

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091619\
 Data File : VX012417.D
 Acq On : 16 Sep 2019 19:52
 Operator : JC/SP
 Sample : K4830-05
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 S13-0273

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_X\METHOD\82X091619W.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	1.070	26	30	42	rBV	655549	778904	49.02%	3.151%
2	1.777	141	146	158	rVB	257728	357377	22.49%	1.446%
3	2.381	238	245	261	rVB	187344	384517	24.20%	1.556%
4	2.594	274	280	292	rVB	46428	84086	5.29%	0.340%
5	2.832	311	319	328	rBV	271265	599808	37.75%	2.427%
6	2.923	328	334	343	rVB	98528	201882	12.70%	0.817%
7	3.161	363	373	390	rBV	589910	1332460	83.85%	5.390%
8	4.130	519	532	544	rBV3	29292	96073	6.05%	0.389%
9	4.301	548	560	566	rVV	66417	196787	12.38%	0.796%
10	4.393	566	575	589	rVV	414826	1218397	76.67%	4.929%
11	4.539	589	599	612	rVB5	16892	65792	4.14%	0.266%
12	5.228	698	712	724	rBV3	40451	146204	9.20%	0.591%
13	5.490	742	755	760	rBV	101373	290417	18.28%	1.175%
14	5.569	760	768	776	rVV	272555	855022	53.81%	3.459%
15	5.655	776	782	786	rVV2	129870	354518	22.31%	1.434%
16	5.722	786	793	805	rVB	205134	631354	39.73%	2.554%
17	5.941	818	829	839	rBV2	64725	198503	12.49%	0.803%
18	6.051	839	847	861	rVV2	120443	318690	20.05%	1.289%
19	6.252	865	880	888	rVV3	100085	353650	22.25%	1.431%
20	6.350	888	896	904	rVV3	174534	530769	33.40%	2.147%
21	6.447	904	912	926	rVB2	117750	332099	20.90%	1.344%
22	6.849	969	978	990	rBV	191799	457758	28.81%	1.852%
23	7.459	1065	1078	1089	rBV	687568	1589103	100.00%	6.429%
24	7.569	1089	1096	1101	rVV2	15849	33677	2.12%	0.136%
25	7.630	1101	1106	1111	rVV2	21905	50761	3.19%	0.205%
26	7.727	1117	1122	1132	rVB2	31207	61260	3.86%	0.248%
27	7.843	1132	1141	1149	rBV2	44503	93931	5.91%	0.380%
28	8.050	1163	1175	1184	rVB3	100190	265411	16.70%	1.074%
29	8.172	1188	1195	1204	rBV	162301	322269	20.28%	1.304%
30	8.386	1223	1230	1236	rBV2	30500	59585	3.75%	0.241%
31	8.660	1268	1275	1278	rBV2	136208	246807	15.53%	0.998%
32	8.709	1278	1283	1297	rVV	577205	984127	61.93%	3.981%
33	8.837	1297	1304	1308	rVV	70746	121400	7.64%	0.491%
34	8.910	1308	1316	1322	rVB	38595	81441	5.12%	0.329%

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35	9.038	1331	1337	1344	rVB	136058	225624	14.20%	0.913%
36	9.160	1349	1357	1363	rBV	66930	113646	7.15%	0.460%
37	9.569	1418	1424	1428	rVV2	38800	61409	3.86%	0.248%
38	9.617	1428	1432	1437	rVV	128189	183808	11.57%	0.744%
39	9.672	1437	1441	1446	rVV	82332	123645	7.78%	0.500%
40	9.886	1469	1476	1490	rVB3	21258	50520	3.18%	0.204%
41	10.111	1507	1513	1519	rVV	388673	536601	33.77%	2.171%
42	10.184	1519	1525	1529	rVV	67317	101501	6.39%	0.411%
43	10.331	1544	1549	1559	rBV4	37280	101088	6.36%	0.409%
44	10.641	1591	1600	1607	rBV3	33127	89887	5.66%	0.364%
45	10.830	1620	1631	1638	rBV2	55358	101042	6.36%	0.409%
46	10.910	1638	1644	1652	rBV4	31521	57462	3.62%	0.232%
47	11.013	1656	1661	1667	rBV	105703	138495	8.72%	0.560%
48	11.135	1675	1681	1686	rBV	470063	602990	37.95%	2.439%
49	11.178	1686	1688	1693	rVV	27764	36813	2.32%	0.149%
50	11.275	1701	1704	1708	rVV3	26998	37304	2.35%	0.151%
51	11.355	1712	1717	1727	rVB	91764	125082	7.87%	0.506%
52	11.672	1763	1769	1777	rBV6	27275	56608	3.56%	0.229%
53	11.763	1777	1784	1787	rBV2	38569	57253	3.60%	0.232%
54	11.806	1787	1791	1795	rVB	24424	30998	1.95%	0.125%
55	11.916	1801	1809	1811	rBV	63399	100096	6.30%	0.405%
56	11.940	1811	1813	1820	rVB	147827	170909	10.76%	0.691%
57	12.074	1830	1835	1840	rBV	530937	653182	41.10%	2.642%
58	12.227	1856	1860	1865	rBV	74862	93502	5.88%	0.378%
59	12.294	1866	1871	1877	rVV	268731	347336	21.86%	1.405%
60	12.367	1877	1883	1893	rVB2	113484	200274	12.60%	0.810%
61	12.458	1893	1898	1903	rBV	106570	139100	8.75%	0.563%
62	12.666	1921	1932	1935	rBV	389379	505302	31.80%	2.044%
63	12.696	1935	1937	1942	rVV	158564	189577	11.93%	0.767%
64	12.757	1942	1947	1953	rVV3	274960	469387	29.54%	1.899%
65	12.812	1953	1956	1962	rVB2	31532	38355	2.41%	0.155%
66	12.891	1962	1969	1974	rVB3	94368	159801	10.06%	0.646%
67	12.970	1974	1982	1987	rBV	304205	439021	27.63%	1.776%
68	13.080	1995	2000	2006	rVB2	55057	89266	5.62%	0.361%
69	13.147	2006	2011	2015	rBV2	54861	84742	5.33%	0.343%
70	13.190	2015	2018	2021	rBV2	71432	79597	5.01%	0.322%
71	13.220	2021	2023	2026	rVB	65806	59441	3.74%	0.240%

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72	13.342	2038	2043	2049	rVB2	713346	1012868	63.74%	4.098%
73	13.421	2054	2056	2059	rVV	38721	41625	2.62%	0.168%
74	13.476	2061	2065	2071	rVB	109101	145003	9.12%	0.587%
75	13.562	2074	2079	2081	rBV2	48338	64974	4.09%	0.263%
76	13.598	2081	2085	2087	rVV2	59024	80114	5.04%	0.324%
77	13.635	2087	2091	2095	rVV2	152211	221254	13.92%	0.895%
78	13.696	2095	2101	2102	rVV2	107992	198315	12.48%	0.802%
79	13.714	2102	2104	2113	rVB2	177839	294877	18.56%	1.193%
80	13.806	2113	2119	2121	rBV	66550	93920	5.91%	0.380%
81	13.848	2121	2126	2131	rVB2	70831	128777	8.10%	0.521%
82	13.909	2131	2136	2140	rVB	81713	107300	6.75%	0.434%
83	13.982	2140	2148	2152	rBV2	136511	201264	12.67%	0.814%
84	14.025	2152	2155	2159	rVV3	55427	73051	4.60%	0.296%
85	14.129	2167	2172	2174	rBV2	48173	66171	4.16%	0.268%
86	14.159	2174	2177	2183	rVB4	33927	45193	2.84%	0.183%
87	14.281	2190	2197	2204	rVB2	112915	240635	15.14%	0.973%
88	14.373	2209	2212	2216	rVB	40679	49135	3.09%	0.199%
89	14.427	2216	2221	2225	rVB3	62949	82209	5.17%	0.333%
90	14.470	2225	2228	2234	rVB	26191	32867	2.07%	0.133%
91	14.537	2234	2239	2249	rBV2	163928	243276	15.31%	0.984%
92	14.690	2257	2264	2267	rVV	150368	222427	14.00%	0.900%
93	14.726	2267	2270	2274	rVV	47895	62447	3.93%	0.253%
94	14.836	2282	2288	2293	rVV2	229036	317117	19.96%	1.283%
95	14.964	2302	2309	2315	rVV8	11714	32509	2.05%	0.132%
96	15.244	2348	2355	2362	rVV2	25526	54096	3.40%	0.219%
97	15.543	2397	2404	2409	rBV	46658	77099	4.85%	0.312%
98	15.683	2420	2427	2430	rBV	61822	101756	6.40%	0.412%
99	15.720	2430	2433	2439	rVB	28582	45565	2.87%	0.184%
100	15.915	2461	2465	2476	rVB2	18096	37570	2.36%	0.152%

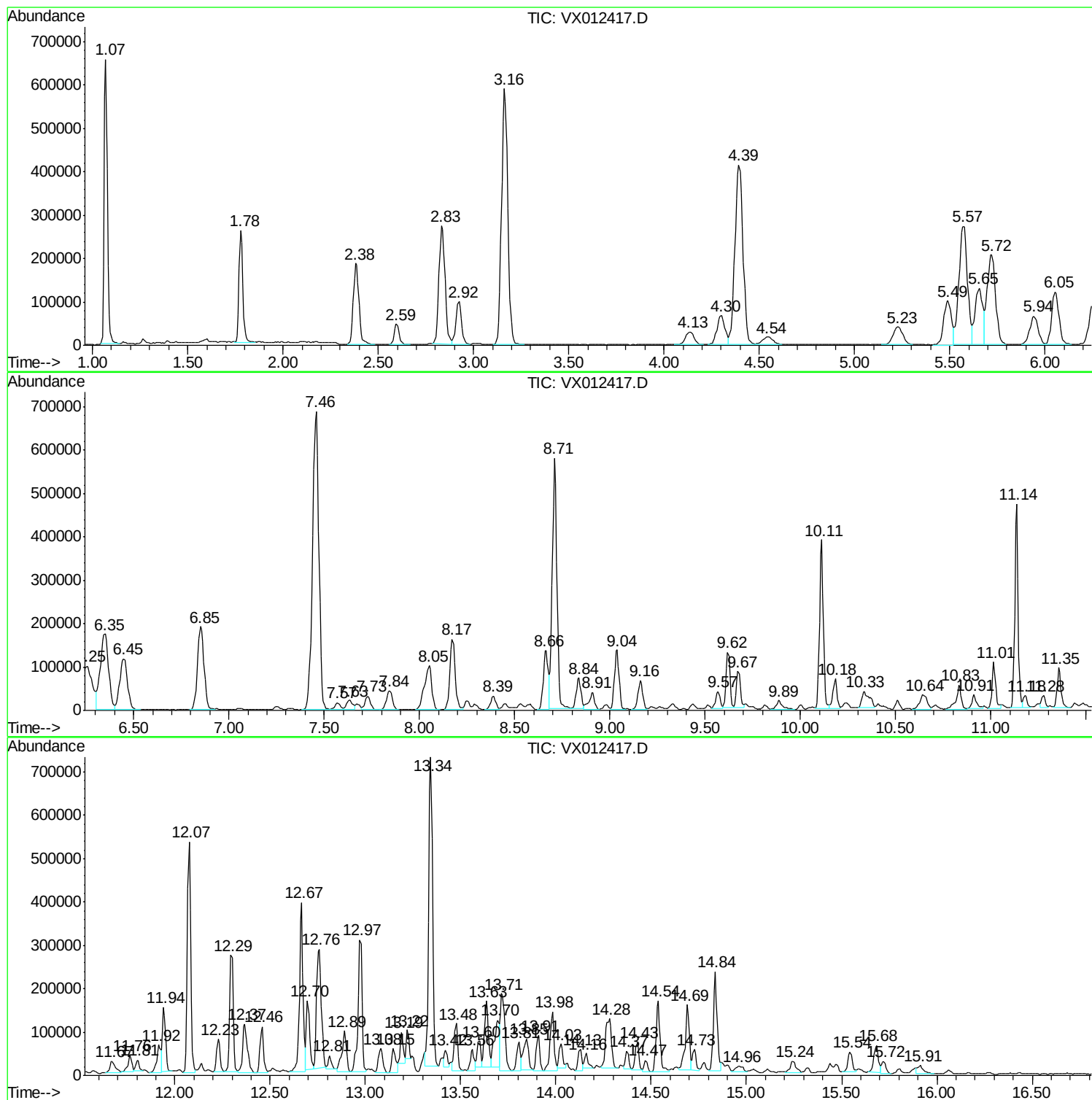
Sum of corrected areas: 24718917

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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



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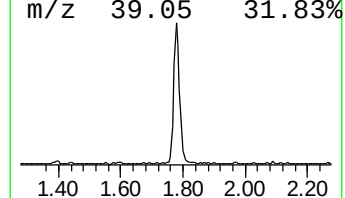
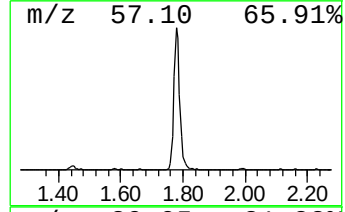
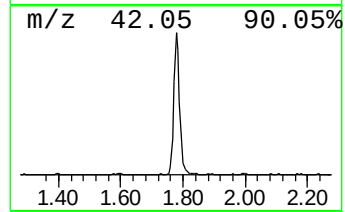
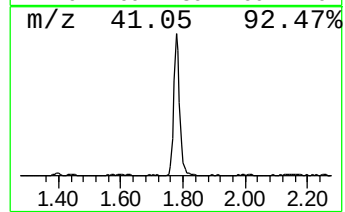
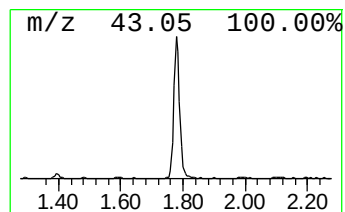
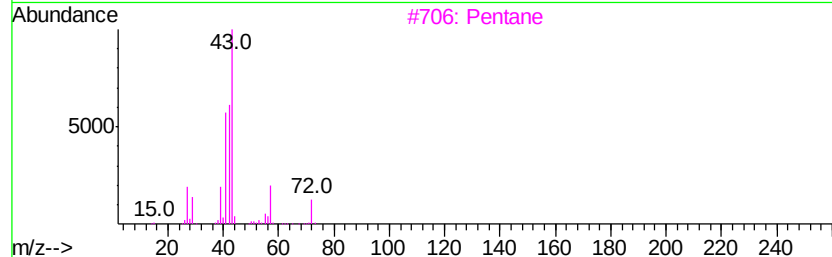
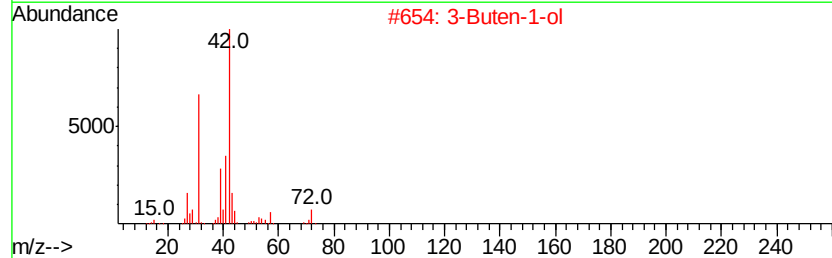
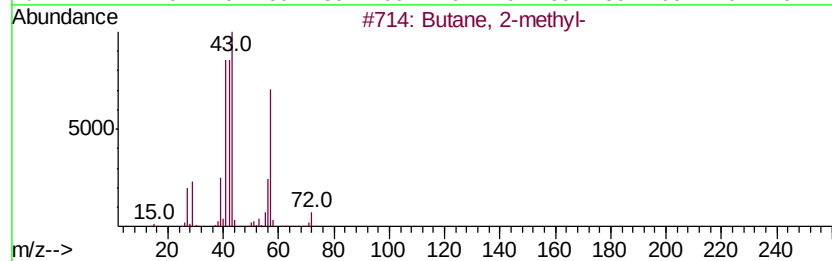
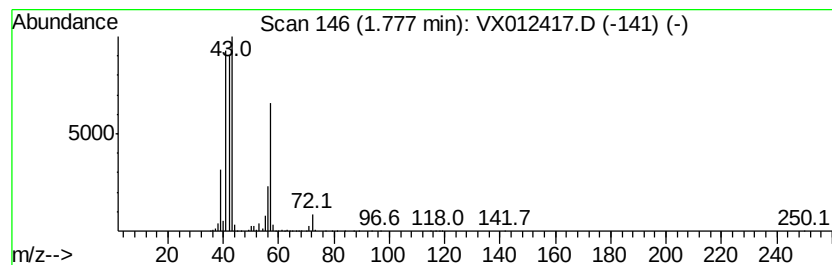
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	50.40 ug/l	357377	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	38
3		Pentane	72	C5H12	000109-66-0	36
4		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5		Cyclobutane, methyl-	70	C5H10	000598-61-8	25



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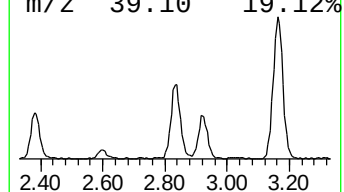
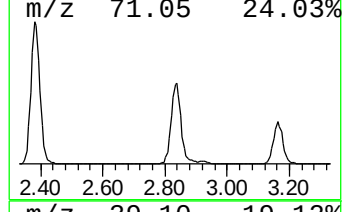
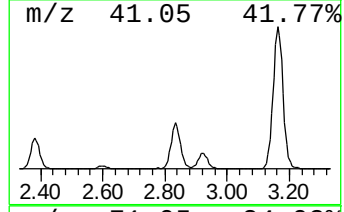
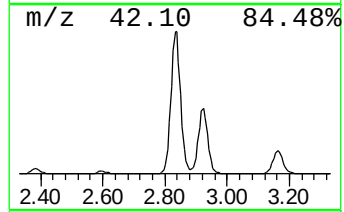
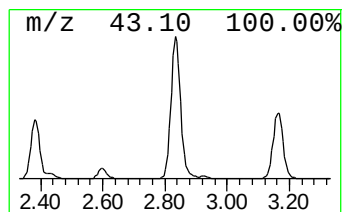
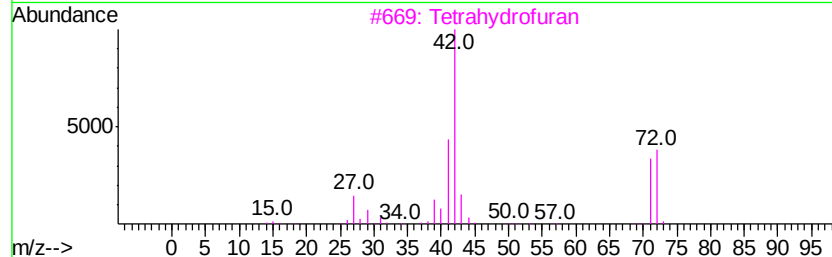
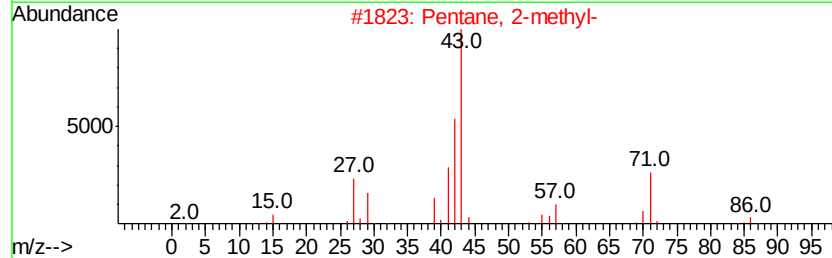
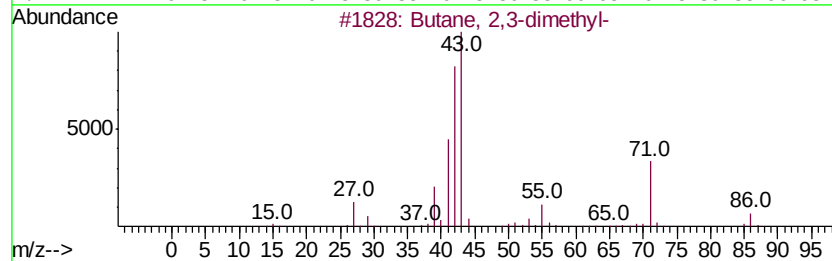
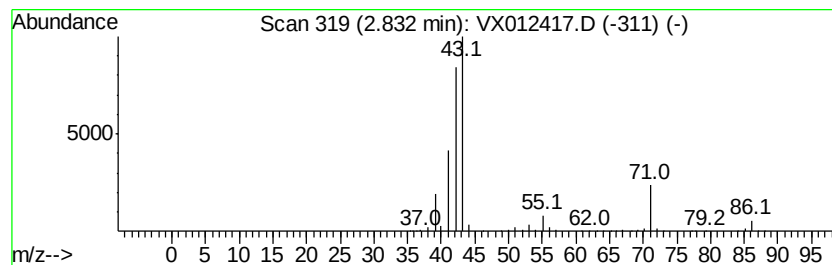
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	84.59 ug/l	599808	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3		Tetrahydrofuran	72	C4H8O	000109-99-9	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	38
5		Cyclobutane, methyl-	70	C5H10	000598-61-8	28



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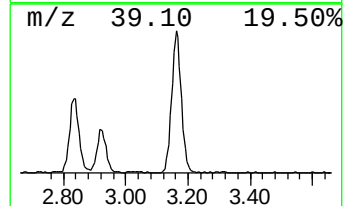
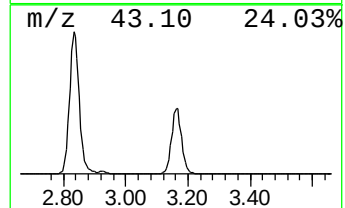
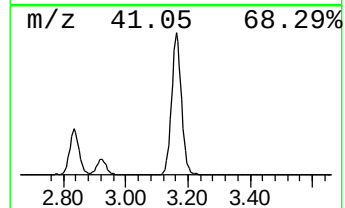
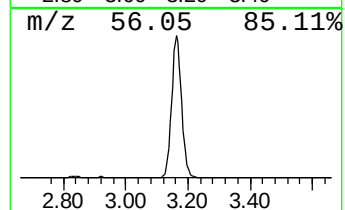
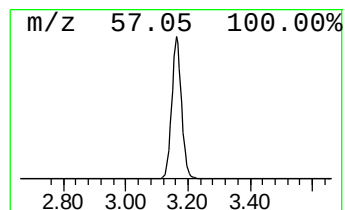
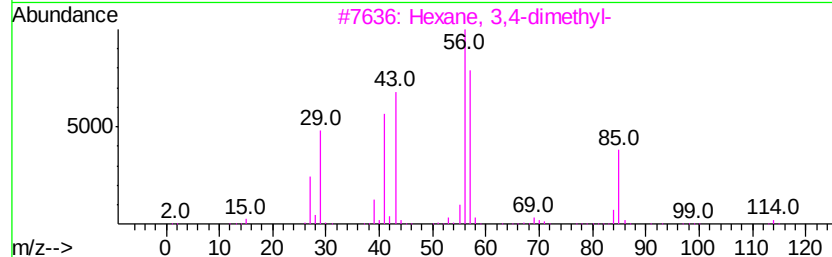
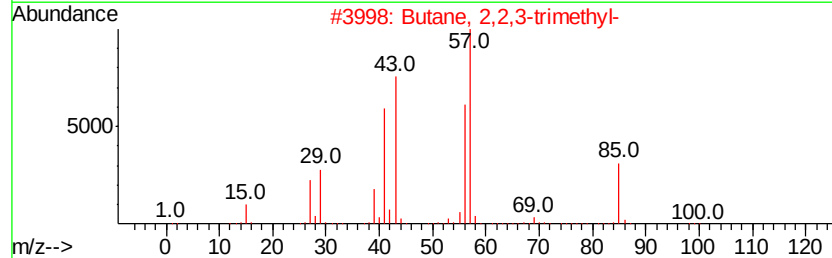
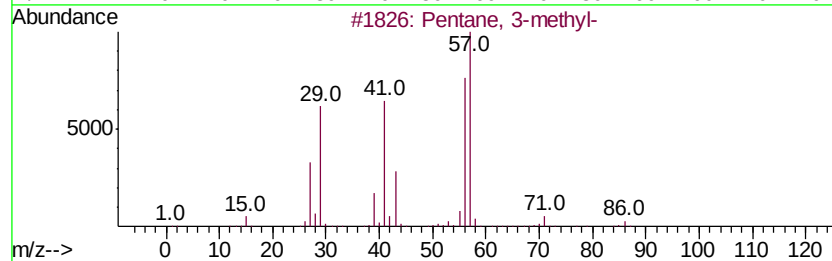
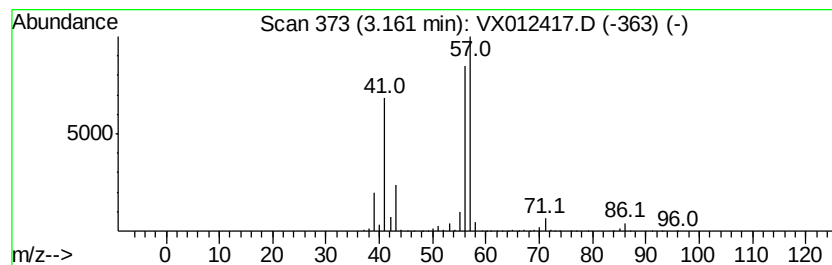
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Peak Number 4 Pentane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	187.93 ug/l	1332460	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	43
4		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	43
5		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0273

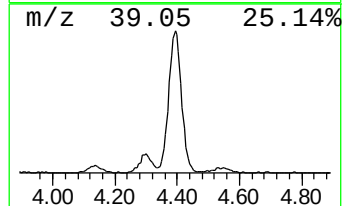
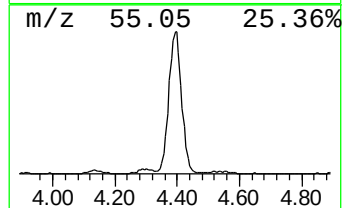
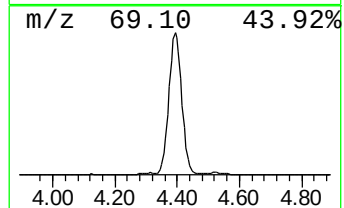
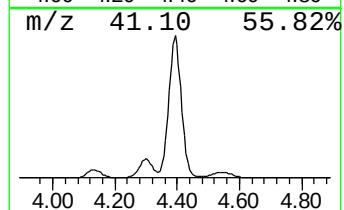
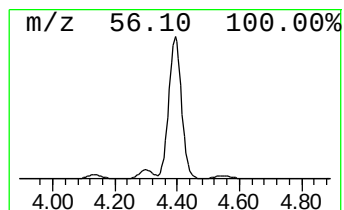
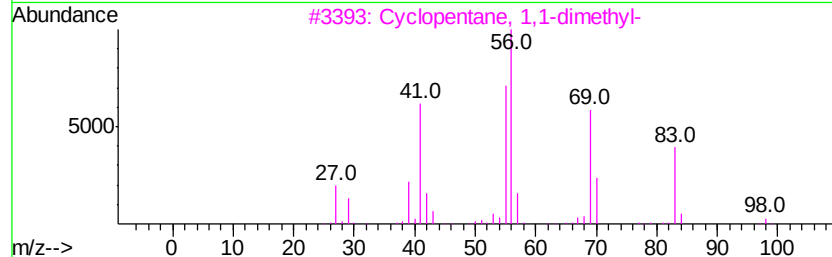
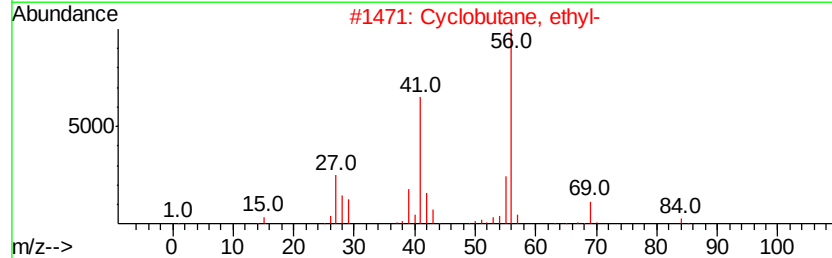
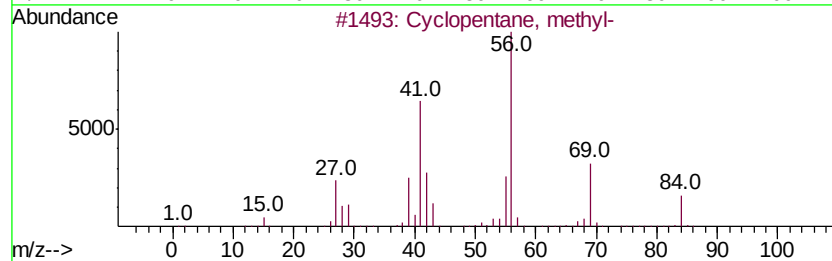
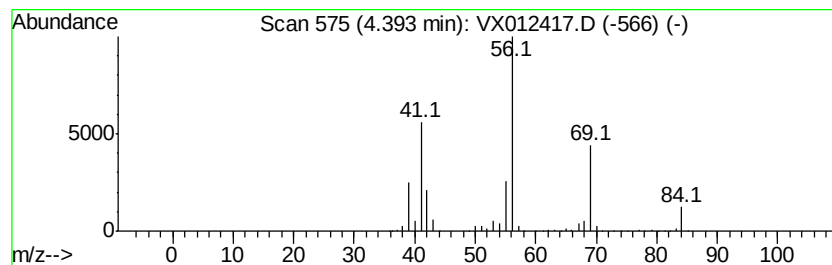
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	171.84 ug/l	1218400	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
S13-0273

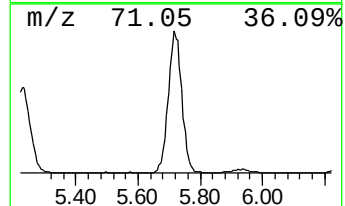
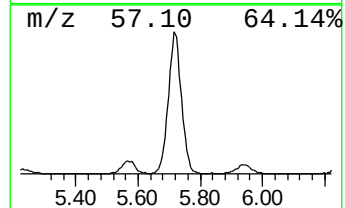
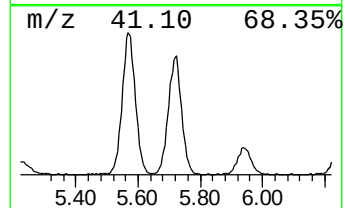
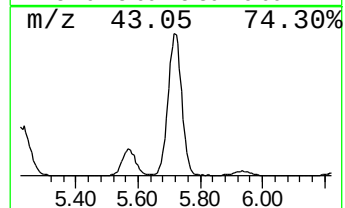
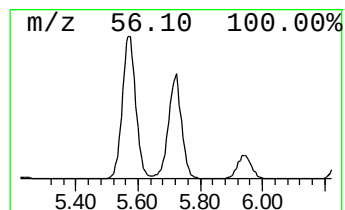
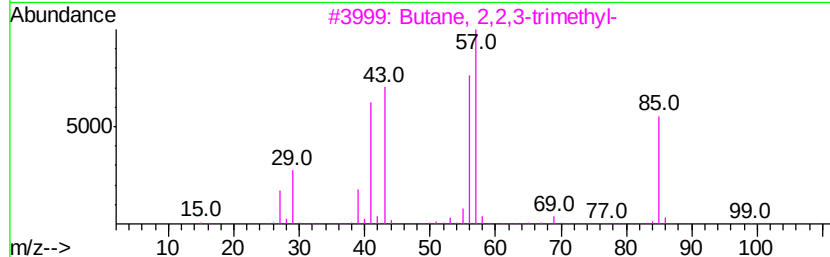
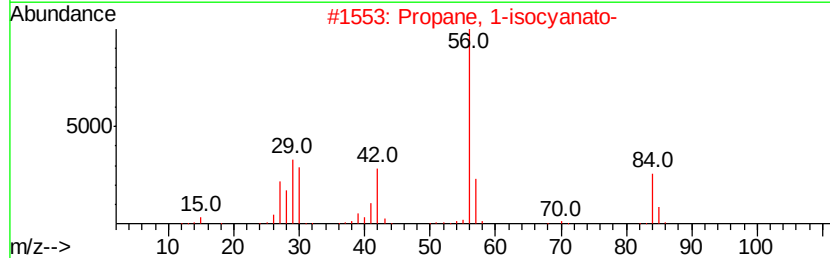
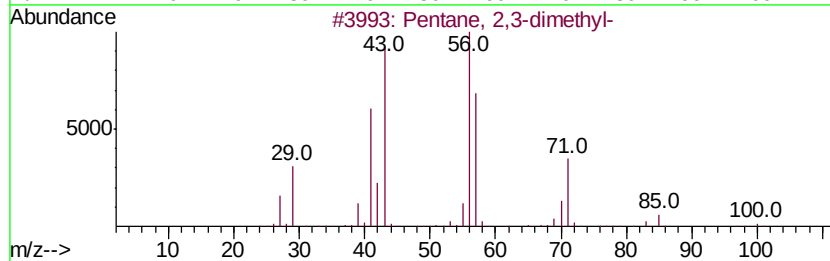
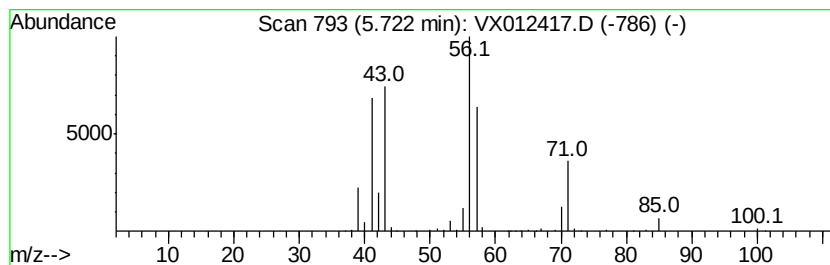
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	89.04 ug/l	631354	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	50
3		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	33
5		Heptane	100	C7H16	000142-82-5	32



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

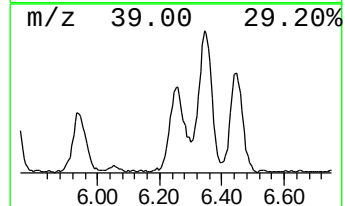
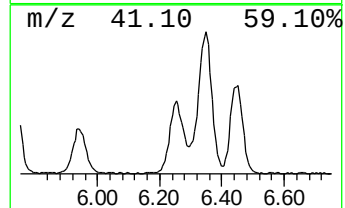
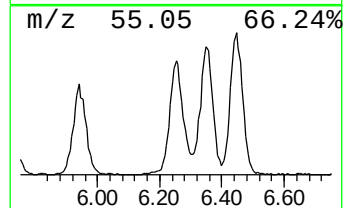
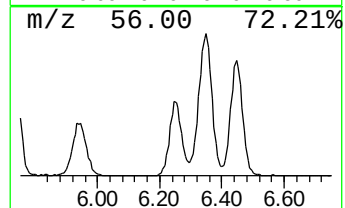
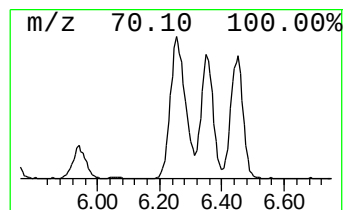
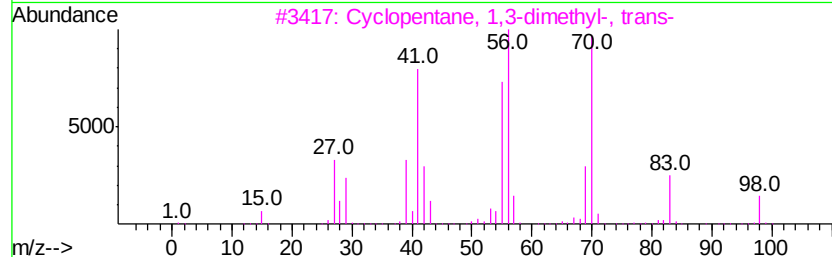
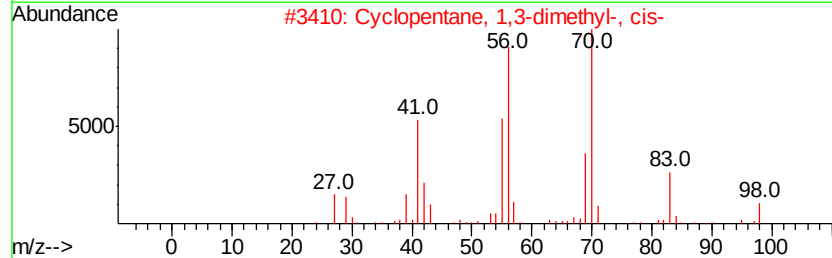
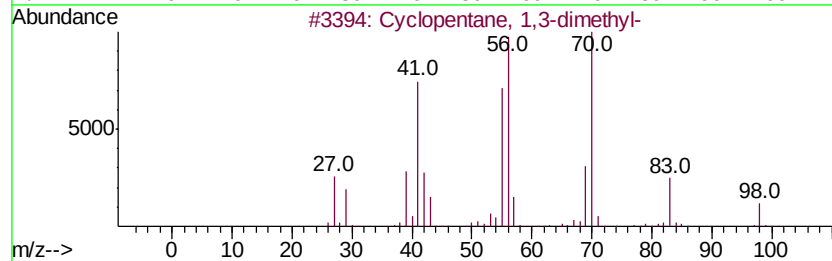
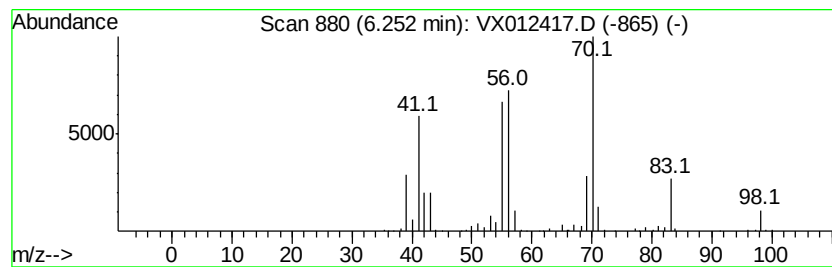
Instrument :
MSVOA_X
ClientSampleID :
S13-0273

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.25	38.63 ug/l	353650	1,4-Difluorobenzene	6.85	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1		Cyclopentane, 1,3-dimethyl-	98 C7H14	002453-00-1	93
2		Cyclopentane, 1,3-dimethyl-, cis-	98 C7H14	002532-58-3	91
3		Cyclopentane, 1,3-dimethyl-, trans-	98 C7H14	001759-58-6	70
4		Cyclopentane, 1,2-dimethyl-, cis-	98 C7H14	001192-18-3	70
5		Cyclopentane, 1,2-dimethyl-	98 C7H14	002452-99-5	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
S13-0273

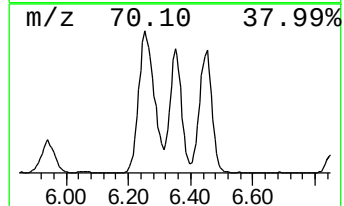
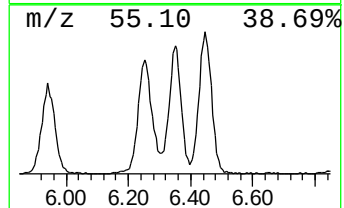
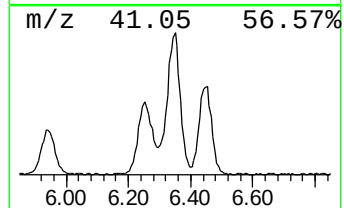
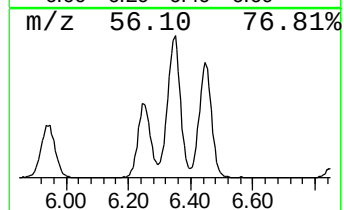
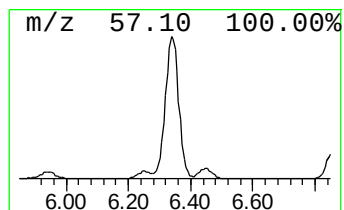
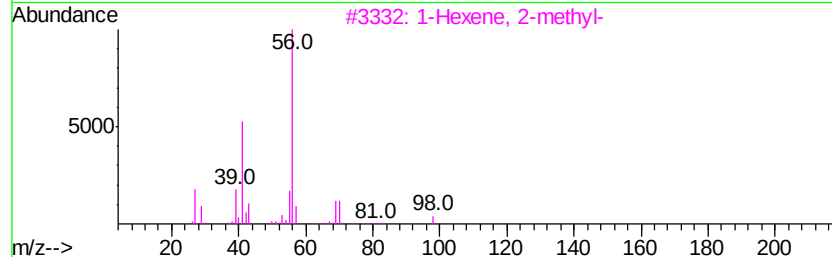
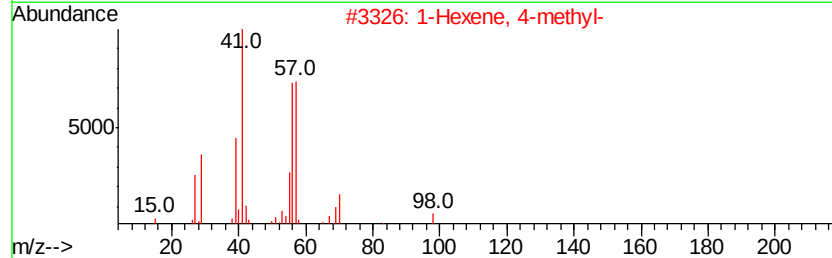
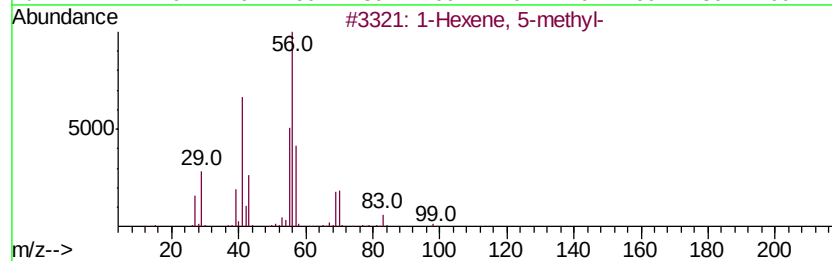
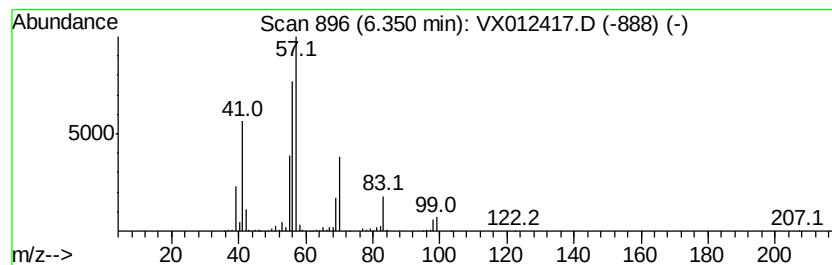
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexene, 5-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	57.97 ug/l	530769	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	59
2		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	56
3		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	52
4		1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	50
5		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0273

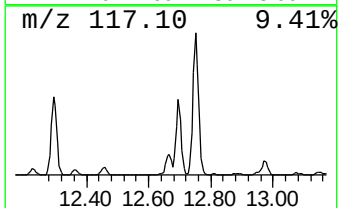
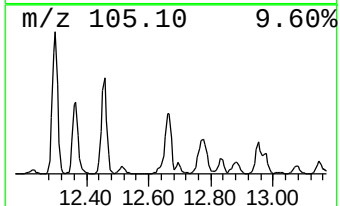
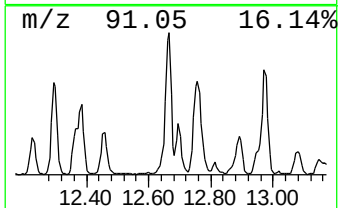
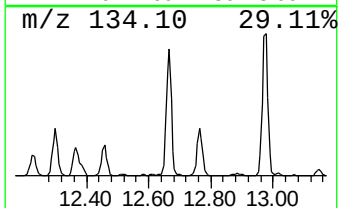
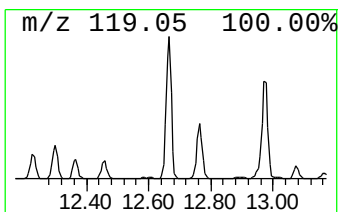
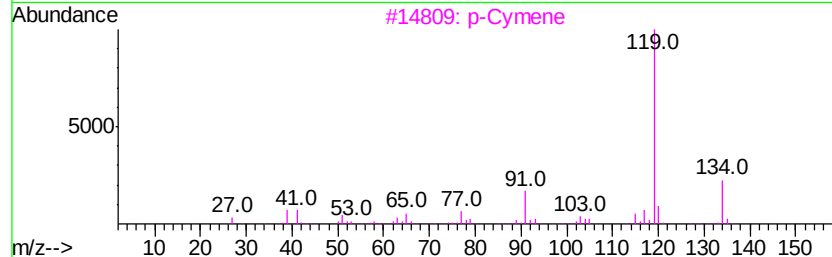
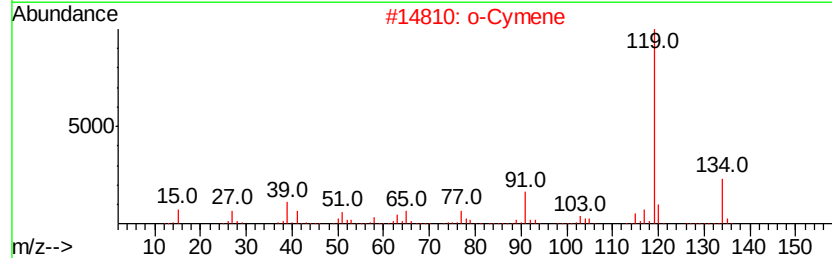
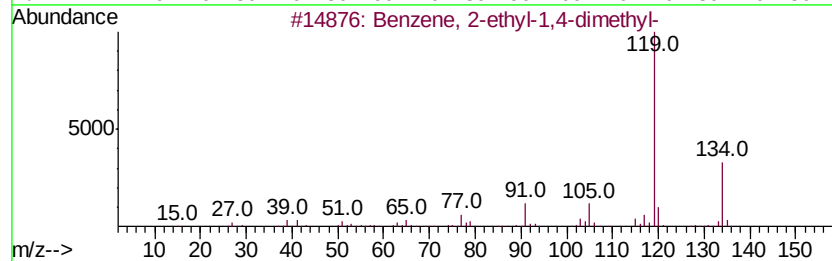
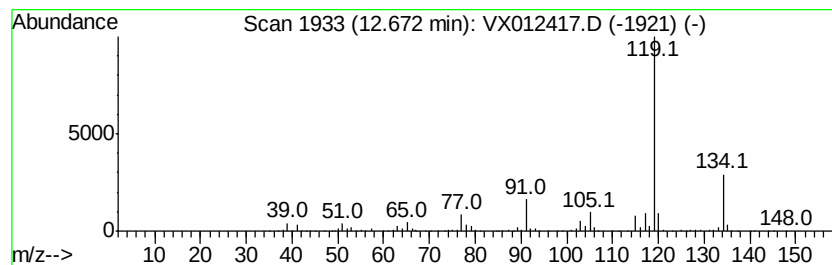
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	38.68 ug/l	505302	1,4-Dichlorobenzene-d4	12.07

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		p-Cymene	134	C10H14	000099-87-6	95
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

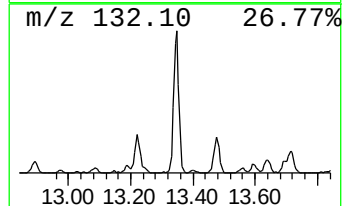
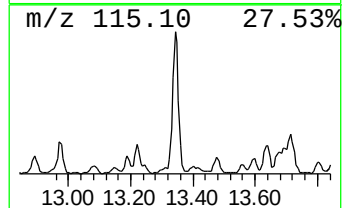
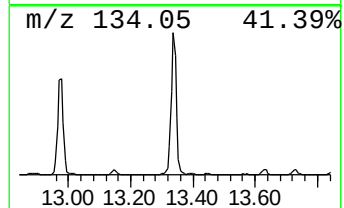
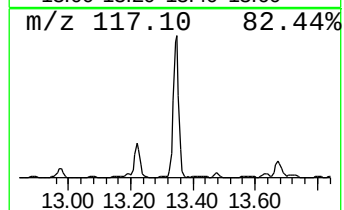
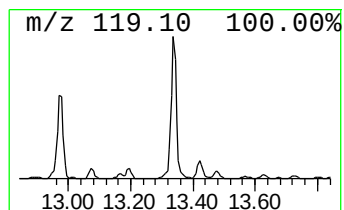
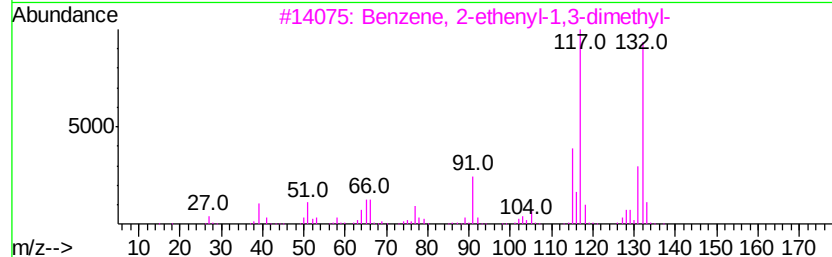
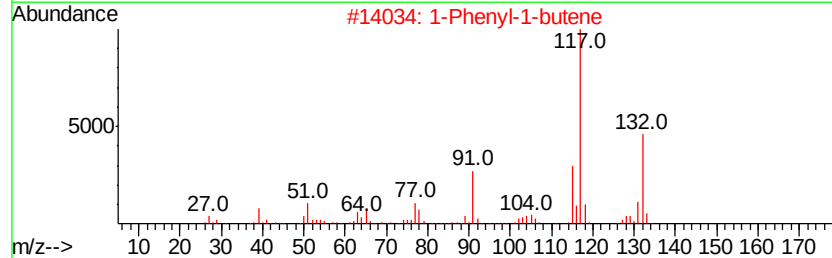
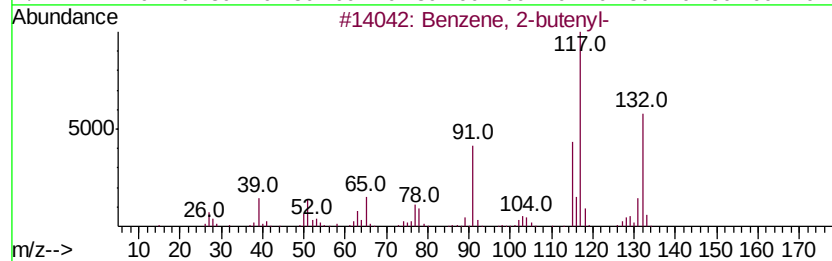
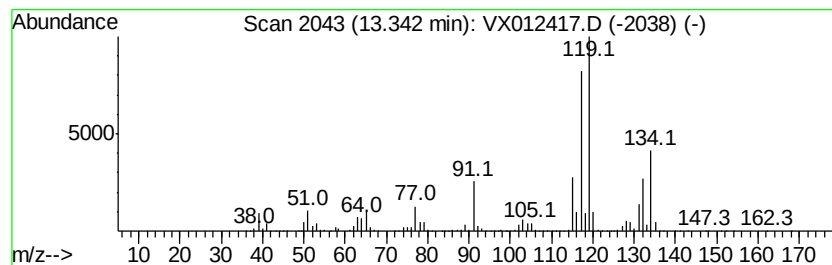
Instrument :
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ClientSampleId :
S13-0273

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-butenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	77.53 ug/l	1012870	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 2-butenyl-	132 C10H12	001560-06-1 87
2		1-Phenyl-1-butene	132 C10H12	000824-90-8 86
3		Benzene, 2-ethenyl-1,3-dimethyl-	132 C10H12	002039-90-9 64
4		Benzene, 1-methyl-4-(2-propenyl)-	132 C10H12	003333-13-9 64
5		3-Phenylbut-1-ene	132 C10H12	000934-10-1 64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091619\
Data File : VX012417.D
Acq On : 16 Sep 2019 19:52
Operator : JC/SP
Sample : K4830-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S13-0273

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091619W.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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Butane, 2,3-dimet...	2.83	84.6	ug/l	599808	1	5.65	354518	50.0
Pentane, 3-methyl-	3.16	187.9	ug/l	1332460	1	5.65	354518	50.0
Cyclopentane, met...	4.39	171.8	ug/l	1218400	1	5.65	354518	50.0
Pentane, 2,3-dime...	5.72	89.0	ug/l	631354	1	5.65	354518	50.0
Cyclopentane, 1,3...	6.25	38.6	ug/l	353650	2	6.85	457758	50.0
1-Hexene, 5-methyl-	6.35	58.0	ug/l	530769	2	6.85	457758	50.0
Benzene, 2-ethyl-...	12.67	38.7	ug/l	505302	4	12.07	653182	50.0
Benzene, 2-butenyl-	13.34	77.5	ug/l	1012870	4	12.07	653182	50.0