

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071018\
 Data File : VU025296.D
 Acq On : 10 Jul 2018 18:06
 Operator : MD/SY
 Sample : J3898-06
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 SS038RW150-180704

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_U\METHOD\82U070918W.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	1.088	138	155	172	rBV	752688	884462	32.44%	2.325%
2	2.320	522	538	548	rBV	34291	64344	2.36%	0.169%
3	2.709	644	659	680	rBV	129649	267811	9.82%	0.704%
4	3.998	1039	1060	1082	rBV2	90315	254355	9.33%	0.669%
5	4.223	1109	1130	1152	rBV3	18861	58621	2.15%	0.154%
6	4.741	1272	1291	1308	rVB6	19205	52241	1.92%	0.137%
7	4.886	1318	1336	1353	rBV	178906	411172	15.08%	1.081%
8	4.989	1353	1368	1384	rVV	270206	598302	21.95%	1.573%
9	5.085	1386	1398	1418	rVB2	41863	102509	3.76%	0.269%
10	5.262	1435	1453	1460	rBV2	96657	221071	8.11%	0.581%
11	5.313	1460	1469	1490	rVB	193076	415479	15.24%	1.092%
12	5.542	1514	1540	1570	rVB	639286	1546669	56.73%	4.066%
13	5.889	1633	1648	1668	rBV	362644	722221	26.49%	1.899%
14	6.397	1789	1806	1820	rBV3	103977	221087	8.11%	0.581%
15	6.480	1820	1832	1844	rBV2	86395	165116	6.06%	0.434%
16	6.593	1853	1867	1885	rVB	135843	288230	10.57%	0.758%
17	6.744	1899	1914	1929	rVB2	114378	231540	8.49%	0.609%
18	6.931	1953	1972	1992	rBV	562355	1119201	41.05%	2.942%
19	7.053	1993	2010	2027	rBV	953078	1926429	70.66%	5.064%
20	7.262	2061	2075	2083	rBV3	49800	101774	3.73%	0.268%
21	7.448	2116	2133	2144	rBV3	15217	37785	1.39%	0.099%
22	7.525	2144	2157	2161	rBV	132082	222348	8.16%	0.584%
23	7.567	2161	2170	2188	rVB	766801	1361849	49.95%	3.580%
24	7.715	2202	2216	2232	rBV	101392	202585	7.43%	0.533%
25	7.863	2248	2262	2270	rBV6	21916	42459	1.56%	0.112%
26	7.918	2270	2279	2288	rBV3	23254	39234	1.44%	0.103%
27	8.050	2312	2320	2331	rVB3	21077	35534	1.30%	0.093%
28	8.133	2331	2346	2366	rVB6	23318	66636	2.44%	0.175%
29	8.332	2387	2408	2417	rBV5	28015	70459	2.58%	0.185%
30	8.400	2417	2429	2440	rVB2	31863	64455	2.36%	0.169%
31	8.487	2440	2456	2471	rBV9	20607	49465	1.81%	0.130%
32	8.609	2483	2494	2503	rBV	68280	126460	4.64%	0.332%
33	8.654	2504	2508	2528	rVV3	24986	52993	1.94%	0.139%
34	8.763	2531	2542	2559	rVB7	18910	46433	1.70%	0.122%

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35	8.850	2559	2569	2581	rBV2	73699	125120	4.59%	0.329%
36	9.091	2632	2644	2667	rBV	519875	990450	36.33%	2.604%
37	9.191	2668	2675	2686	rVV2	62198	107891	3.96%	0.284%
38	9.258	2686	2696	2706	rVB4	19365	35274	1.29%	0.093%
39	9.368	2719	2730	2746	rVB5	71032	155220	5.69%	0.408%
40	9.448	2746	2755	2782	rVB3	77772	176171	6.46%	0.463%
41	9.574	2782	2794	2810	rBV2	83826	144655	5.31%	0.380%
42	9.750	2826	2849	2860	rVV7	102392	352055	12.91%	0.925%
43	9.808	2860	2867	2878	rVB	35577	62062	2.28%	0.163%
44	9.927	2892	2904	2907	rBV3	101987	171008	6.27%	0.450%
45	9.956	2907	2913	2924	rVB	214855	347793	12.76%	0.914%
46	10.053	2933	2943	2959	rBV7	111774	228292	8.37%	0.600%
47	10.168	2971	2979	2986	rVB	69795	100623	3.69%	0.265%
48	10.223	2986	2996	3012	rVB6	131500	245422	9.00%	0.645%
49	10.310	3012	3023	3035	rBV	528281	835089	30.63%	2.195%
50	10.381	3035	3045	3061	rBV8	134236	269701	9.89%	0.709%
51	10.455	3062	3068	3072	rVV3	26788	37442	1.37%	0.098%
52	10.500	3073	3082	3092	rVB4	241623	386769	14.19%	1.017%
53	10.644	3115	3127	3136	rBV6	64646	169239	6.21%	0.445%
54	10.702	3137	3145	3155	rVB5	109730	213740	7.84%	0.562%
55	10.818	3174	3181	3188	rBV4	51374	73174	2.68%	0.192%
56	10.869	3189	3197	3217	rVB9	51726	111319	4.08%	0.293%
57	10.985	3220	3233	3249	rBV2	192591	391878	14.37%	1.030%
58	11.101	3261	3269	3278	rVB	154683	228071	8.37%	0.600%
59	11.149	3278	3284	3289	rBV4	39530	59865	2.20%	0.157%
60	11.294	3312	3329	3335	rBV	486976	919475	33.73%	2.417%
61	11.326	3335	3339	3354	rVB	362095	551618	20.23%	1.450%
62	11.487	3379	3389	3403	rBV	604932	946061	34.70%	2.487%
63	11.615	3420	3429	3441	rBV7	44053	123973	4.55%	0.326%
64	11.692	3442	3453	3470	rVB	602590	991183	36.36%	2.606%
65	11.782	3470	3481	3494	rBV2	340822	563341	20.66%	1.481%
66	11.860	3495	3505	3525	rVB4	376432	739330	27.12%	1.944%
67	12.194	3602	3609	3615	rBV8	22135	35894	1.32%	0.094%
68	12.255	3615	3628	3635	rVV	1735700	2726211	100.00%	7.167%
69	12.291	3635	3639	3650	rVV2	510127	780699	28.64%	2.052%
70	12.358	3650	3660	3679	rVV3	993392	2380028	87.30%	6.257%
71	12.438	3679	3685	3695	rVB	154674	245274	9.00%	0.645%

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72	12.541	3696	3717	3731	rVB2	593528	1218563	44.70%	3.203%
73	12.654	3731	3752	3764	rBV2	932392	1774776	65.10%	4.665%
74	12.725	3765	3774	3785	rVV3	122375	204708	7.51%	0.538%
75	12.792	3785	3795	3806	rVB2	190789	306157	11.23%	0.805%
76	12.882	3813	3823	3830	rBV	224685	341515	12.53%	0.898%
77	12.927	3830	3837	3845	rVB	192899	274937	10.08%	0.723%
78	13.001	3853	3860	3869	rVB	133309	199794	7.33%	0.525%
79	13.123	3870	3898	3908	rBV2	1072029	1903356	69.82%	5.003%
80	13.239	3928	3934	3949	rBV2	85602	169160	6.20%	0.445%
81	13.409	3980	3987	3993	rBV3	32091	49479	1.81%	0.130%
82	13.458	3994	4002	4010	rVV	96152	159640	5.86%	0.420%
83	13.512	4010	4019	4027	rVV2	315306	484601	17.78%	1.274%
84	13.583	4027	4041	4045	rVV3	162953	389736	14.30%	1.025%
85	13.612	4046	4050	4067	rVV2	209783	365873	13.42%	0.962%
86	13.731	4079	4087	4097	rVB3	83546	135268	4.96%	0.356%
87	13.792	4097	4106	4117	rVB2	65791	105192	3.86%	0.277%
88	13.879	4118	4133	4142	rBV6	87585	209453	7.68%	0.551%
89	13.956	4149	4157	4168	rVV4	48603	92729	3.40%	0.244%
90	14.017	4170	4176	4184	rVB5	26185	36729	1.35%	0.097%
91	14.155	4208	4219	4222	rBV5	26845	47403	1.74%	0.125%
92	14.339	4268	4276	4288	rVB2	47638	95154	3.49%	0.250%
93	14.480	4315	4320	4330	rVB7	18025	28687	1.05%	0.075%
94	14.541	4333	4339	4353	rVB4	24432	46887	1.72%	0.123%
95	14.683	4372	4383	4401	rBV4	53059	111784	4.10%	0.294%
96	14.933	4454	4461	4478	rVB5	26341	55216	2.03%	0.145%
97	15.069	4492	4503	4520	rVB3	73476	141327	5.18%	0.372%

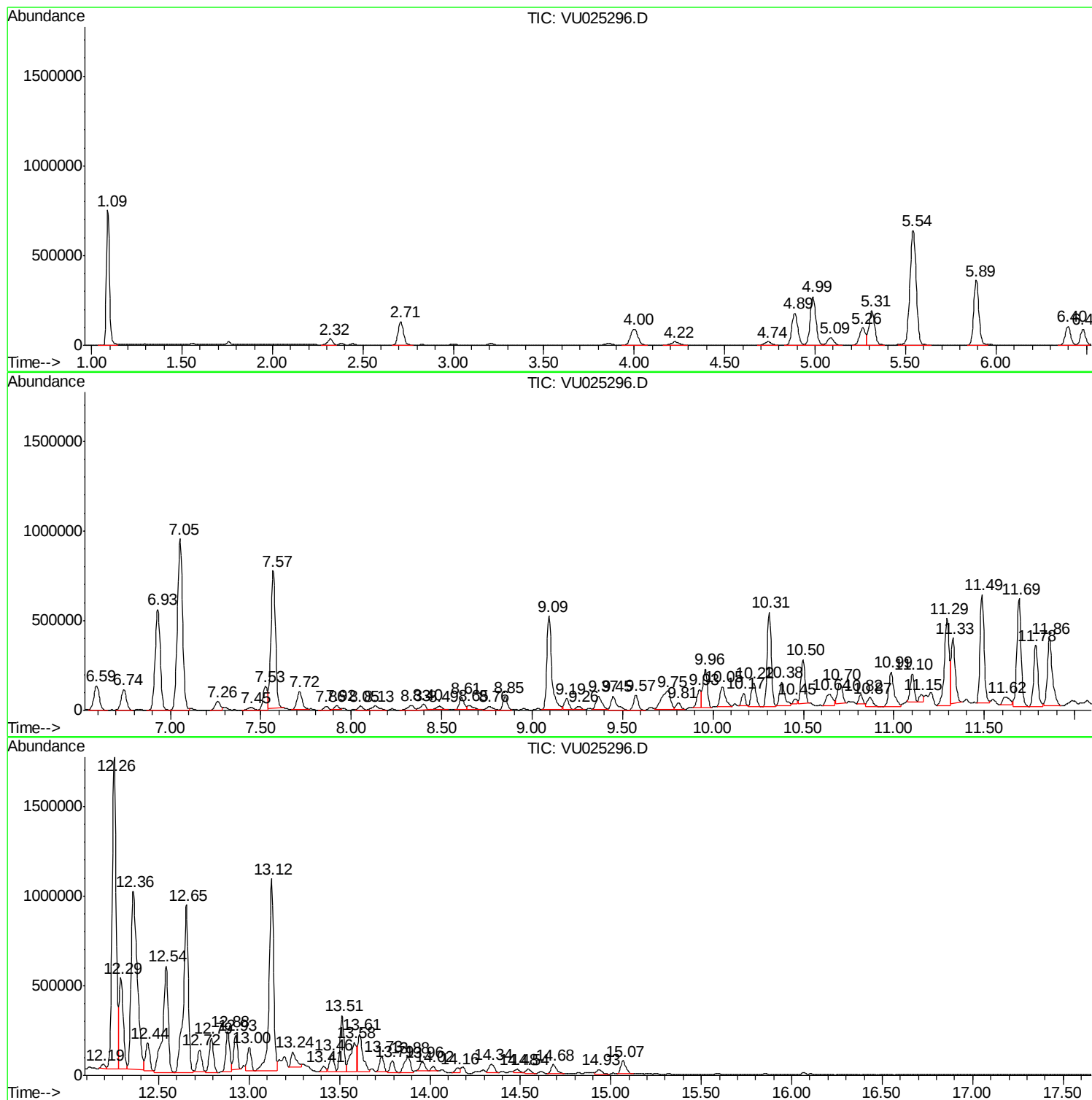
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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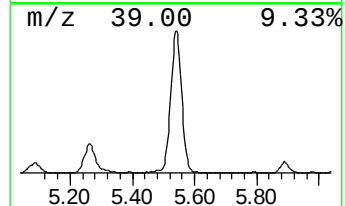
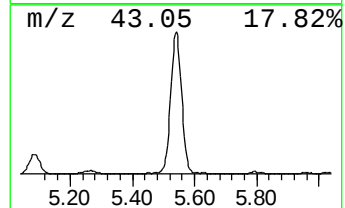
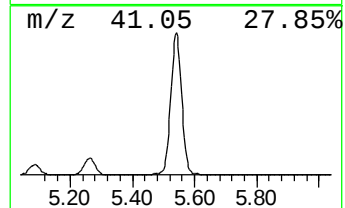
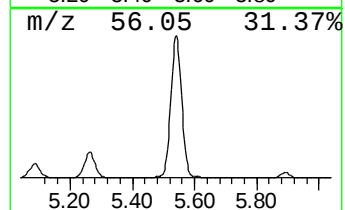
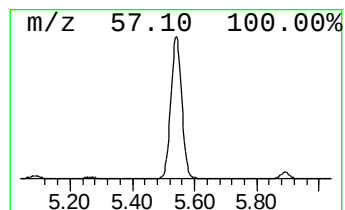
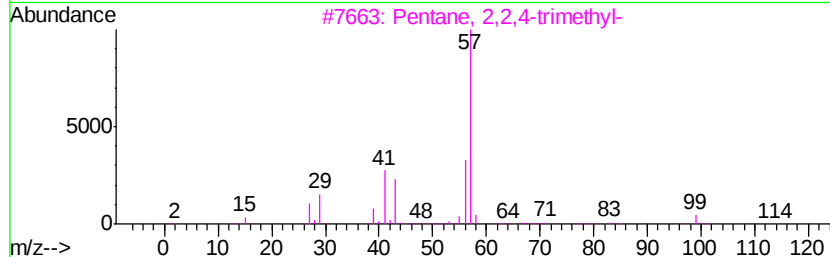
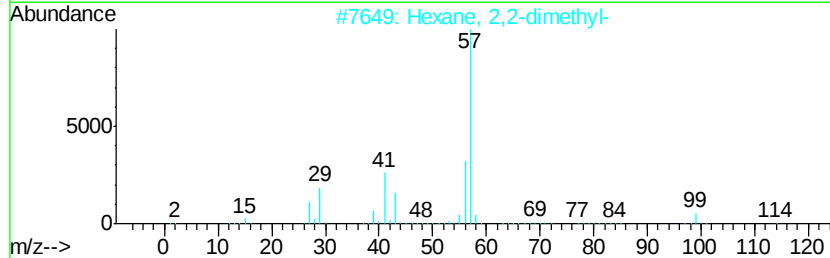
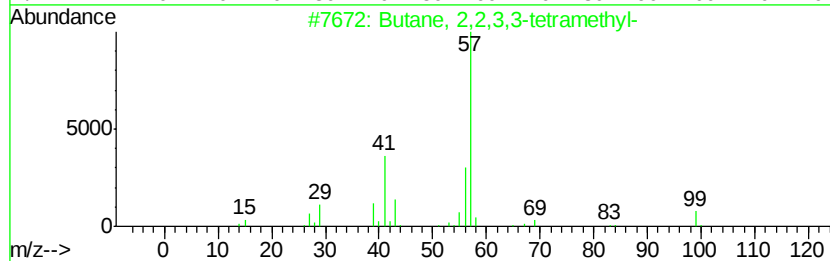
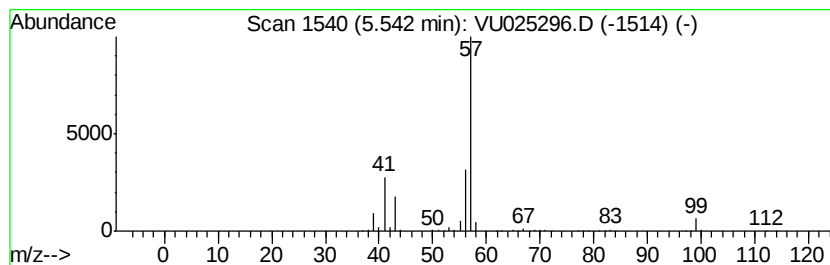
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U070918W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	107.08 ug/l	1546670	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	50



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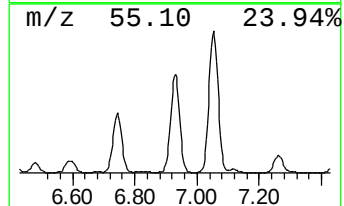
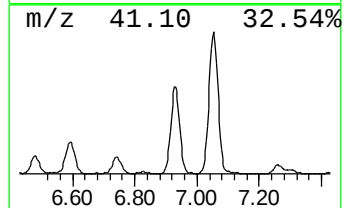
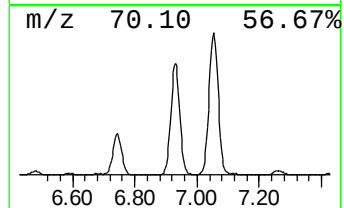
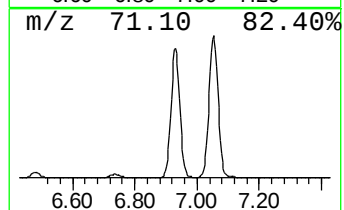
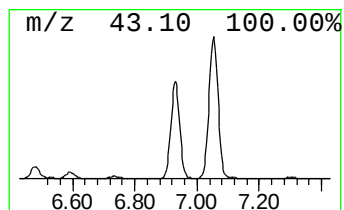
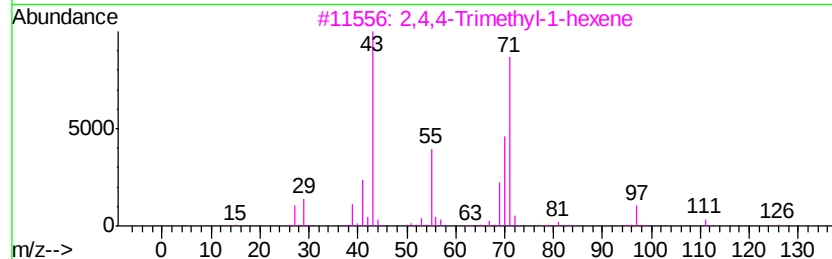
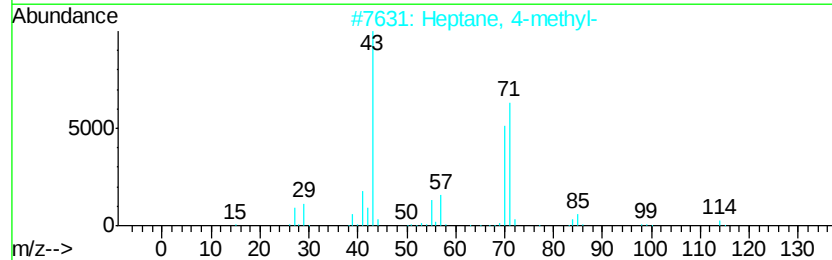
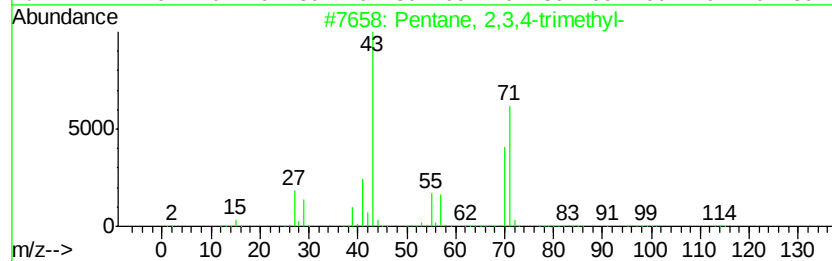
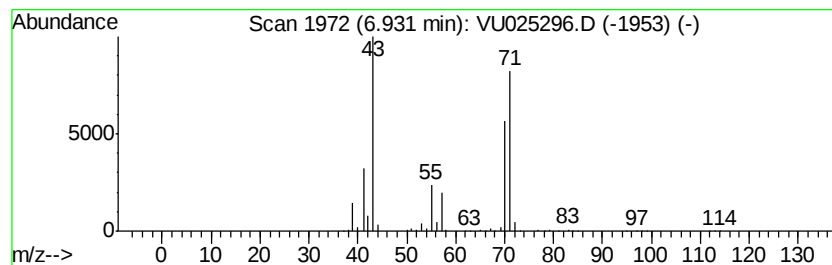
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	77.48 ug/l	1119200	1,4-Difluorobenzene	5.89

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	83
3		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	74



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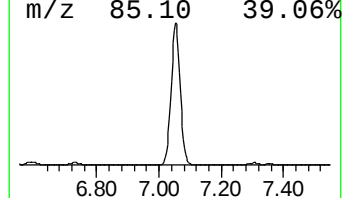
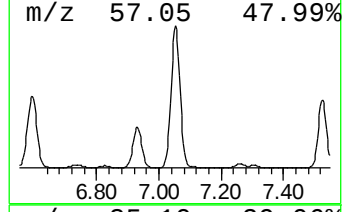
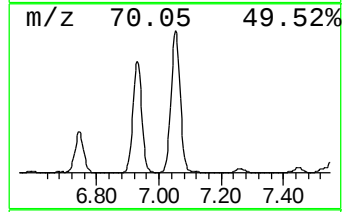
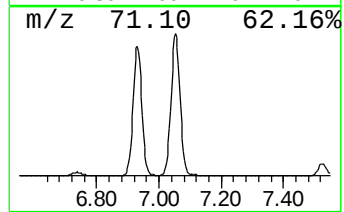
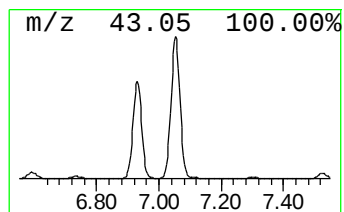
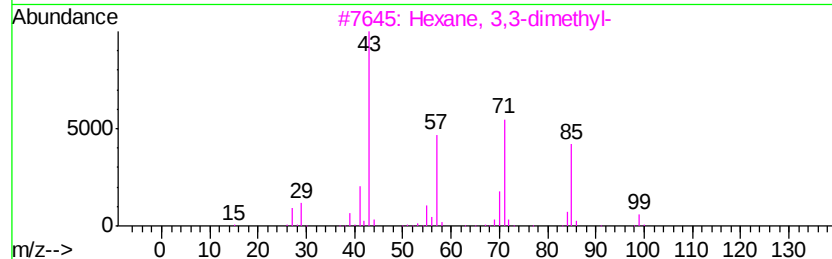
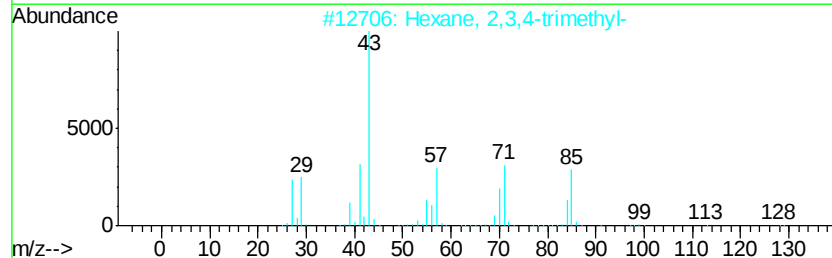
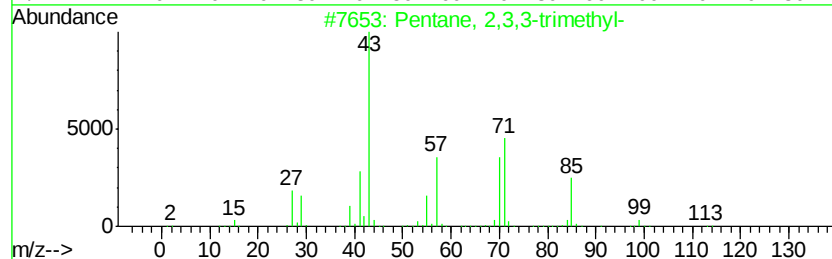
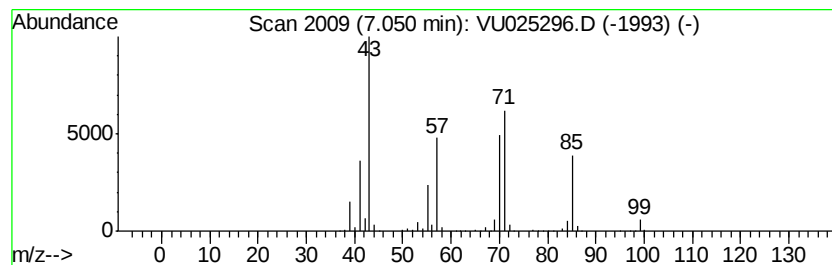
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	133.37 ug/l	1926430	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

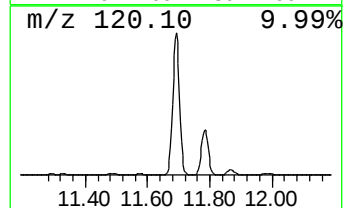
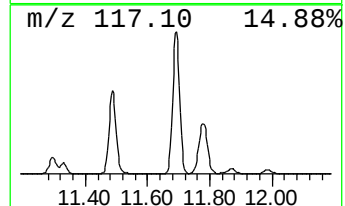
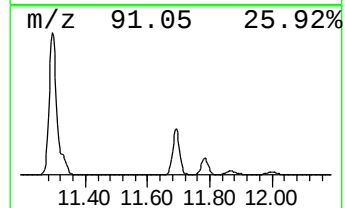
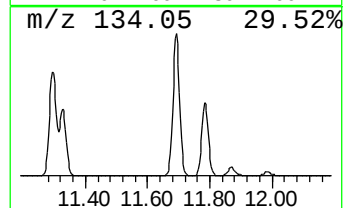
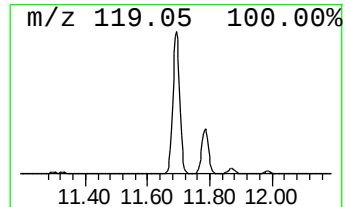
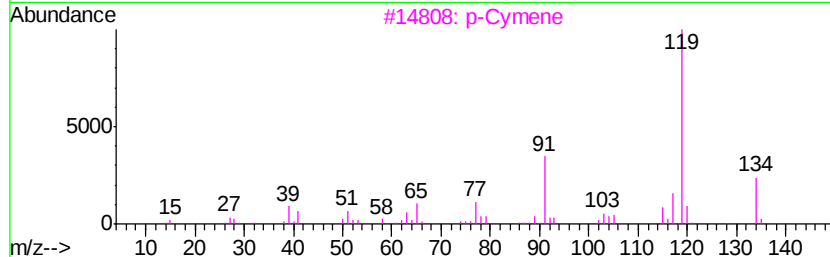
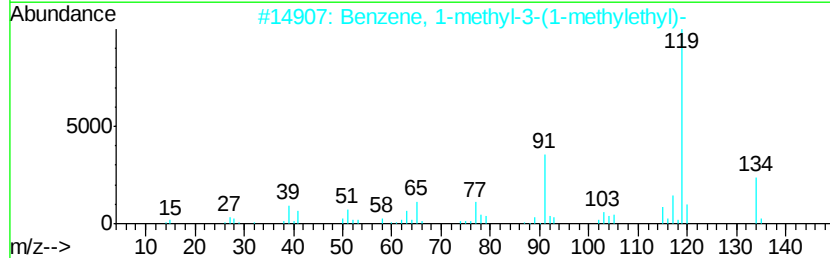
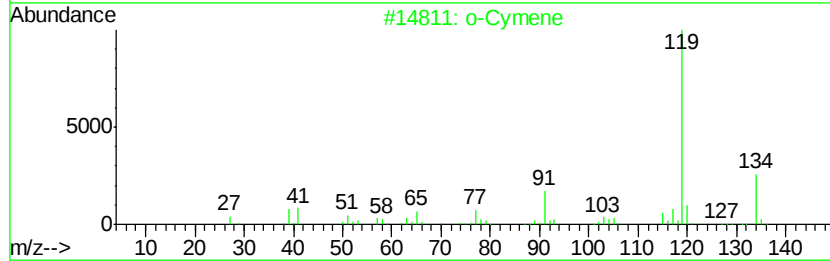
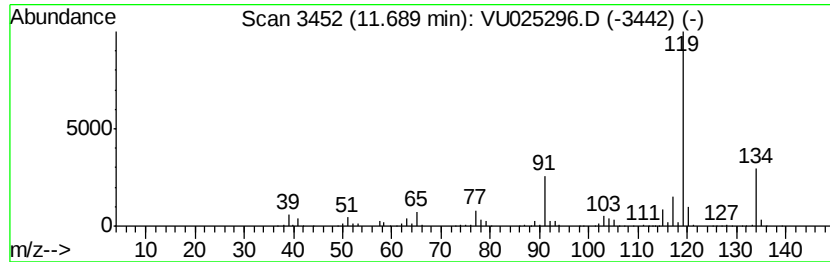
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	52.38 ug/l	991183	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	97
2		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
3		p-Cymene	134	C10H14	000099-87-6	95
4		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
5		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

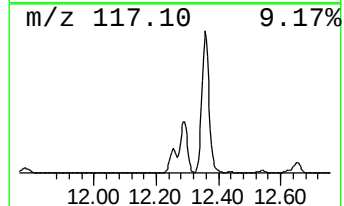
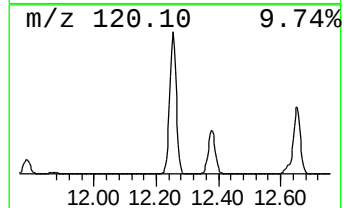
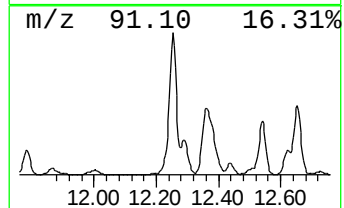
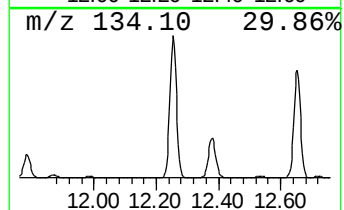
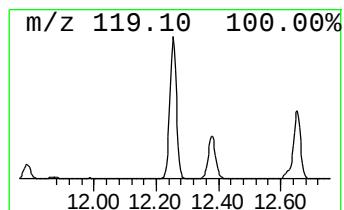
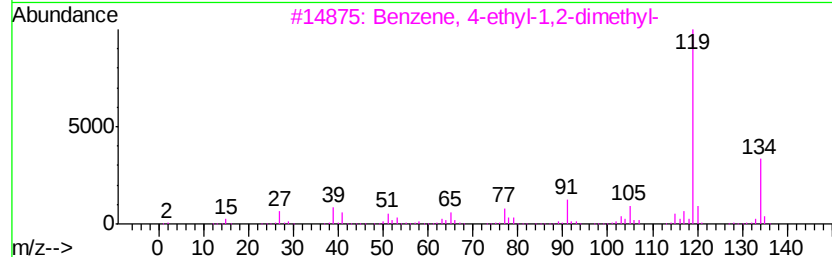
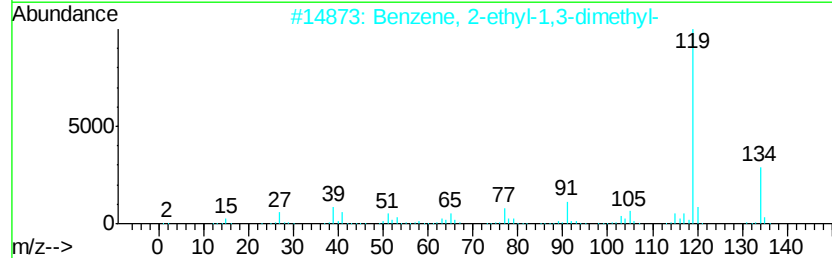
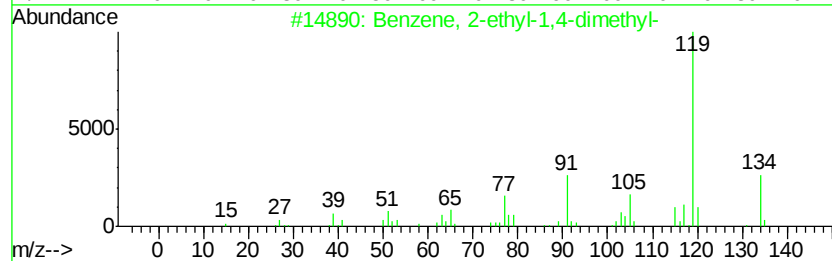
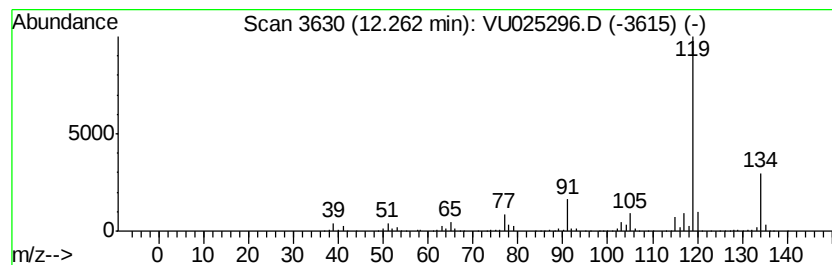
Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U070918W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	144.08 ug/l	2726210	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14	001758-88-9 96
2		Benzene, 2-ethyl-1,3-dimethyl-	134 C10H14	002870-04-4 95
3		Benzene, 4-ethyl-1,2-dimethyl-	134 C10H14	000934-80-5 95
4		o-Cymene	134 C10H14	000527-84-4 95
5		Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14	000933-98-2 95



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

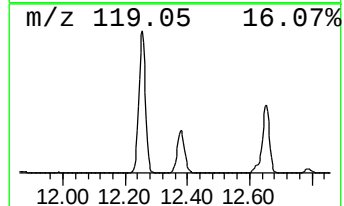
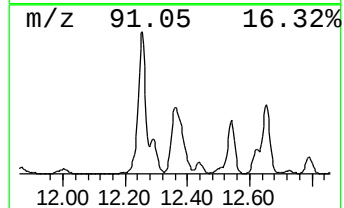
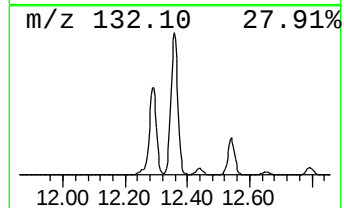
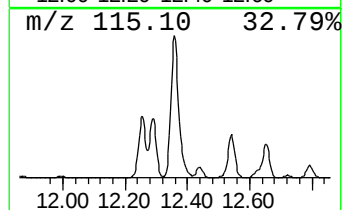
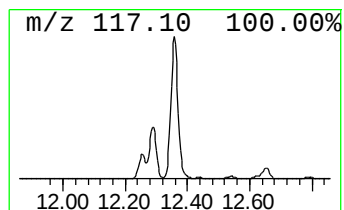
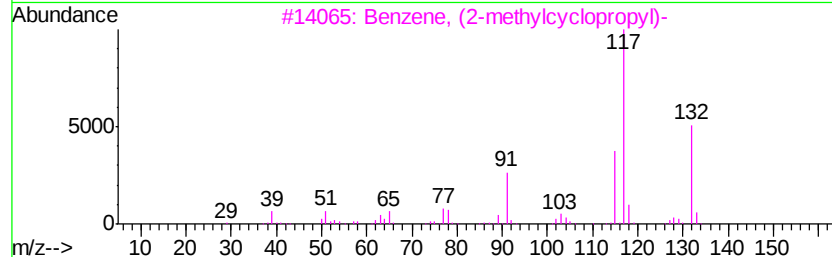
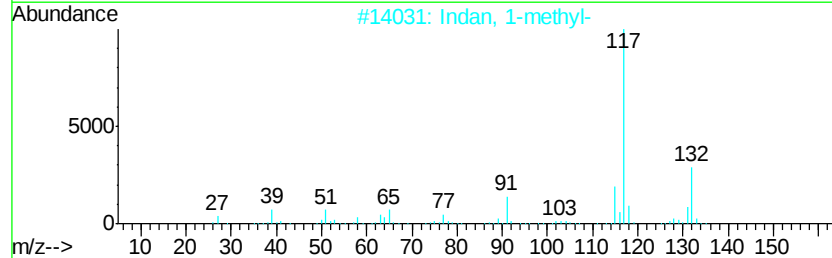
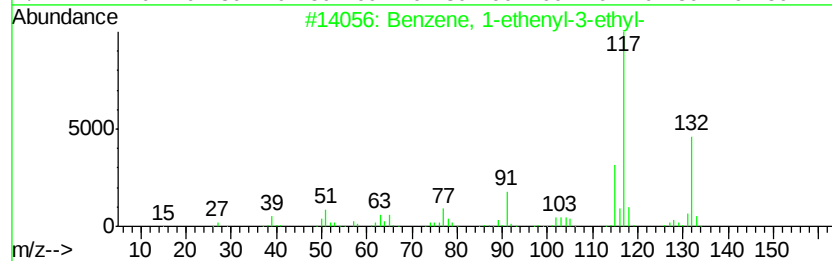
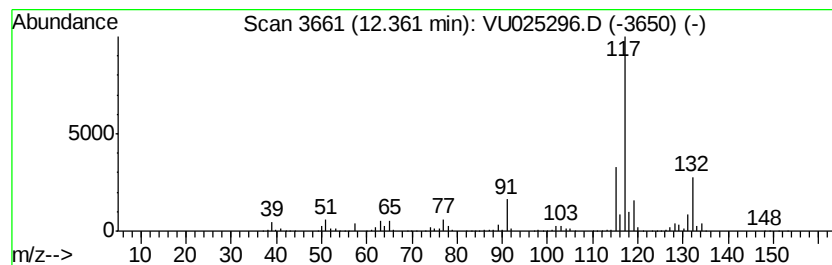
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	125.79 ug/l	2380030	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2		Indan, 1-methyl-	132	C10H12	000767-58-8	87
3		Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	83
4		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
5		Benzene, (1-methyl-1-propenyl)-, ...	132	C10H12	000768-00-3	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

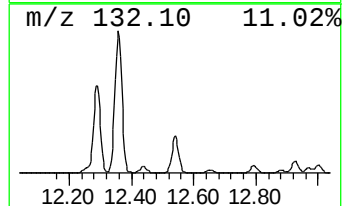
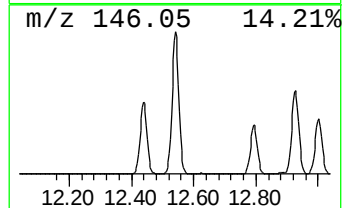
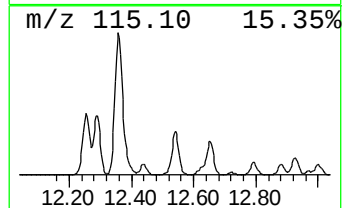
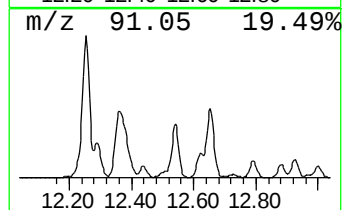
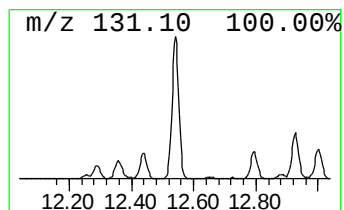
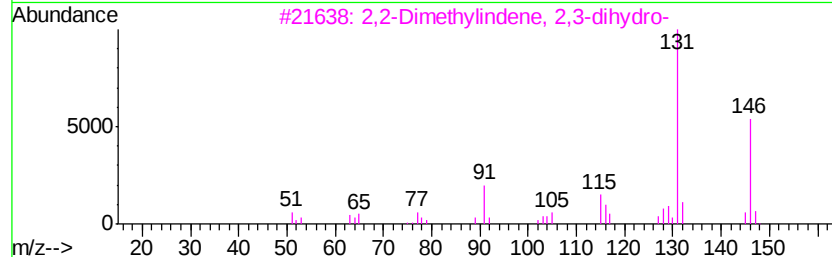
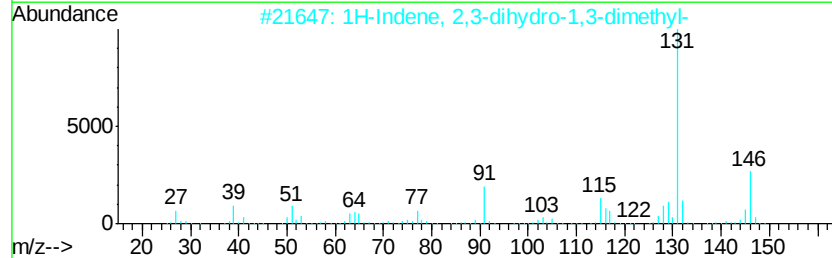
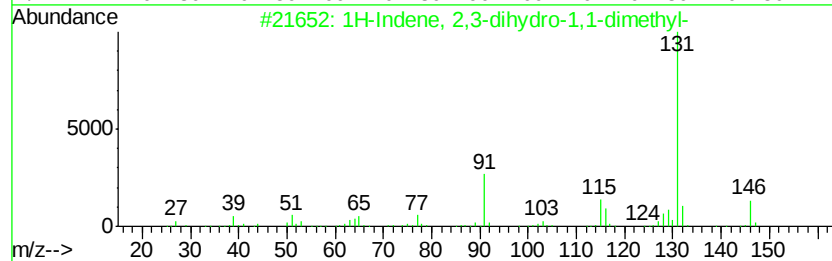
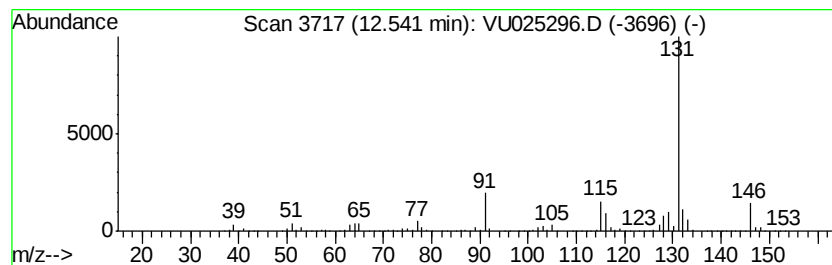
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-1,1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	64.40 ug/l	1218560	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	95
2		1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91
3		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	90
4		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
5		1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

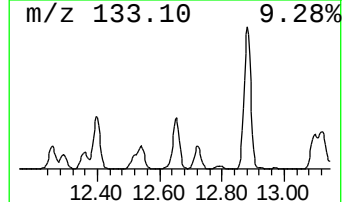
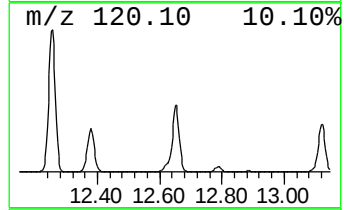
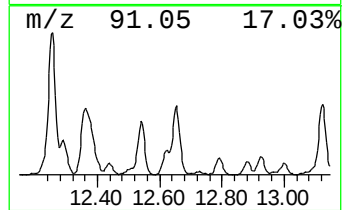
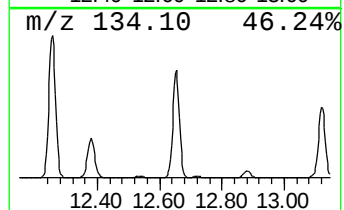
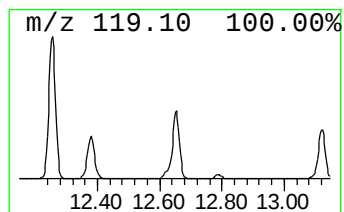
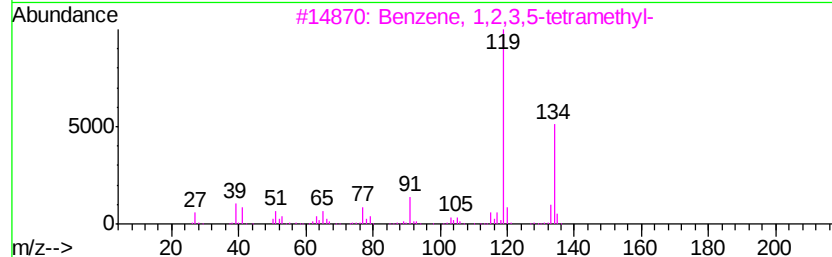
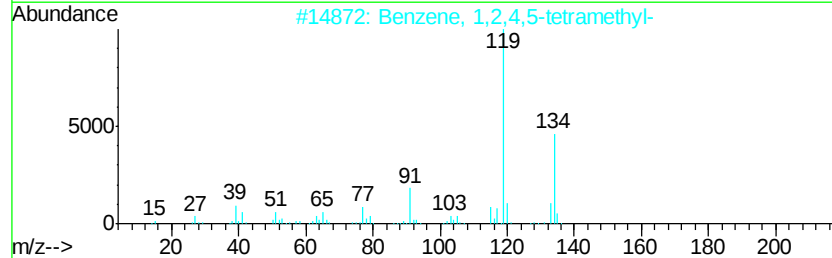
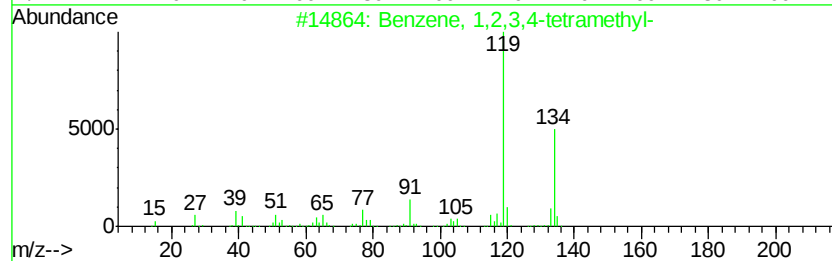
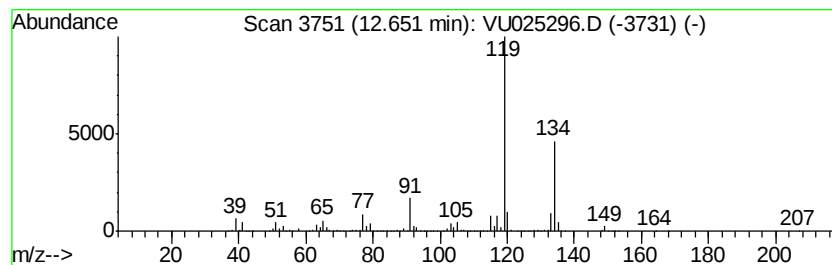
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	93.80 ug/l	1774780	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4		o-Cymene	134	C10H14	000527-84-4	93
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

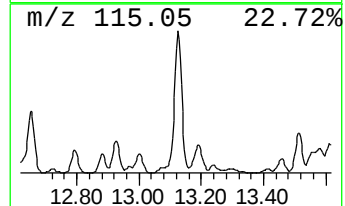
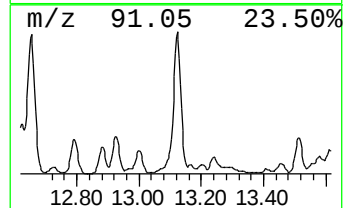
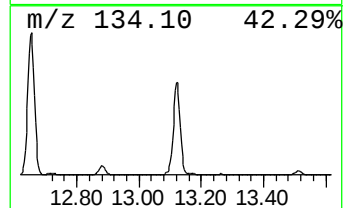
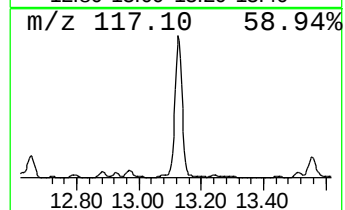
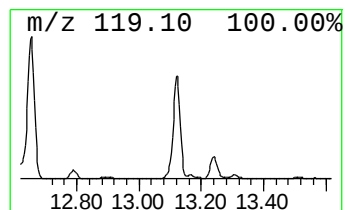
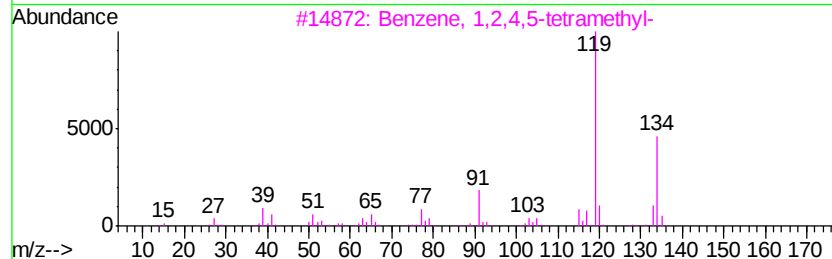
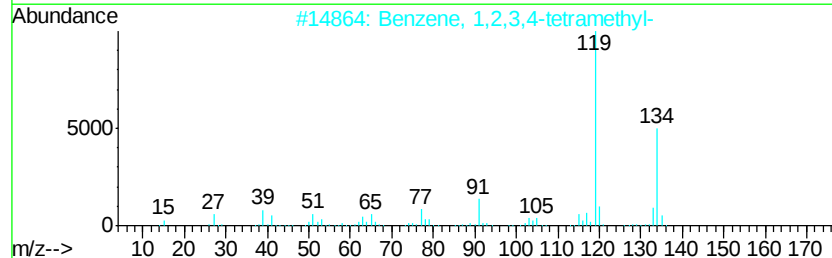
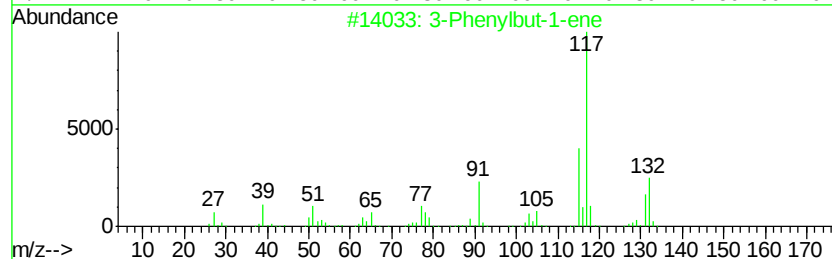
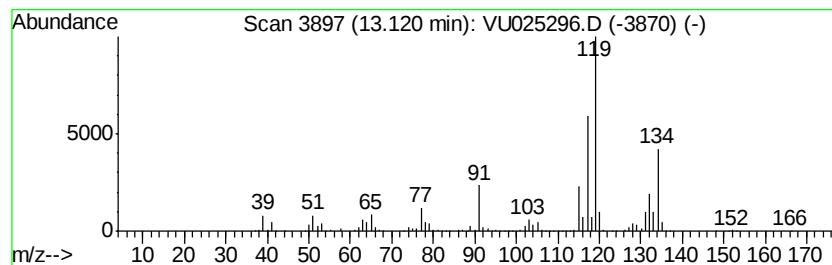
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U070918W.M
Quant Title : SW846 8260

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

Peak Number 10 3-Phenylbut-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	100.59 ug/l	1903360	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
4		p-Cymene	134	C10H14	000099-87-6	60
5		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU071018\
Data File : VU025296.D
Acq On : 10 Jul 2018 18:06
Operator : MD/SY
Sample : J3898-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SS038RW150-180704

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U070918W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentane, 2,3,4-tr...	6.93	77.5	ug/l	1119200	2	5.89	722221	50.0
Pentane, 2,3,3-tr...	7.05	133.4	ug/l	1926430	2	5.89	722221	50.0
o-Cymene	11.69	52.4	ug/l	991183	4	11.49	946061	50.0
Benzene, 2-ethyl-...	12.26	144.1	ug/l	2726210	4	11.49	946061	50.0
Benzene, 1-etheny...	12.36	125.8	ug/l	2380030	4	11.49	946061	50.0
1H-Indene, 2,3-di...	12.54	64.4	ug/l	1218560	4	11.49	946061	50.0
Benzene, 1,2,3,4-...	12.65	93.8	ug/l	1774780	4	11.49	946061	50.0
3-Phenylbut-1-ene	13.12	100.6	ug/l	1903360	4	11.49	946061	50.0