10	8109	16890	1.05%	0.089%
34	11.277	2955	2966	2972	rBV5	15717	31213	1.94%	0.165%

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35	11.379	2985	2998	3016	rBV	876951	1557555	96.99%	8.228%
36	12.225	3249	3261	3275	rBV	255377	415871	25.90%	2.197%
37	12.376	3293	3308	3327	rBV	714602	1232279	76.73%	6.509%
38	12.566	3356	3367	3383	rVB	519456	837741	52.17%	4.425%
39	12.868	3451	3461	3470	rVV2	21550	34737	2.16%	0.183%
40	13.013	3498	3506	3520	rVB3	13241	21925	1.37%	0.116%
41	13.135	3532	3544	3565	rBV4	63574	162867	10.14%	0.860%
42	13.318	3588	3601	3621	rBV	795448	1382945	86.12%	7.305%
43	13.418	3626	3632	3640	rVV3	12024	20378	1.27%	0.108%
44	13.489	3640	3654	3656	rVV2	174945	231201	14.40%	1.221%
45	13.518	3657	3663	3673	rVV	475365	790593	49.23%	4.176%
46	13.569	3673	3679	3694	rVV2	88625	159892	9.96%	0.845%
47	13.649	3694	3704	3714	rVB	53772	84007	5.23%	0.444%
48	13.788	3737	3747	3758	rBV4	25480	44316	2.76%	0.234%
49	13.865	3758	3771	3781	rBV	278555	438447	27.30%	2.316%
50	13.923	3781	3789	3794	rVV3	24836	39541	2.46%	0.209%
51	13.971	3794	3804	3818	rVV2	195153	333284	20.75%	1.761%
52	14.042	3818	3826	3835	rVB8	13629	23533	1.47%	0.124%
53	14.183	3853	3870	3884	rBV	181527	317129	19.75%	1.675%
54	14.267	3888	3896	3905	rBV3	27810	46806	2.91%	0.247%
55	14.341	3913	3919	3926	rBV5	19275	30028	1.87%	0.159%
56	14.453	3944	3954	3963	rBV3	57074	97915	6.10%	0.517%
57	14.501	3963	3969	3976	rVB4	14377	19919	1.24%	0.105%
58	14.566	3976	3989	4000	rBV5	74600	160293	9.98%	0.847%
59	14.627	4000	4008	4019	rBV3	33537	57416	3.58%	0.303%
60	14.826	4061	4070	4080	rBV4	48026	74296	4.63%	0.392%
61	14.926	4092	4101	4116	rVB6	42715	88342	5.50%	0.467%
62	15.106	4143	4157	4170	rBV	173778	311897	19.42%	1.648%
63	15.382	4236	4243	4255	rBV5	13133	26363	1.64%	0.139%
64	15.662	4320	4330	4343	rBV2	23942	44948	2.80%	0.237%
65	15.730	4343	4351	4360	rVB2	10712	18672	1.16%	0.099%
66	16.315	4522	4533	4547	rVB3	23789	51018	3.18%	0.269%

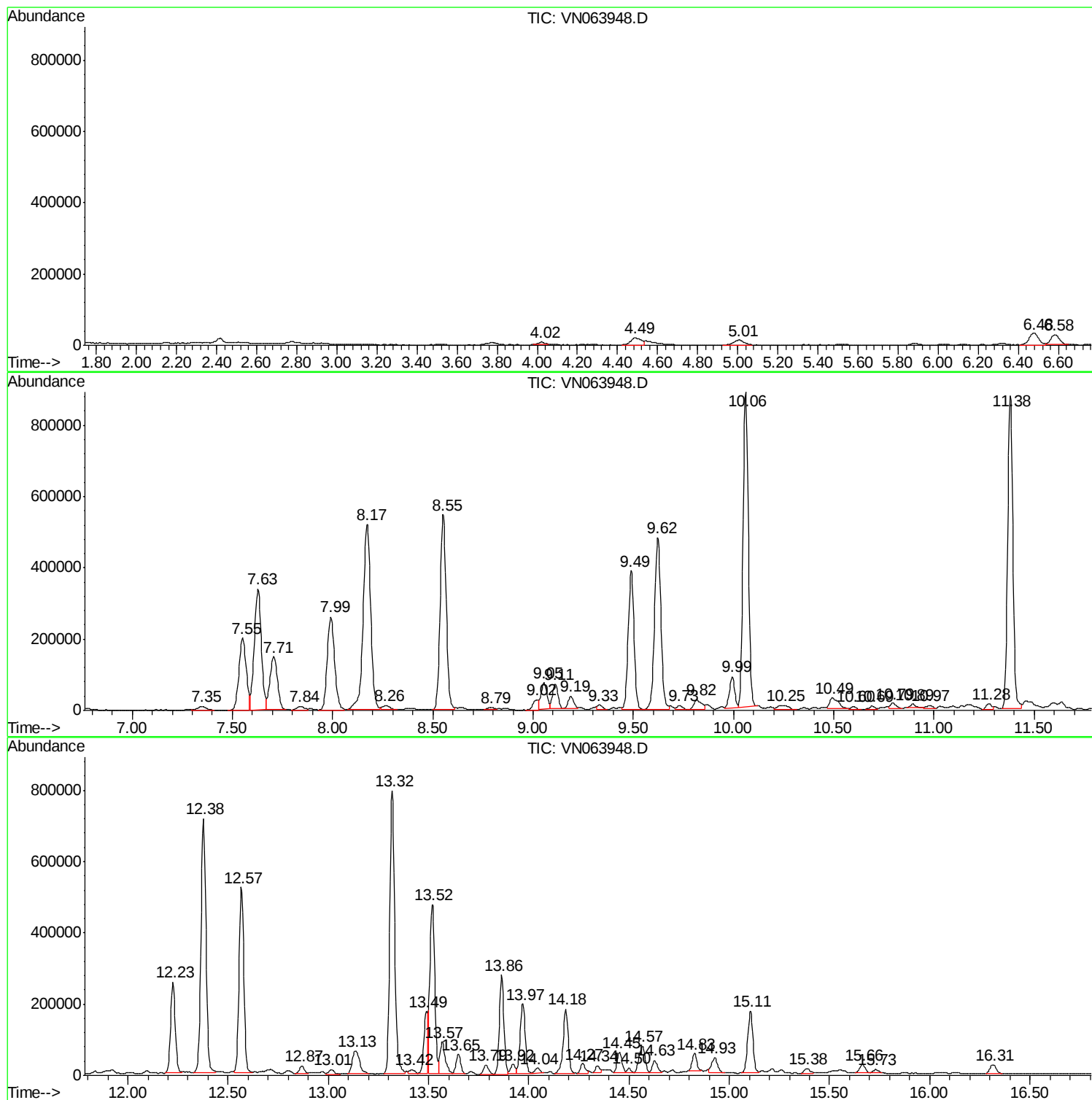
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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



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Instrument :
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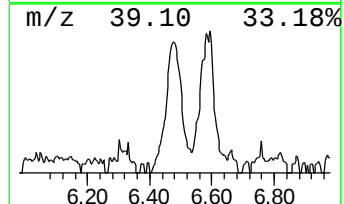
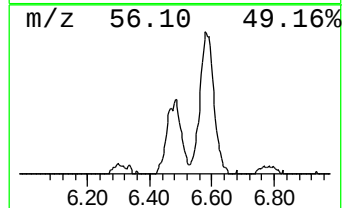
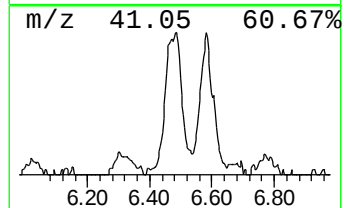
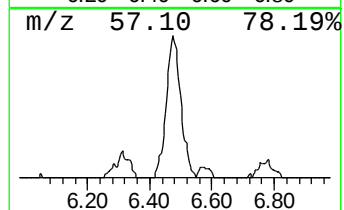
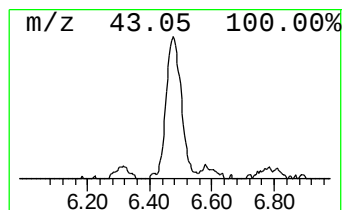
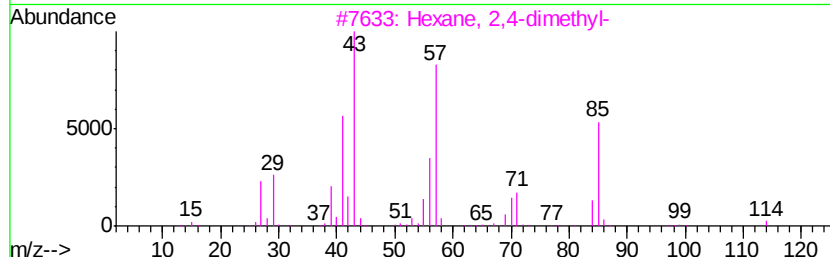
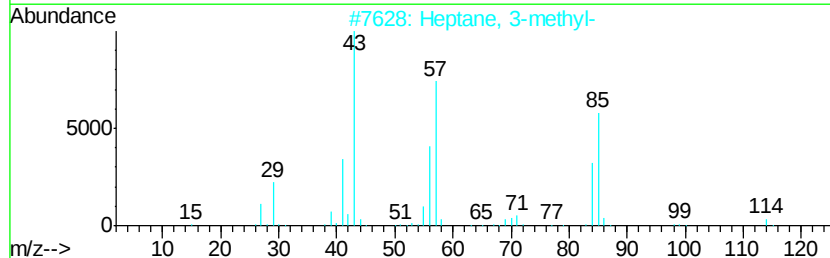
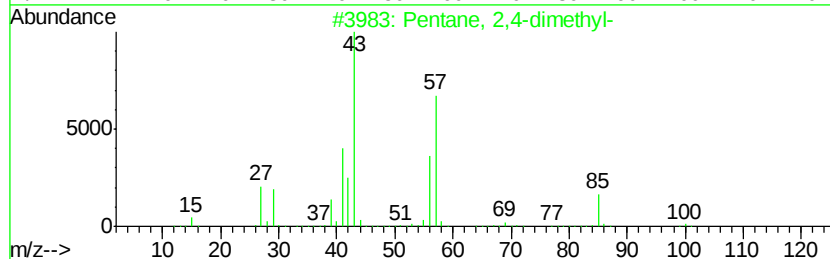
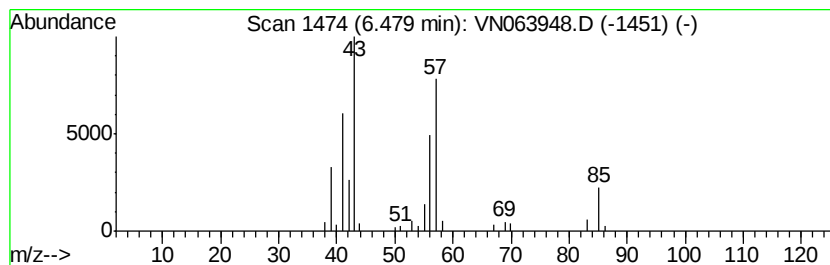
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	6.64 ug/l	109779	Pentafluorobenzene	7.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	78
2			Heptane, 3-methyl-	114	C8H18	000589-81-1	72
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	56
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	43
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	42



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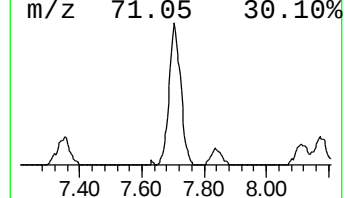
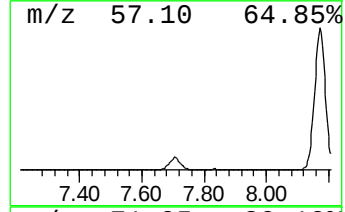
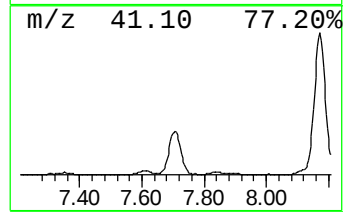
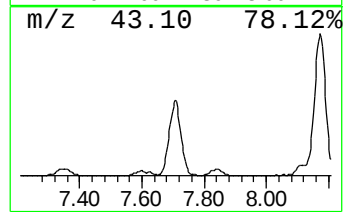
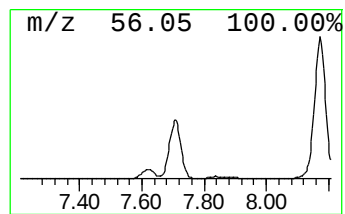
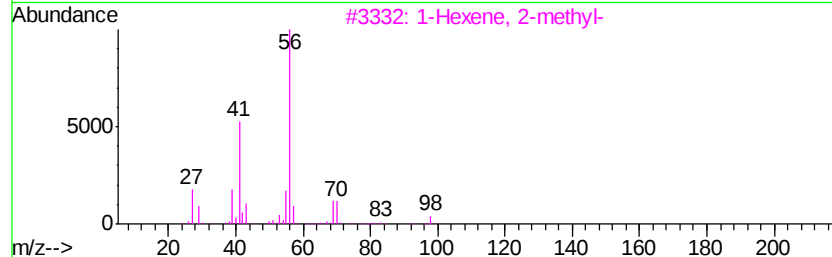
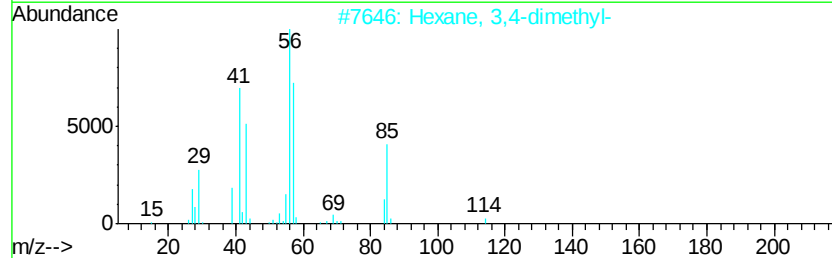
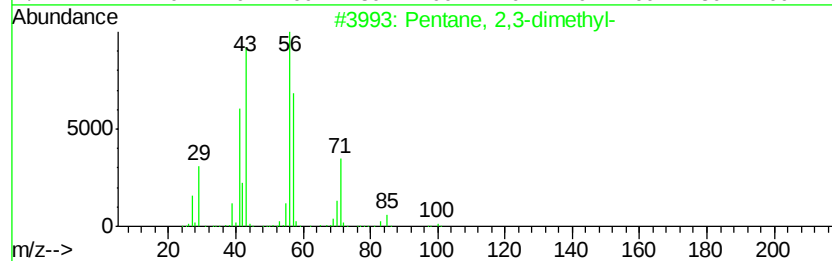
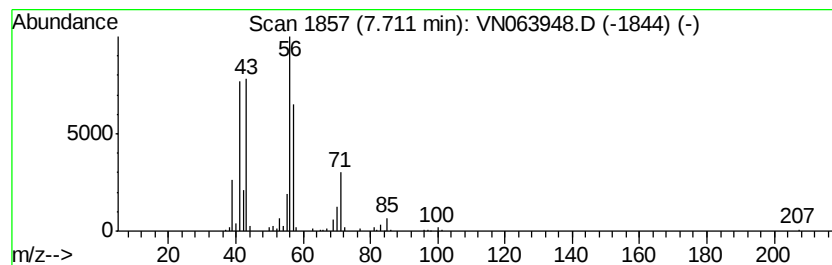
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	23.34 ug/l	385931	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	53
3		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
4		Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	40
5		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38



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ALS Vial : 19 Sample Multiplier: 1

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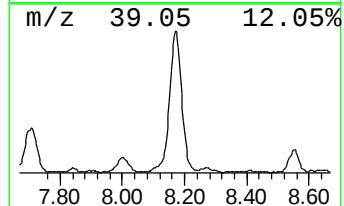
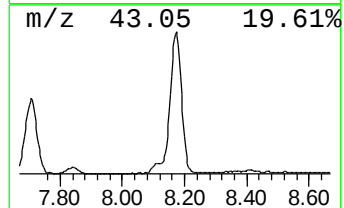
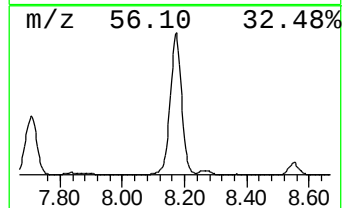
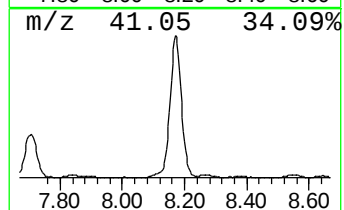
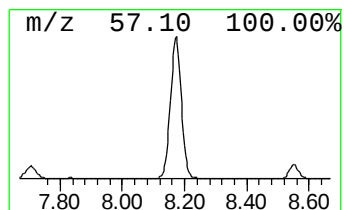
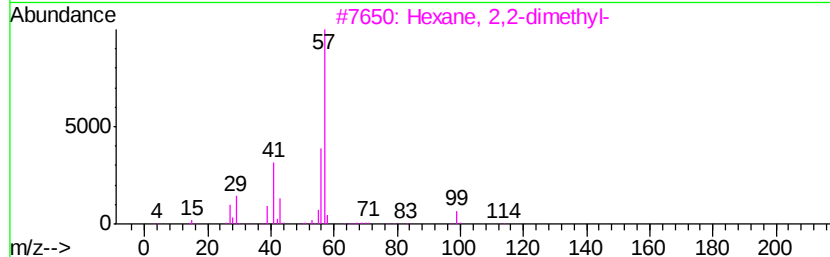
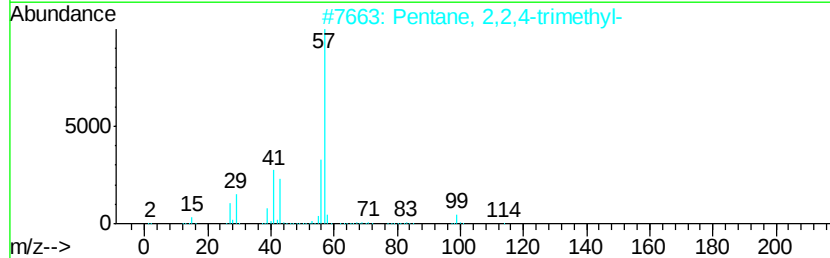
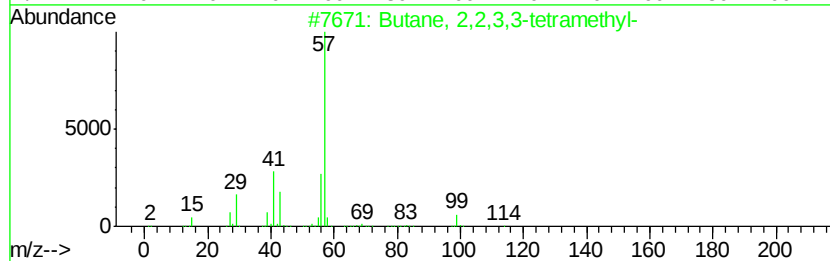
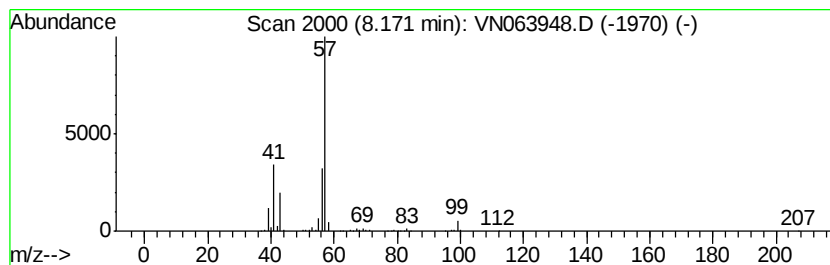
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	58.96 ug/l	1366650	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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ClientSampled :
MW-06

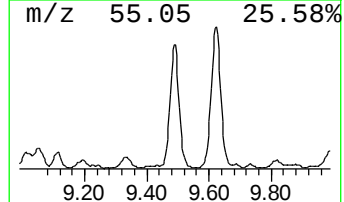
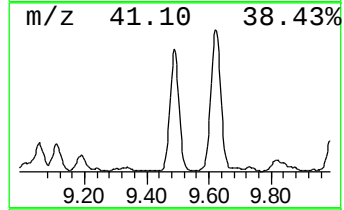
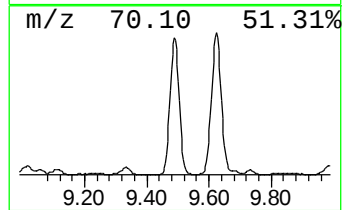
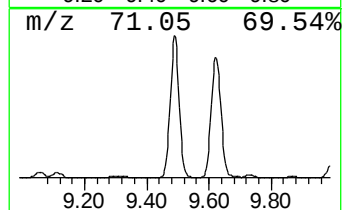
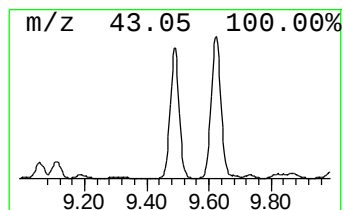
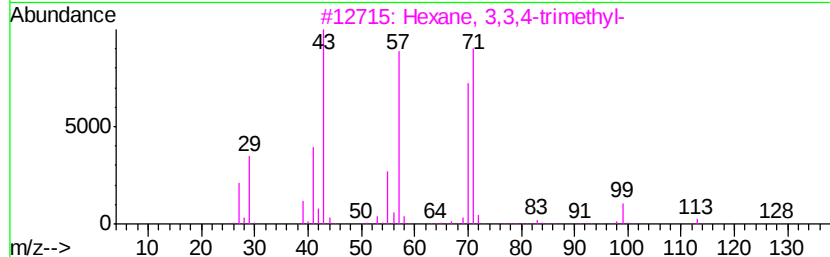
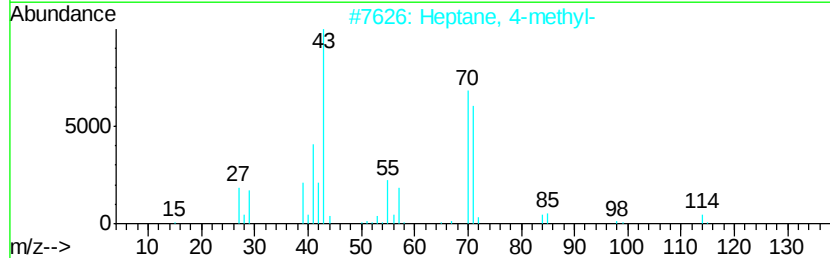
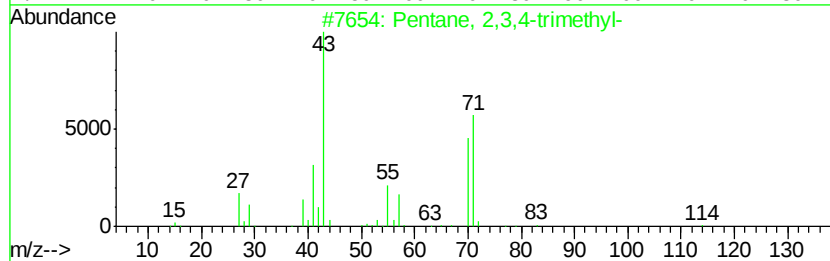
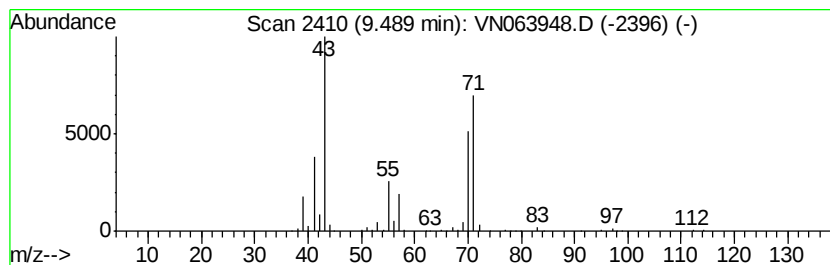
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.49	33.82 ug/l	783876	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56
4		Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	56
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-06

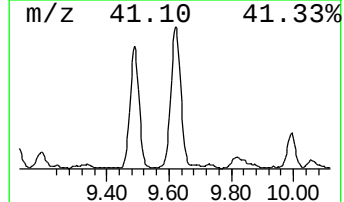
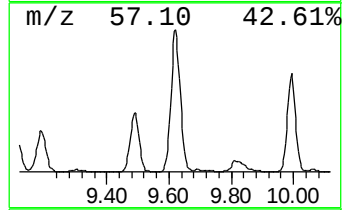
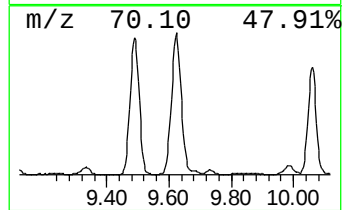
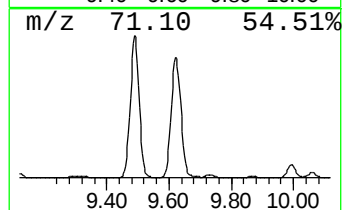
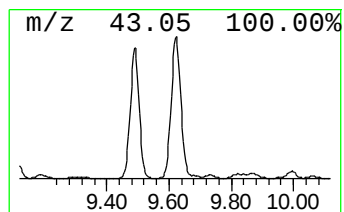
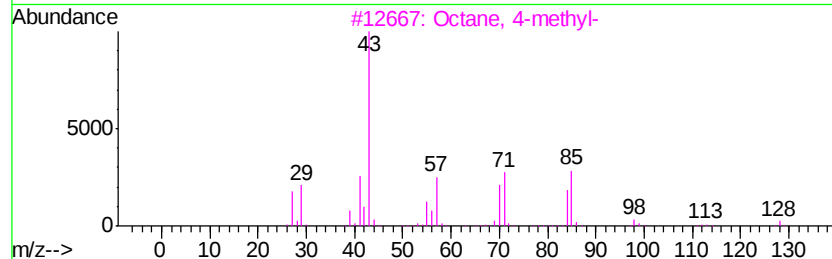
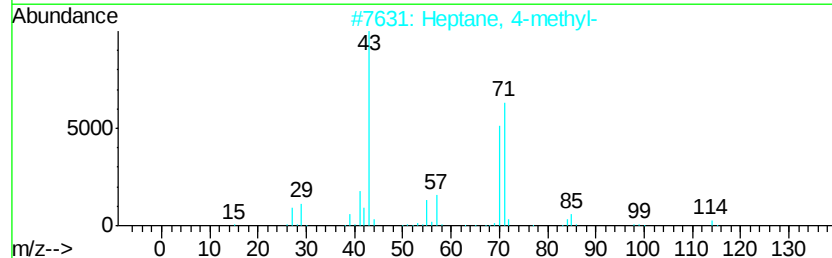
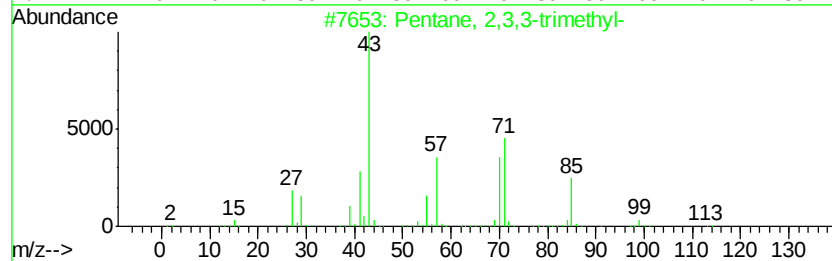
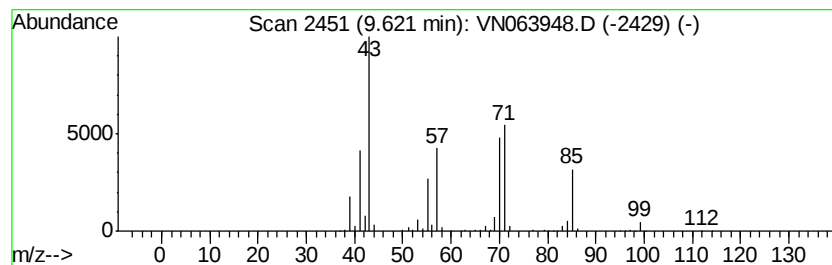
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	46.21 ug/l	1071090	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		Octane, 4-methyl-	128	C9H20	002216-34-4	64
4		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 19 Sample Multiplier: 1

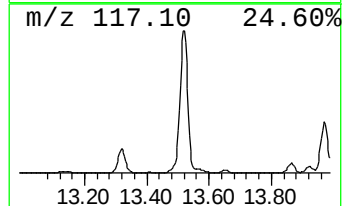
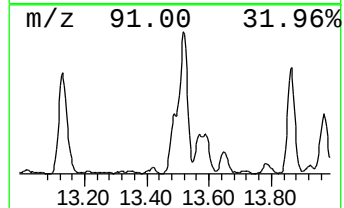
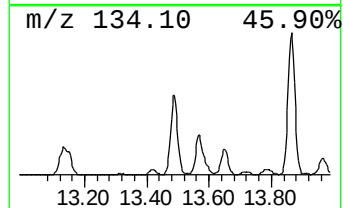
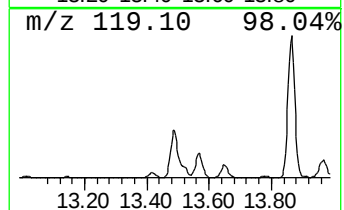
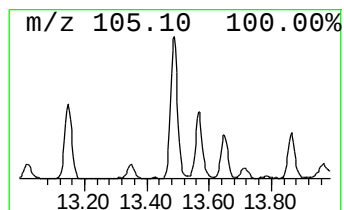
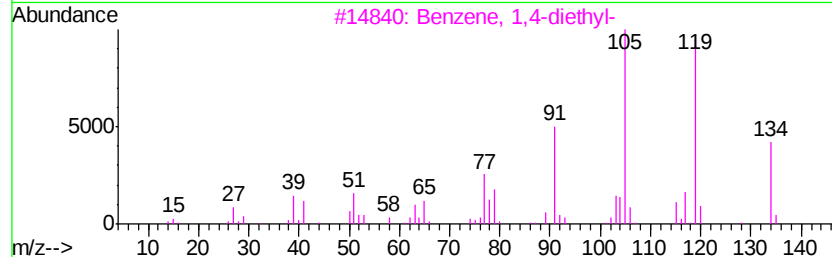
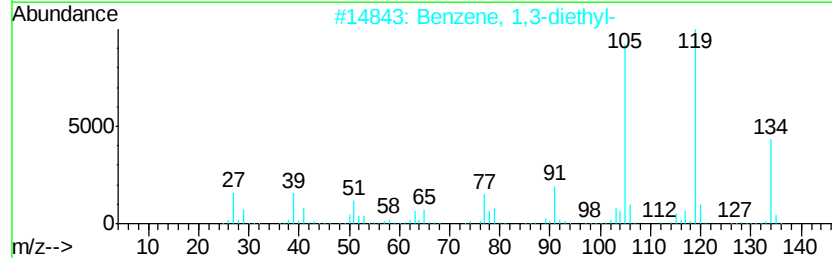
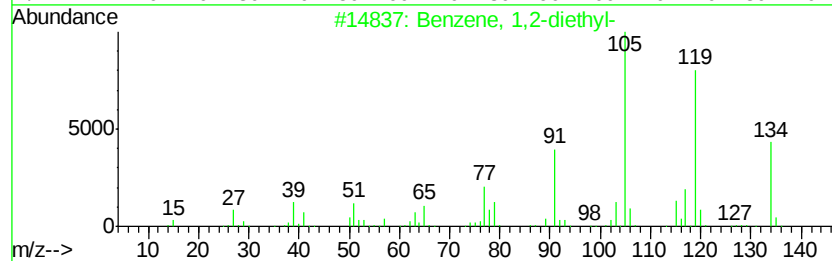
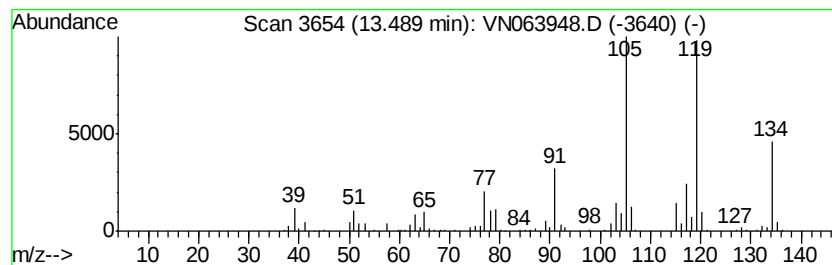
Instrument :
MSVOA_N
ClientSampleId :
MW-06

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2-diethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	8.36 ug/l	231201	1,4-Dichlorobenzene-d4	13.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1,2-diethyl-	134 C10H14	000135-01-3 95
2		Benzene, 1,3-diethyl-	134 C10H14	000141-93-5 90
3		Benzene, 1,4-diethyl-	134 C10H14	000105-05-5 90
4		Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14	000933-98-2 80
5		Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14	000934-74-7 74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-06

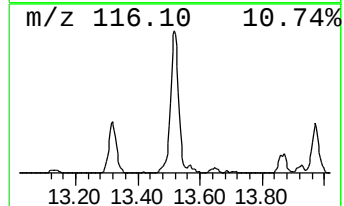
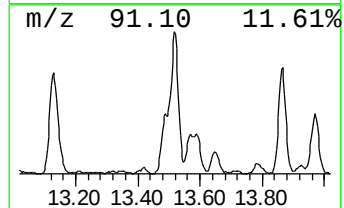
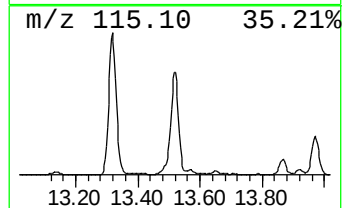
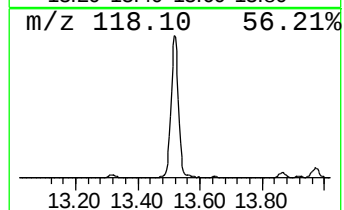
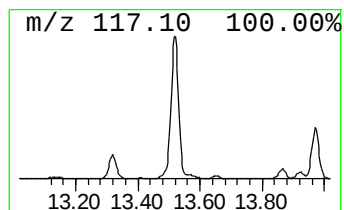
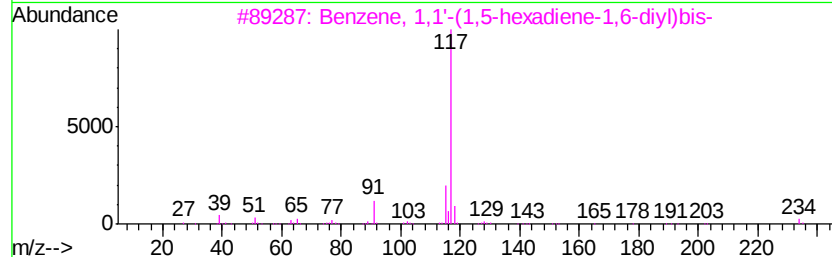
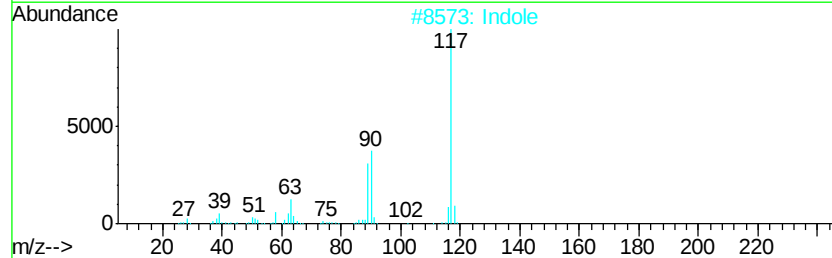
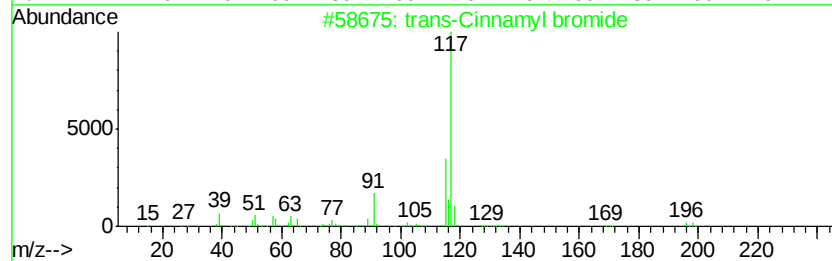
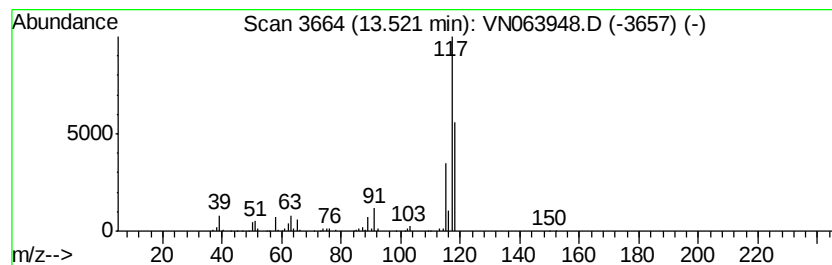
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Quant Title : SW846 8260

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

Peak Number 7 trans-Cinnamyl bromide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	28.58 ug/l	790593	1,4-Dichlorobenzene-d4	13.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
2			Indole	117	C8H7N	000120-72-9	47
3			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	45
4			Benzyl nitrile	117	C8H7N	000140-29-4	43
5			5H-1-Pyridine	117	C8H7N	000270-91-7	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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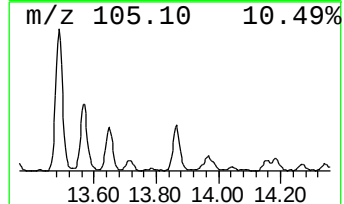
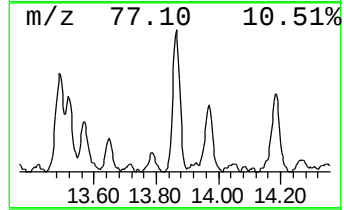
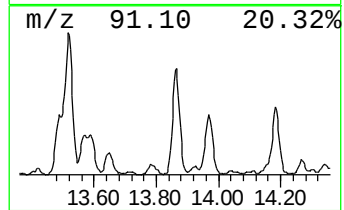
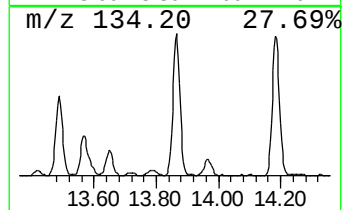
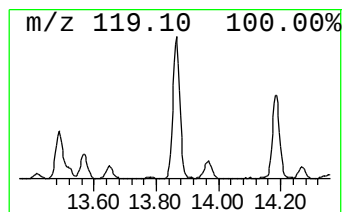
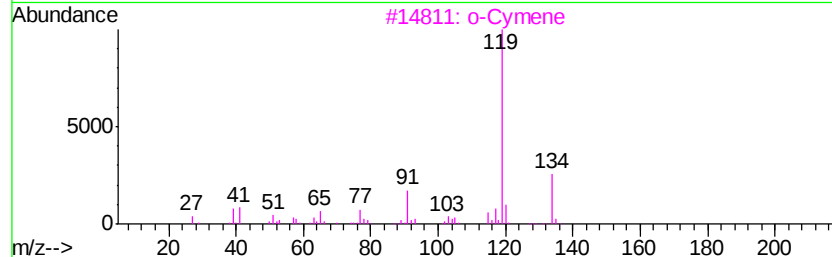
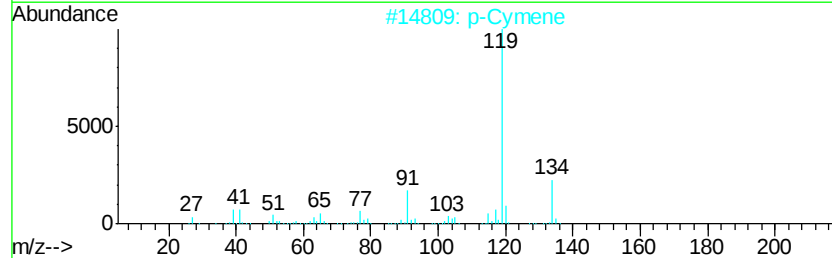
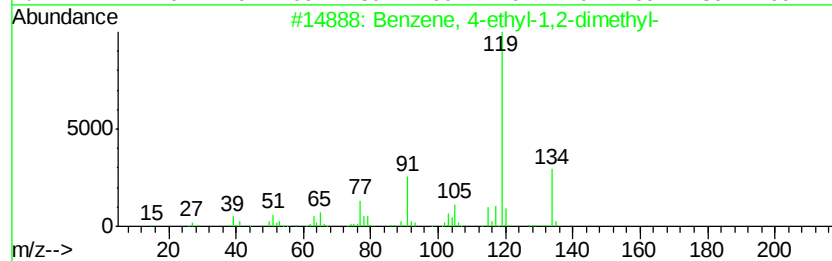
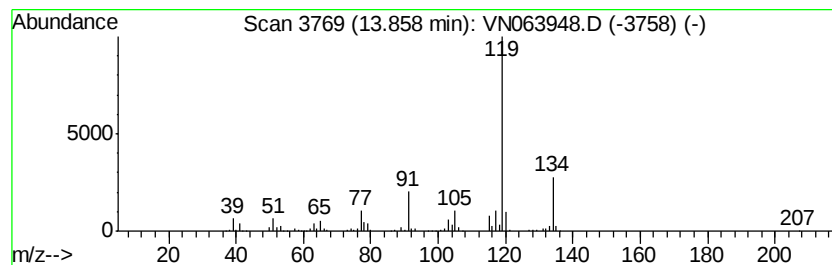
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	15.85 ug/l	438447	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2		p-Cymene	134	C10H14	000099-87-6	95
3		o-Cymene	134	C10H14	000527-84-4	95
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 19 Sample Multiplier: 1

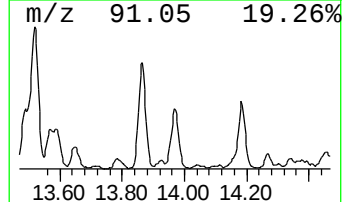
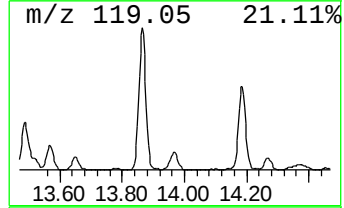
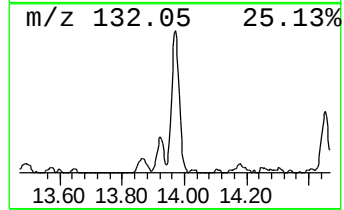
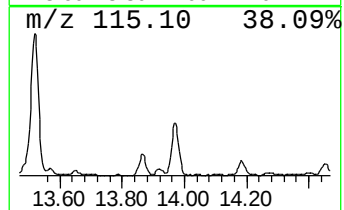
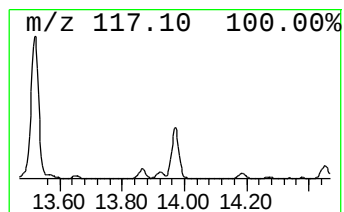
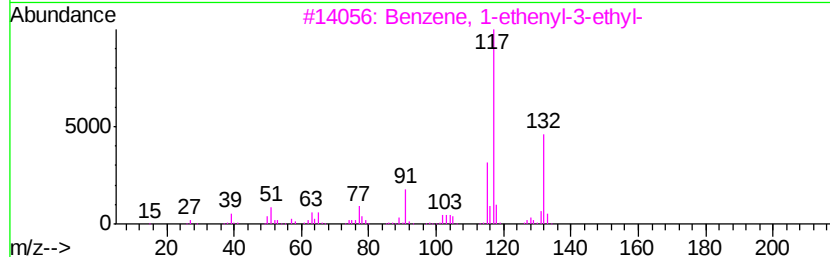
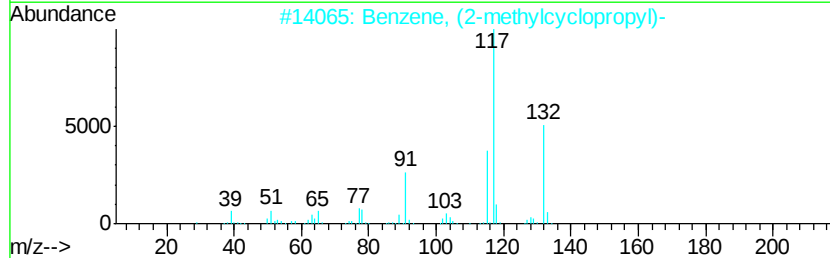
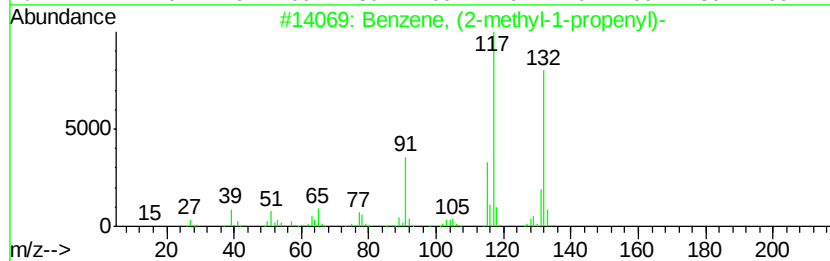
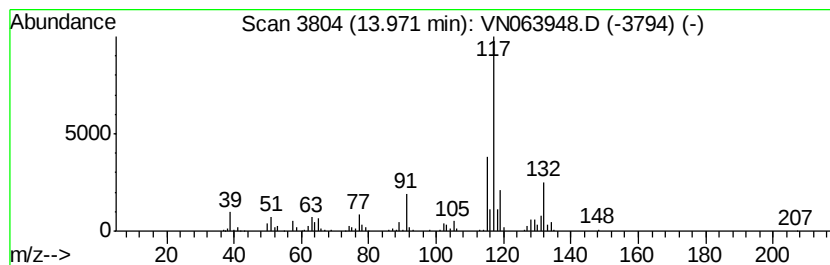
Instrument :
MSVOA_N
ClientSampled :
MW-06

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, (2-methyl-1-propen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	12.05 ug/l	333284	1,4-Dichlorobenzene-d4	13.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, (2-methyl-1-propenyl)-	132 C10H12	000768-49-0 83
2		Benzene, (2-methylcyclopropyl)-	132 C10H12	1000327-39-0 76
3		Benzene, 1-ethenyl-3-ethyl-	132 C10H12	007525-62-4 74
4		Benzene, 1-methyl-2-(2-propenyl)-	132 C10H12	001587-04-8 74
5		3-Phenylbut-1-ene	132 C10H12	000934-10-1 72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-06

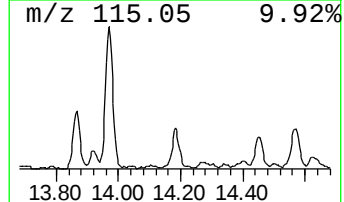
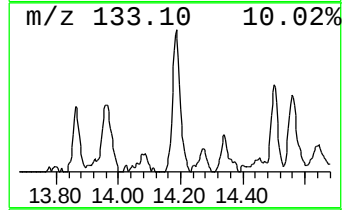
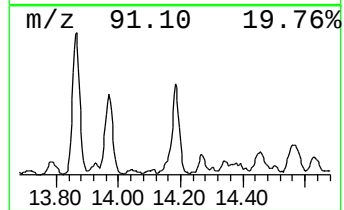
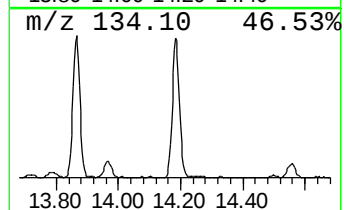
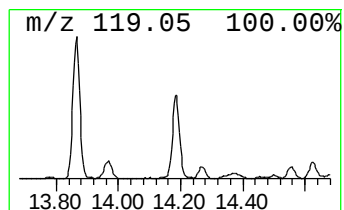
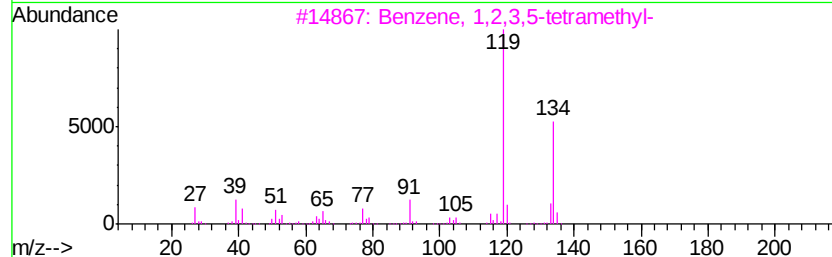
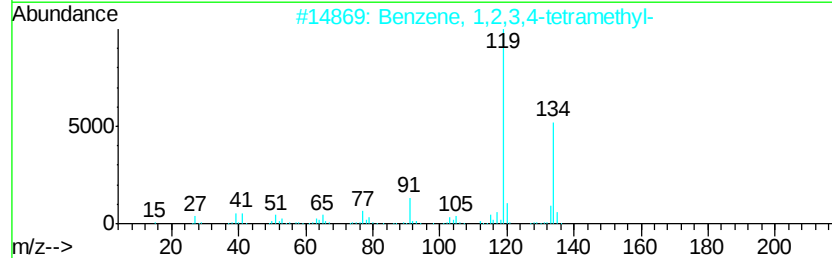
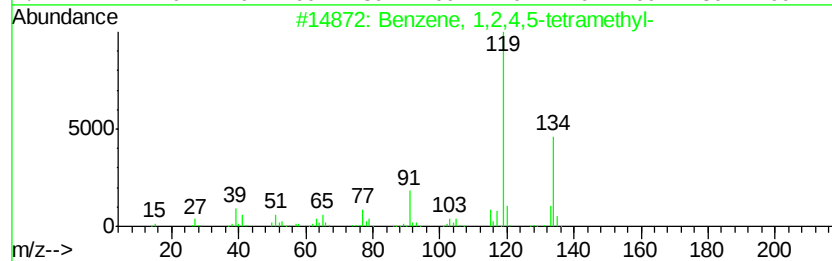
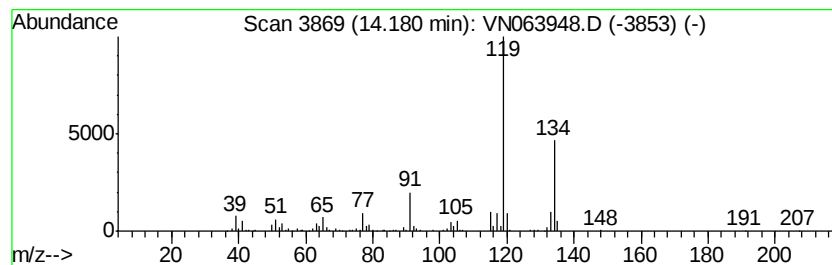
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	11.47 ug/l	317129	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	93
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100720\
Data File : VN063948.D
Acq On : 7 Oct 2020 17:19
Operator : JC/MD
Sample : L4250-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-06

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N093020W.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
Pentane, 2,4-dime...	6.48	6.6	ug/l	109779	1	7.63	826653	50.0
Pentane, 2,3-dime...	7.71	23.3	ug/l	385931	1	7.63	826653	50.0
Butane, 2,2,3,3-t...	8.17	59.0	ug/l	1366650	2	8.55	1158960	50.0
Pentane, 2,3,4-tr...	9.49	33.8	ug/l	783876	2	8.55	1158960	50.0
Pentane, 2,3,3-tr...	9.62	46.2	ug/l	1071090	2	8.55	1158960	50.0
Benzene, 1,2-diet...	13.49	8.4	ug/l	231201	4	13.32	1382950	50.0
trans-Cinnamyl br...	13.52	28.6	ug/l	790593	4	13.32	1382950	50.0
Benzene, 4-ethyl-...	13.86	15.9	ug/l	438447	4	13.32	1382950	50.0
Benzene, (2-methy...	13.97	12.1	ug/l	333284	4	13.32	1382950	50.0
Benzene, 1,2,4,5-...	14.18	11.5	ug/l	317129	4	13.32	1382950	50.0