

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081718\
 Data File : VX004135.D
 Acq On : 17 Aug 2018 16:36
 Operator : JC/MD
 Sample : J4522-06
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-1R

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\82X081418W.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	1.075	75	80	94	rBV	1752236	2314568	70.13%	8.060%
2	1.404	130	134	138	rVB	30453	33690	1.02%	0.117%
3	1.788	192	197	209	rVB	537667	768489	23.28%	2.676%
4	2.398	290	297	312	rVB	54666	121471	3.68%	0.423%
5	2.599	323	330	341	rBV	90964	167456	5.07%	0.583%
6	2.849	362	371	382	rBV	261069	656736	19.90%	2.287%
7	2.934	382	385	395	rVB2	33001	68506	2.08%	0.239%
8	3.044	395	403	413	rVB	28595	65304	1.98%	0.227%
9	3.178	413	425	441	rBV3	463787	1482407	44.92%	5.162%
10	4.148	575	584	590	rBV	12620	37985	1.15%	0.132%
11	4.306	599	610	620	rBV2	117932	354668	10.75%	1.235%
12	4.404	620	626	636	rVB	15643	42604	1.29%	0.148%
13	4.556	636	651	666	rBV7	16359	74163	2.25%	0.258%
14	4.757	674	684	698	rVB	11522	39529	1.20%	0.138%
15	5.233	744	762	783	rBV8	23190	114116	3.46%	0.397%
16	5.507	795	807	822	rBV	184618	543922	16.48%	1.894%
17	5.666	822	833	837	rVV	246204	692994	21.00%	2.413%
18	5.720	837	842	862	rVB	303744	935097	28.33%	3.256%
19	5.940	867	878	889	rVV4	32617	111739	3.39%	0.389%
20	6.068	889	899	907	rVV	193687	505808	15.33%	1.761%
21	6.147	907	912	919	rVV	33143	87834	2.66%	0.306%
22	6.257	920	930	936	rVV3	144517	446649	13.53%	1.555%
23	6.348	936	945	957	rVV2	481809	1627316	49.31%	5.667%
24	6.452	957	962	975	rVB3	48580	135817	4.12%	0.473%
25	6.861	1018	1029	1039	rBV	385259	931451	28.22%	3.244%
26	7.257	1082	1094	1100	rVB7	13828	37373	1.13%	0.130%
27	7.440	1115	1124	1135	rBV3	73975	177764	5.39%	0.619%
28	7.574	1138	1146	1151	rBV	50293	103502	3.14%	0.360%
29	7.635	1151	1156	1160	rVV	67191	142088	4.31%	0.495%
30	7.677	1160	1163	1171	rVB2	38974	74433	2.26%	0.259%
31	7.848	1183	1191	1199	rVB3	48275	103778	3.14%	0.361%
32	8.055	1211	1225	1236	rVB	282493	602496	18.26%	2.098%
33	8.177	1236	1245	1254	rBV	473246	960374	29.10%	3.344%
34	8.257	1254	1258	1263	rVB	59307	92114	2.79%	0.321%

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Integration Parameters: RTEINT.P

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

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 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\82X081418W.M
 Title : SW846 8260

35	8.385	1273	1279	1285	rBV6	30972	68053	2.06%	0.237%
36	8.452	1285	1290	1294	rVV2	22830	39869	1.21%	0.139%
37	8.513	1294	1300	1307	rVV2	81889	177001	5.36%	0.616%
38	8.586	1307	1312	1319	rVB2	56803	101817	3.09%	0.355%
39	8.671	1319	1326	1329	rBV2	91372	187390	5.68%	0.653%
40	8.714	1329	1333	1344	rVB	979109	1551979	47.02%	5.404%
41	8.836	1349	1353	1357	rVV2	35498	55114	1.67%	0.192%
42	8.885	1357	1361	1363	rVV	25241	37239	1.13%	0.130%
43	8.915	1363	1366	1373	rVB	33017	49391	1.50%	0.172%
44	9.037	1381	1386	1392	rVB2	35461	64928	1.97%	0.226%
45	9.165	1392	1407	1412	rBV3	75586	155139	4.70%	0.540%
46	9.220	1412	1416	1420	rBV	48299	75366	2.28%	0.262%
47	9.439	1447	1452	1456	rBV3	22873	36296	1.10%	0.126%
48	9.525	1457	1466	1471	rVV	495120	758168	22.97%	2.640%
49	9.567	1471	1473	1479	rVB2	40799	61479	1.86%	0.214%
50	10.116	1558	1563	1569	rVB	774495	1046638	31.71%	3.645%
51	10.311	1589	1595	1609	rVB6	27482	95055	2.88%	0.331%
52	10.640	1639	1649	1656	rBV7	14000	40357	1.22%	0.141%
53	10.842	1675	1682	1689	rBV5	16184	44419	1.35%	0.155%
54	11.073	1716	1720	1724	rBV	25233	33102	1.00%	0.115%
55	11.140	1725	1731	1736	rBV	827613	1043940	31.63%	3.635%
56	11.671	1815	1818	1826	rVB2	25019	36943	1.12%	0.129%
57	11.768	1827	1834	1843	rBV4	22488	41270	1.25%	0.144%
58	11.945	1860	1863	1867	rVB	31354	37547	1.14%	0.131%
59	12.079	1880	1885	1893	rBV	1024651	1244158	37.70%	4.332%
60	12.232	1906	1910	1914	rVB	29384	35444	1.07%	0.123%
61	12.299	1914	1921	1927	rVV	2734430	3300361	100.00%	11.493%
62	12.372	1928	1933	1942	rVB	146063	197396	5.98%	0.687%
63	12.463	1942	1948	1952	rBV	54338	72264	2.19%	0.252%
64	12.530	1954	1959	1964	rVB	82777	106402	3.22%	0.371%
65	12.701	1983	1987	1992	rVV	173111	218586	6.62%	0.761%
66	12.756	1992	1996	2003	rVB	450833	594274	18.01%	2.069%
67	12.896	2012	2019	2025	rVB2	38194	60545	1.83%	0.211%
68	12.981	2025	2033	2038	rBV2	67167	119830	3.63%	0.417%
69	13.085	2045	2050	2058	rVB2	67539	114138	3.46%	0.397%
70	13.195	2058	2068	2070	rBV2	45223	79412	2.41%	0.277%
71	13.225	2070	2073	2076	rBV	65064	70405	2.13%	0.245%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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72	13.353	2089	2094	2099	rBV	798323	971125	29.42%	3.382%
73	13.402	2099	2102	2106	rVB3	25324	36229	1.10%	0.126%
74	13.481	2112	2115	2120	rVB2	37309	48739	1.48%	0.170%
75	13.646	2137	2142	2145	rVV2	87671	130535	3.96%	0.455%
76	13.719	2145	2154	2160	rVB3	137501	294440	8.92%	1.025%
77	13.981	2192	2197	2201	rBV	60558	80647	2.44%	0.281%
78	14.030	2201	2205	2209	rBV	54570	66597	2.02%	0.232%
79	14.134	2217	2222	2226	rBV	46052	57266	1.74%	0.199%
80	14.274	2240	2245	2251	rBV	51376	81566	2.47%	0.284%
81	14.377	2259	2262	2267	rBV	29349	36455	1.10%	0.127%
82	14.432	2267	2271	2276	rVB2	46691	64073	1.94%	0.223%
83	14.542	2284	2289	2294	rBV2	37941	59185	1.79%	0.206%
84	14.658	2302	2308	2313	rBV3	22479	47554	1.44%	0.166%
85	14.847	2334	2339	2343	rBV4	20160	36979	1.12%	0.129%

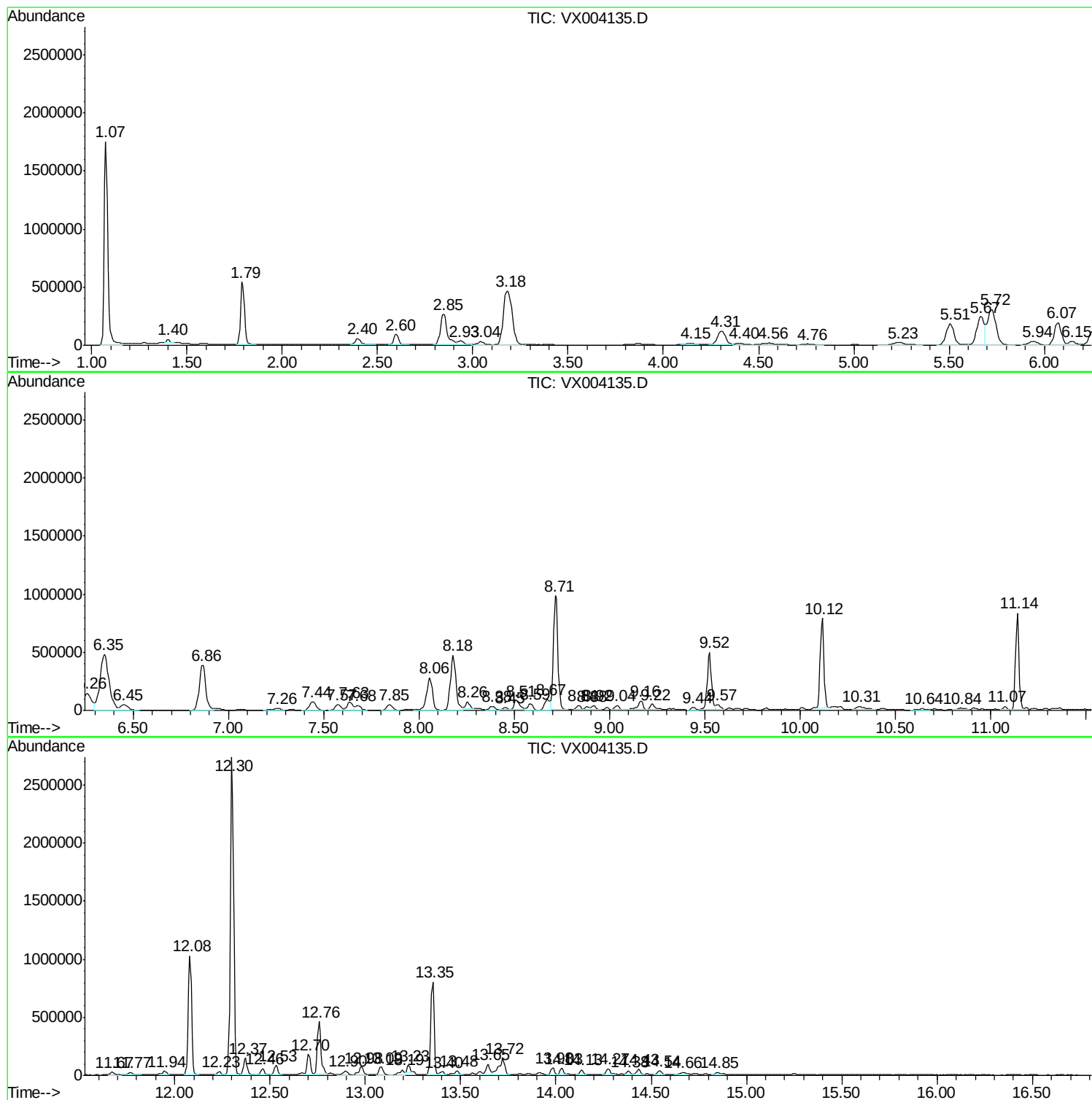
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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



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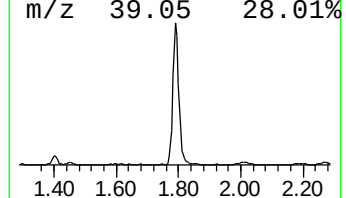
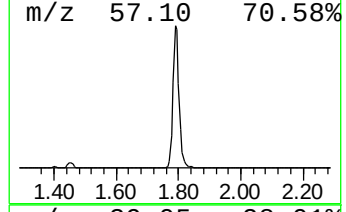
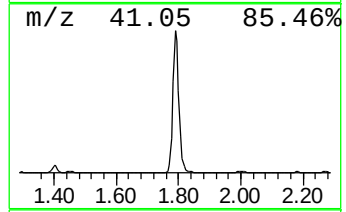
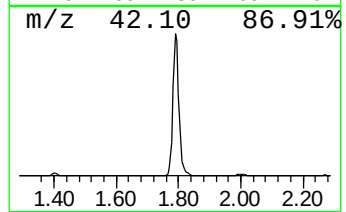
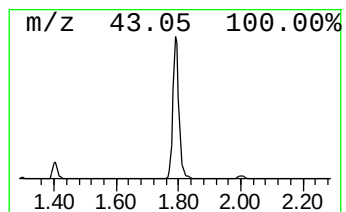
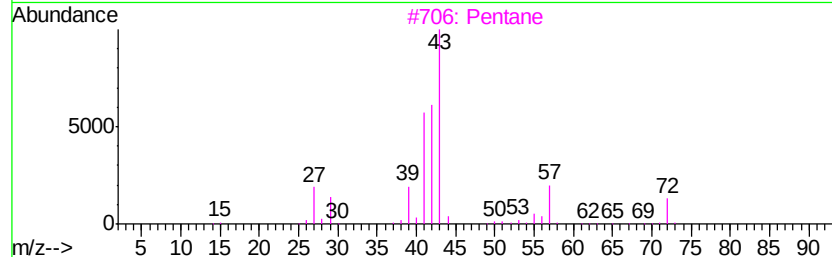
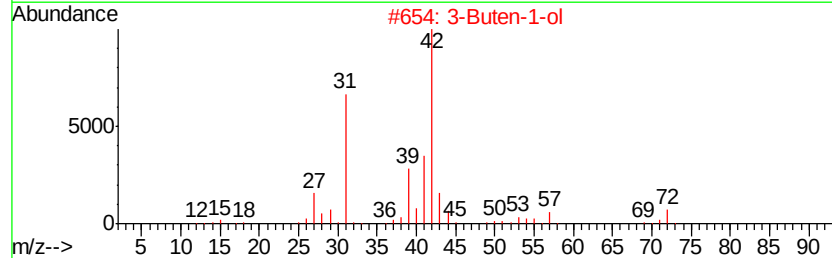
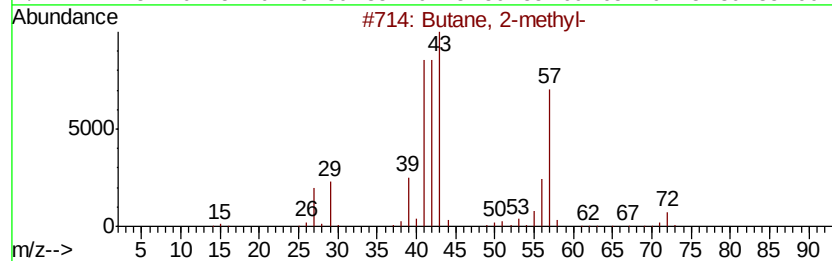
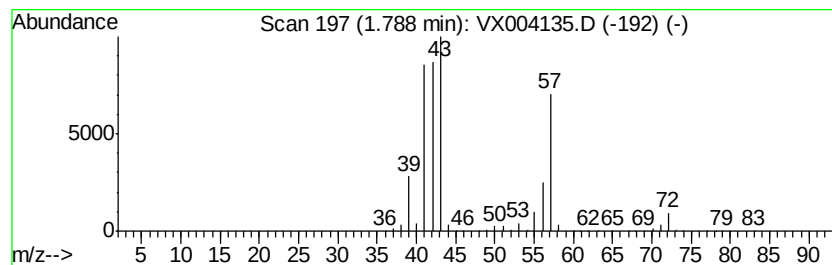
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	55.45 ug/l	768489	Pentafluorobenzene	5.67

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	47
3		Pentane	72	C5H12	000109-66-0	39
4		1-Butene	56	C4H8	000106-98-9	10
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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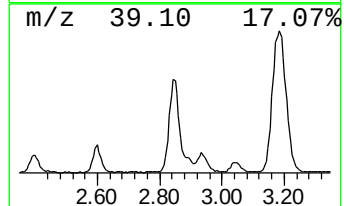
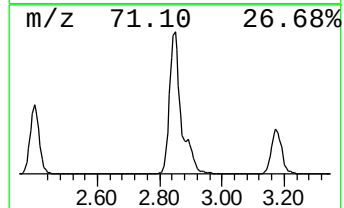
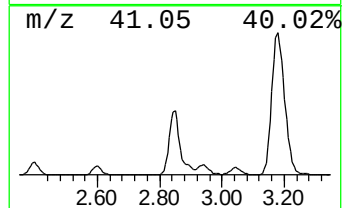
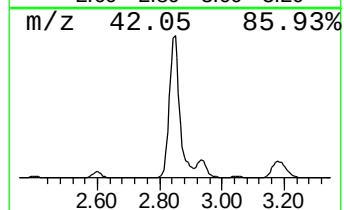
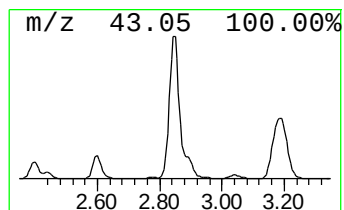
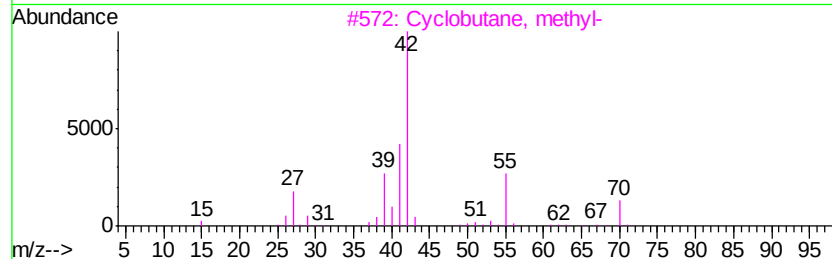
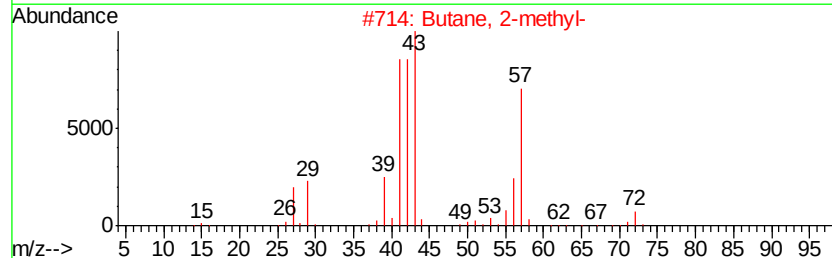
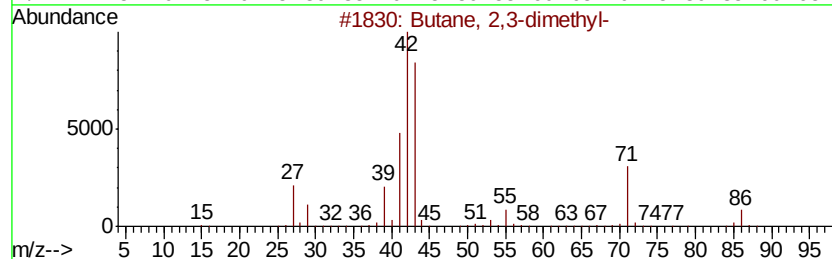
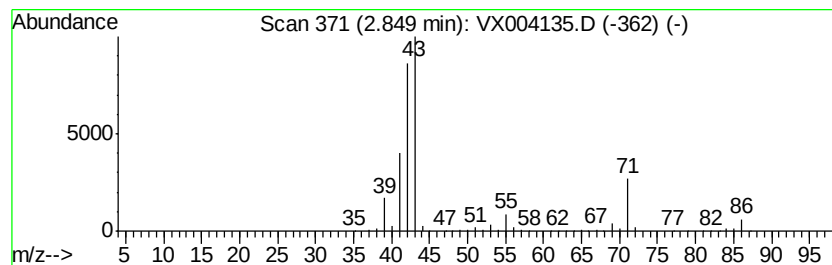
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	47.38 ug/l	656736	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2		Butane, 2-methyl-	72	C5H12	000078-78-4	38
3		Cyclobutane, methyl-	70	C5H10	000598-61-8	38
4		Pentane, 2-methyl-	86	C6H14	000107-83-5	38
5		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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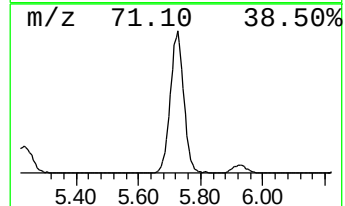
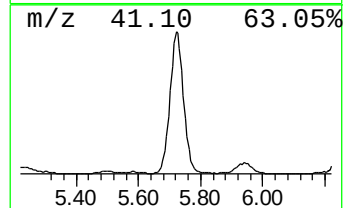
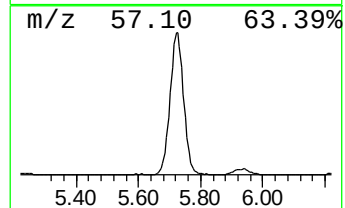
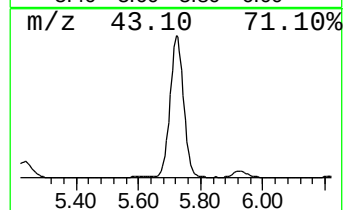
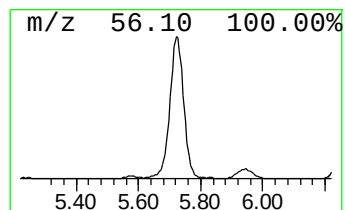
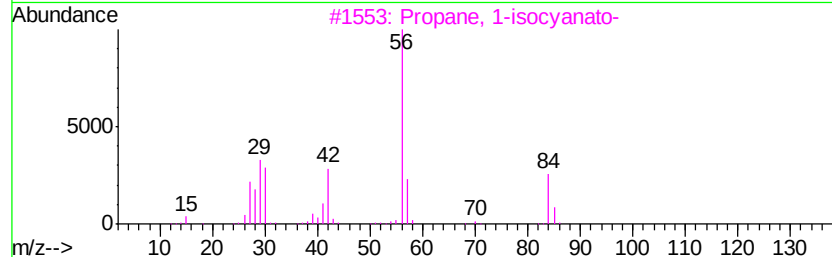
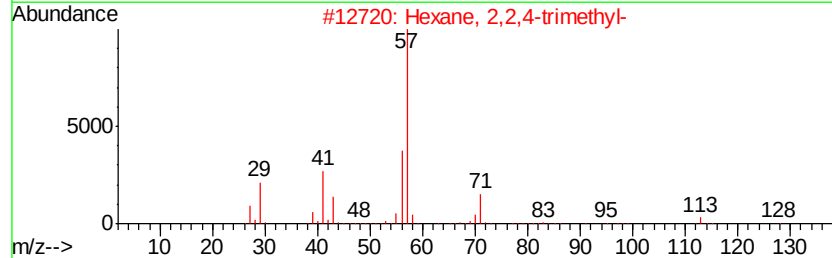
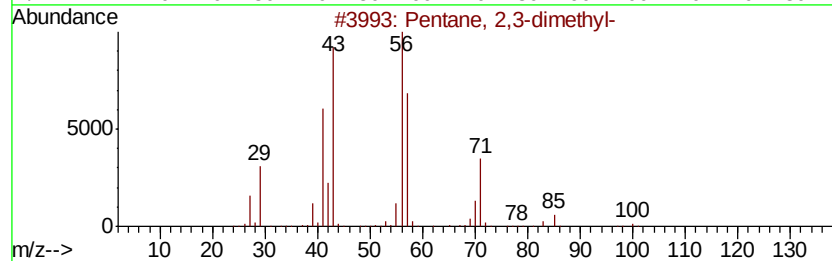
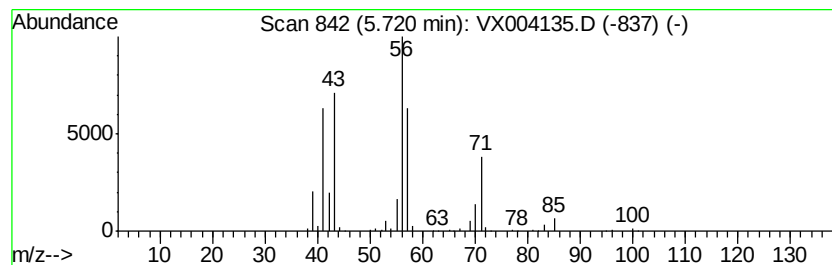
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	67.47 ug/l	935097	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50
3		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38
4		4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	37
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	37



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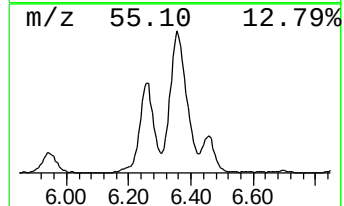
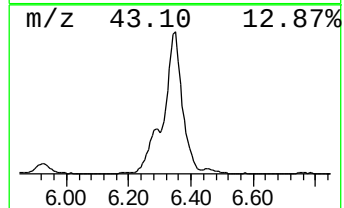
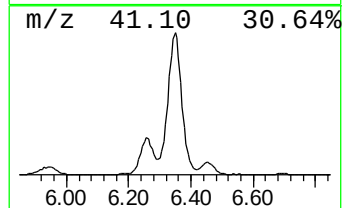
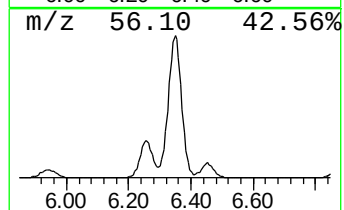
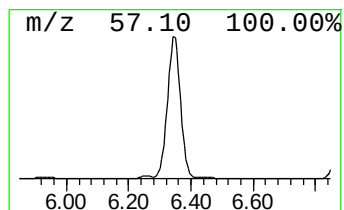
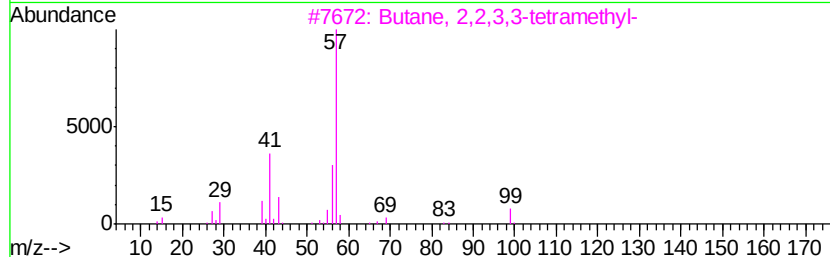
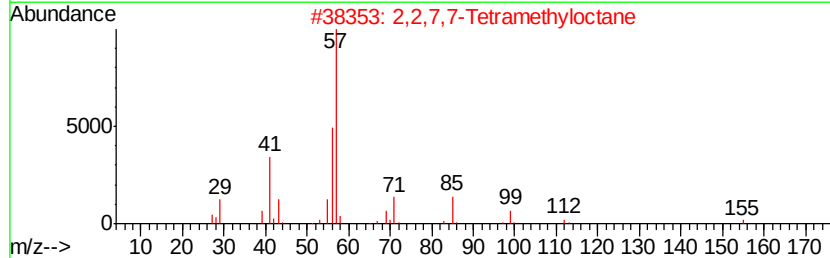
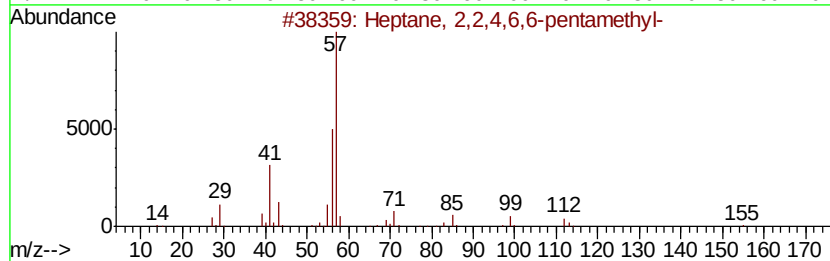
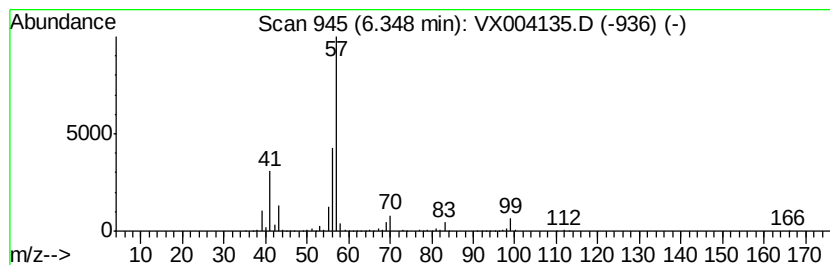
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Quant Title : SW846 8260

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

Peak Number 5 Heptane, 2,2,4,6,6-pentamet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	87.35 ug/l	1627320	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
2		2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	64
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
4		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
5		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004135.D
Acq On : 17 Aug 2018 16:36
Operator : JC/MD
Sample : J4522-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

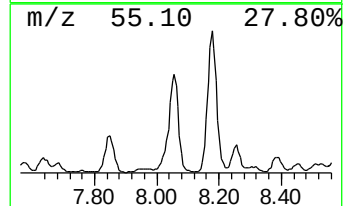
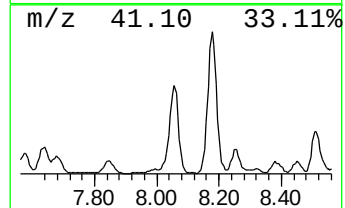
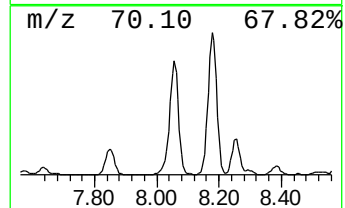
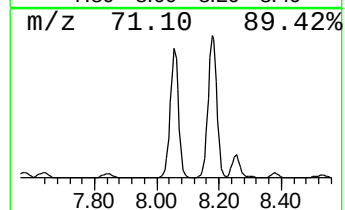
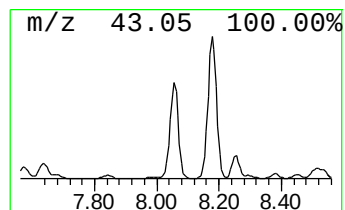
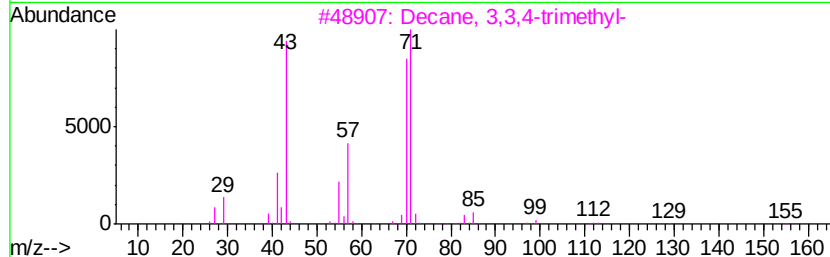
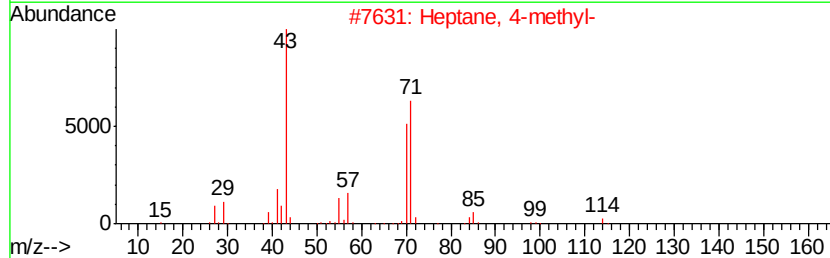
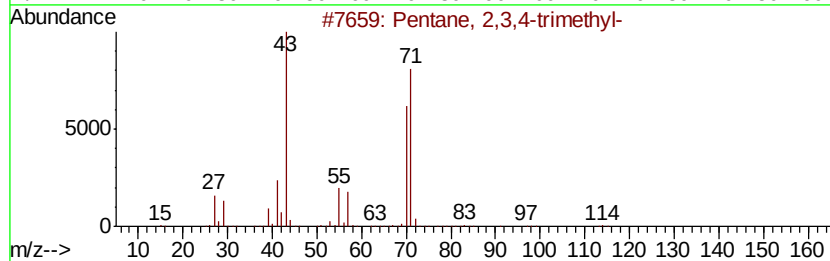
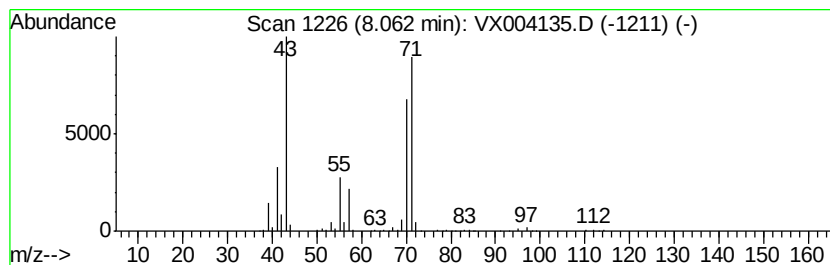
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	32.34 ug/l	602496	1,4-Difluorobenzene	6.87

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		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78
4		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
5		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004135.D
Acq On : 17 Aug 2018 16:36
Operator : JC/MD
Sample : J4522-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

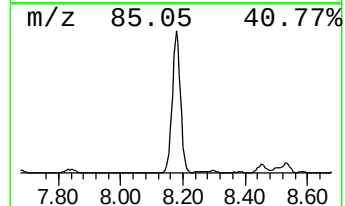
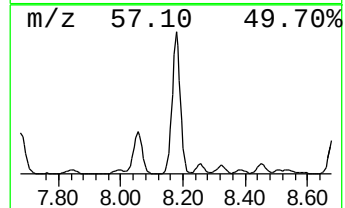
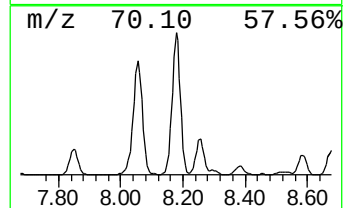
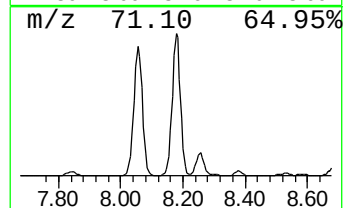
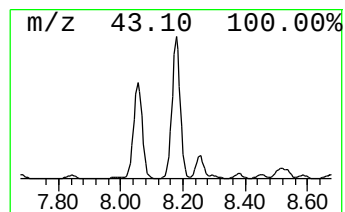
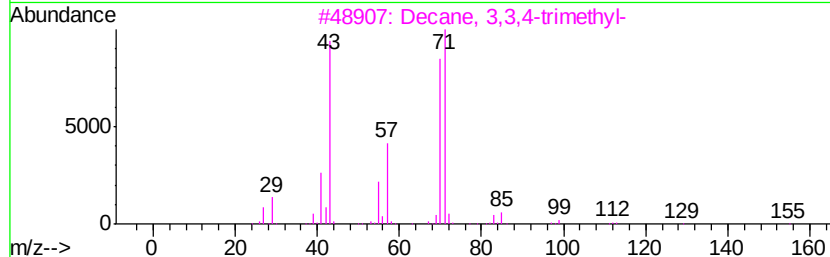
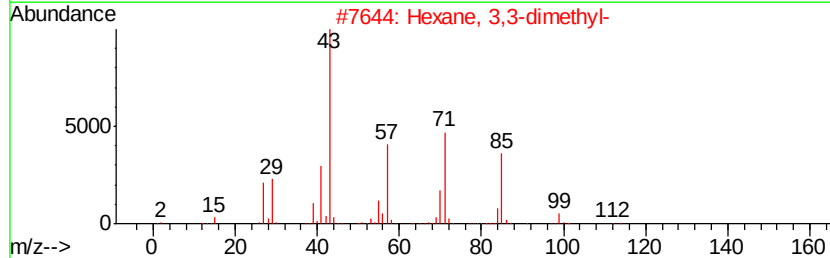
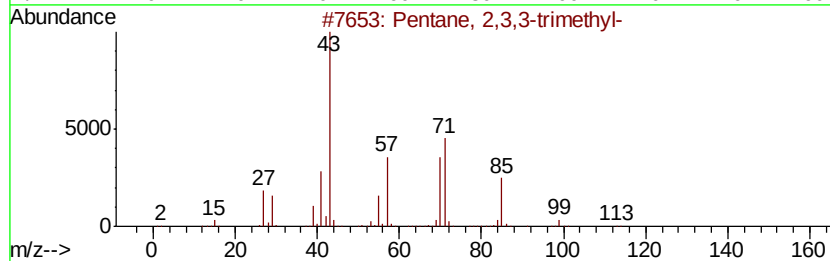
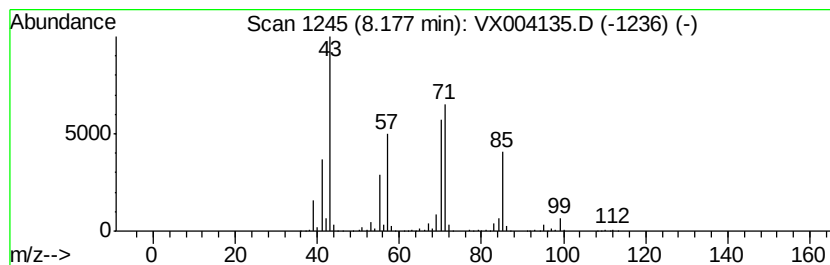
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	51.55 ug/l	960374	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
4		Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	50
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004135.D
Acq On : 17 Aug 2018 16:36
Operator : JC/MD
Sample : J4522-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-1R

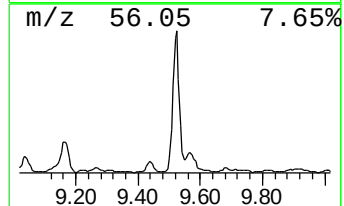
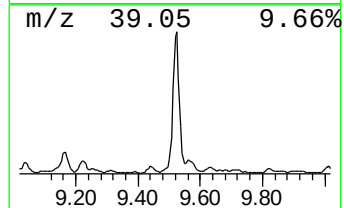
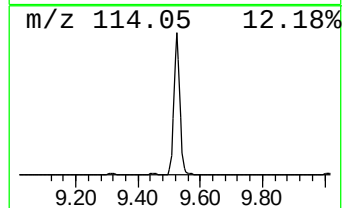
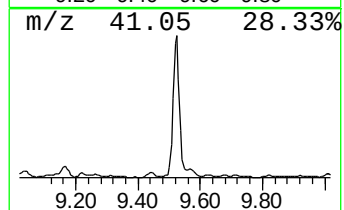
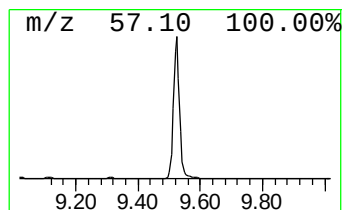
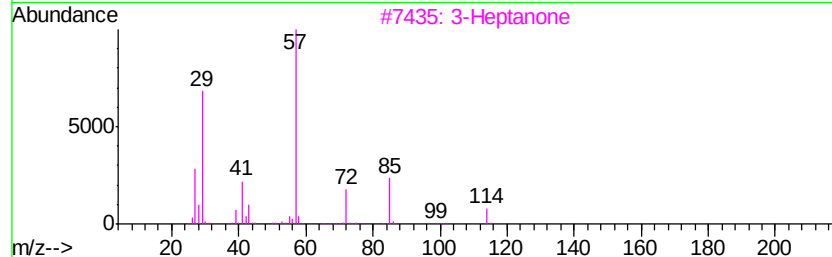
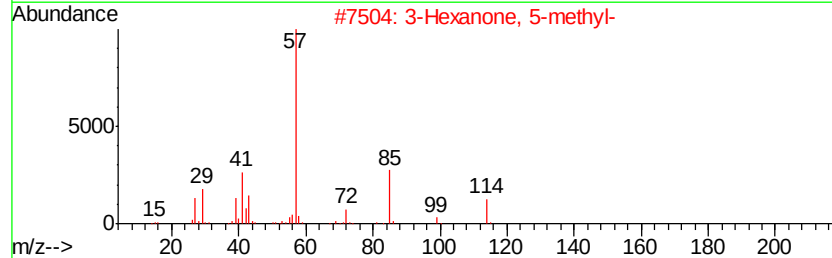
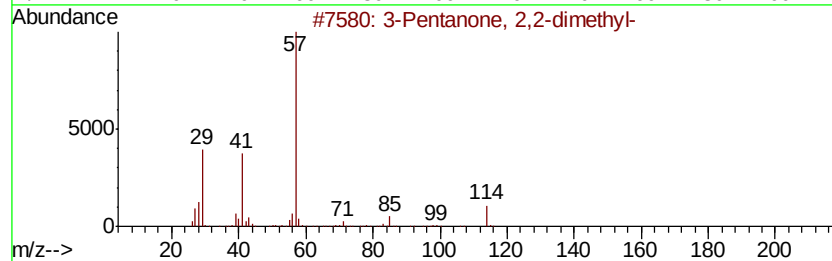
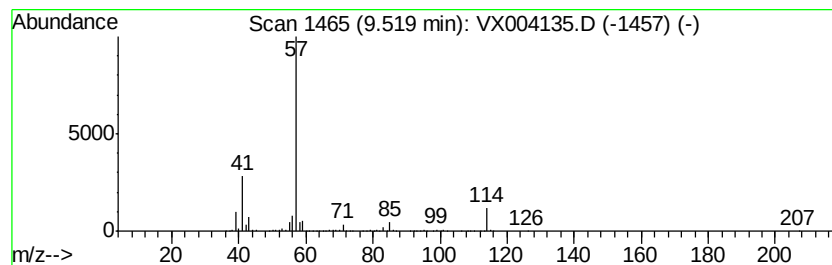
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Quant Title : SW846 8260

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

Peak Number 8 3-Pentanone, 2,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	36.22 ug/l	758168	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	83
2		3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
3		3-Heptanone	114	C7H14O	000106-35-4	50
4		Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	40
5		3,4-Hexanedione	114	C6H10O2	004437-51-8	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004135.D
Acq On : 17 Aug 2018 16:36
Operator : JC/MD
Sample : J4522-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

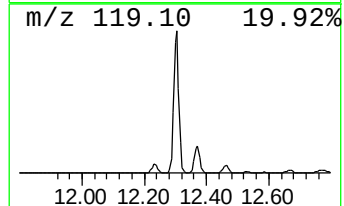
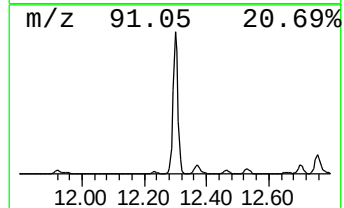
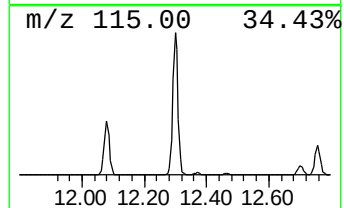
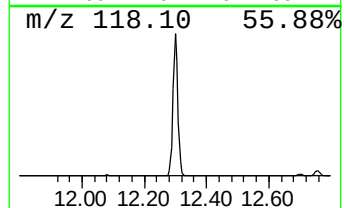
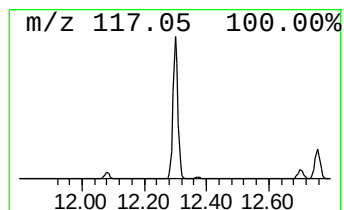
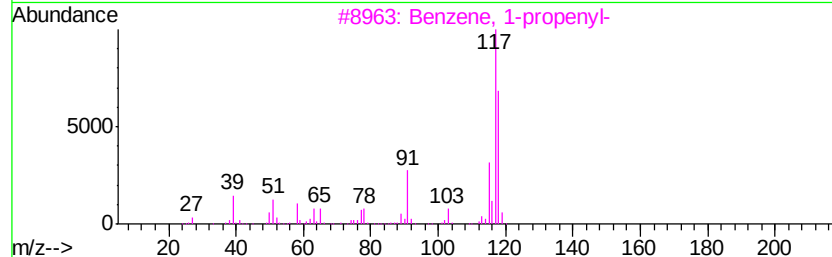
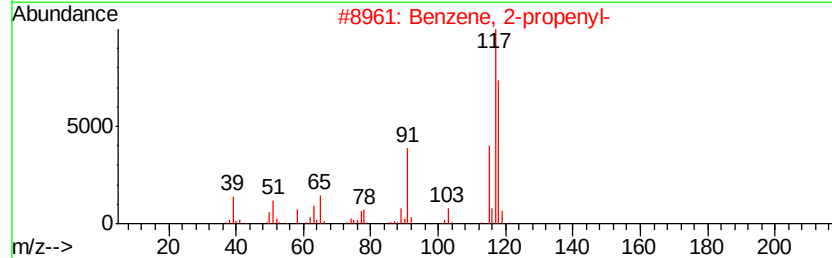
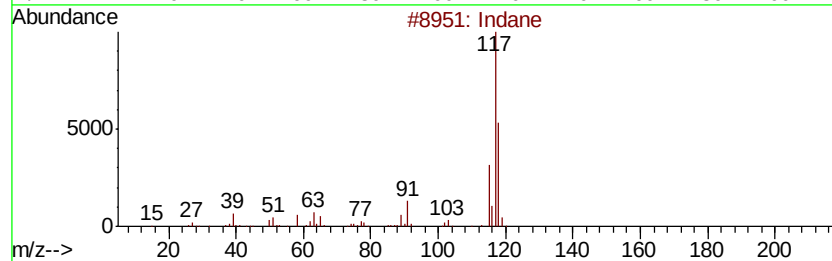
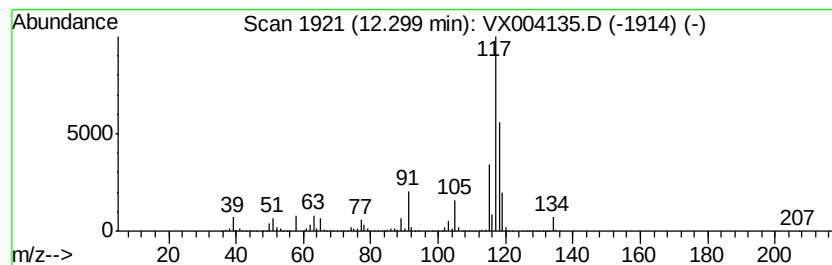
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	132.63 ug/l	3300360	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	70
2		Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3		Benzene, 1-propenyl-	118	C9H10	000637-50-3	62
4		Benzene, cyclopropyl-	118	C9H10	000873-49-4	62
5		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081718\
Data File : VX004135.D
Acq On : 17 Aug 2018 16:36
Operator : JC/MD
Sample : J4522-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

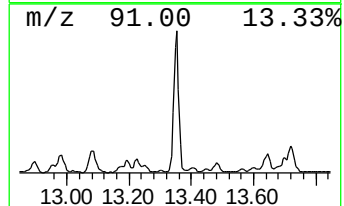
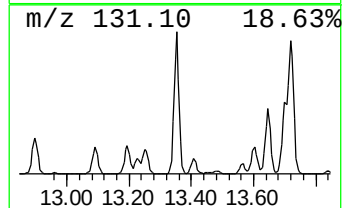
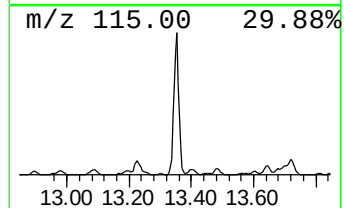
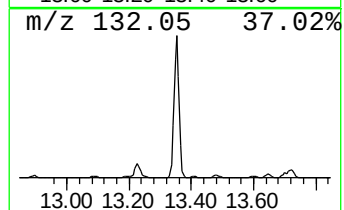
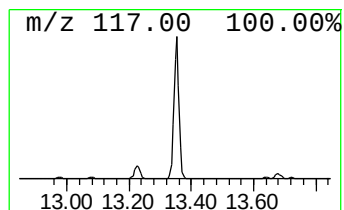
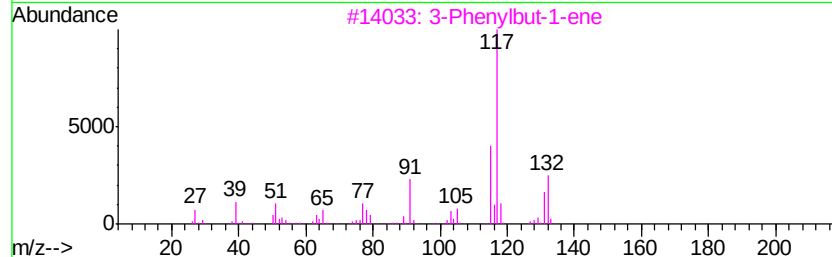
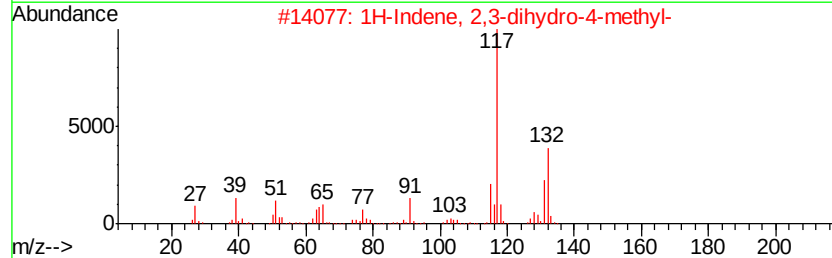
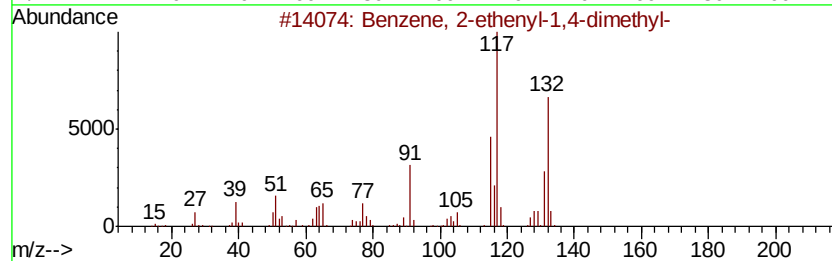
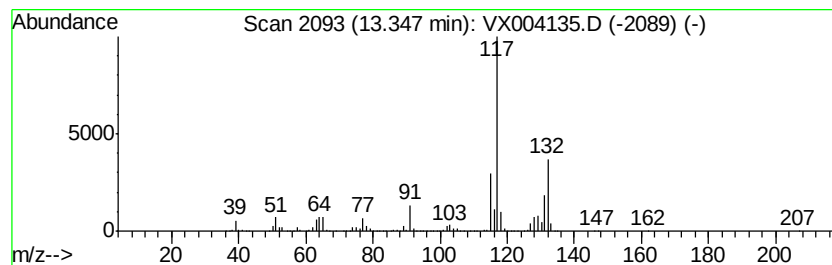
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	39.03 ug/l	971125	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
2		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX081718\
Data File : VX004135.D
Acq On : 17 Aug 2018 16:36
Operator : JC/MD
Sample : J4522-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.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-	1.79	55.5	ug/l	768489	1	5.67	692994	50.0
Butane, 2,3-dimet...	2.85	47.4	ug/l	656736	1	5.67	692994	50.0
Pentane, 2,3-dime...	5.72	67.5	ug/l	935097	1	5.67	692994	50.0
Heptane, 2,2,4,6,...	6.35	87.3	ug/l	1627320	2	6.87	931451	50.0
Pentane, 2,3,4-tr...	8.06	32.3	ug/l	602496	2	6.87	931451	50.0
Pentane, 2,3,3-tr...	8.18	51.5	ug/l	960374	2	6.87	931451	50.0
3-Pentanone, 2,2-...	9.52	36.2	ug/l	758168	3	10.12	1046640	50.0
Indane	12.30	132.6	ug/l	3300360	4	12.08	1244160	50.0
Benzene, 2-etheny...	13.35	39.0	ug/l	971125	4	12.08	1244160	50.0