

Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX111618\
 Data File : VX006049.D
 Acq On : 16 Nov 2018 14:55
 Operator : JC/MD
 Sample : J5965-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 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\82X110718W.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	1.404	36	41	45	rBV	11488	11599	1.21%	0.126%
2	1.623	65	77	84	rVB8	4778	15365	1.61%	0.167%
3	1.782	98	103	117	rVB	155684	229003	23.95%	2.492%
4	2.391	196	203	215	rBV	16405	35652	3.73%	0.388%
5	2.617	234	240	249	rVB	12563	22696	2.37%	0.247%
6	2.843	268	277	288	rBV	88930	218510	22.85%	2.378%
7	2.934	288	292	300	rVV2	12897	28170	2.95%	0.307%
8	3.019	300	306	309	rVV	4230	9807	1.03%	0.107%
9	3.062	309	313	322	rVV	8263	17437	1.82%	0.190%
10	3.172	322	331	348	rVB3	118106	440813	46.10%	4.797%
11	4.135	480	489	495	rBV2	3542	11341	1.19%	0.123%
12	4.300	504	516	525	rBV2	35467	107034	11.19%	1.165%
13	4.397	526	532	542	rVB3	7830	21064	2.20%	0.229%
14	4.537	542	555	574	rVB9	5383	25815	2.70%	0.281%
15	5.232	658	669	689	rVB5	7756	33622	3.52%	0.366%
16	5.501	702	713	724	rBV	78291	223380	23.36%	2.431%
17	5.665	729	740	745	rVV	141629	410825	42.96%	4.471%
18	5.726	745	750	766	rVB2	102822	298356	31.20%	3.247%
19	5.940	772	785	797	rBV6	10278	33694	3.52%	0.367%
20	6.068	797	806	814	rVV	85148	225235	23.55%	2.451%
21	6.141	814	818	826	rVV2	14027	38071	3.98%	0.414%
22	6.257	828	837	843	rVV3	46292	143792	15.04%	1.565%
23	6.348	843	852	863	rVV2	158707	528082	55.23%	5.747%
24	6.452	863	869	882	rVB3	15027	43386	4.54%	0.472%
25	6.860	926	936	946	rBV2	185987	465980	48.73%	5.071%
26	7.256	989	1001	1008	rVB4	4690	10641	1.11%	0.116%
27	7.445	1023	1032	1044	rBV3	22172	53816	5.63%	0.586%
28	7.573	1044	1053	1058	rBV2	14609	30742	3.21%	0.335%
29	7.634	1058	1063	1067	rVV3	19720	42363	4.43%	0.461%
30	7.677	1068	1070	1077	rVB2	11208	18041	1.89%	0.196%
31	7.848	1090	1098	1105	rVB3	14796	30792	3.22%	0.335%
32	7.988	1105	1121	1123	rBV6	3834	12398	1.30%	0.135%
33	8.055	1123	1132	1142	rVB	88958	184228	19.27%	2.005%
34	8.177	1144	1152	1160	rBV	140818	286552	29.97%	3.118%

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Integration Parameters: RTEINT.P

Integrator: RTE
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35	8.256	1160	1165	1170	rBV	16655	27139	2.84%	0.295%
36	8.384	1179	1186	1192	rBV6	9673	21821	2.28%	0.237%
37	8.451	1192	1197	1201	rVV	7049	11485	1.20%	0.125%
38	8.506	1201	1206	1214	rVV2	21044	44140	4.62%	0.480%
39	8.579	1214	1218	1226	rVB	16169	27977	2.93%	0.304%
40	8.671	1226	1233	1235	rBV2	28043	50171	5.25%	0.546%
41	8.714	1235	1240	1251	rVB	388486	604726	63.24%	6.581%
42	8.835	1256	1260	1264	rVV2	10771	16234	1.70%	0.177%
43	8.878	1264	1267	1270	rVV2	6967	11317	1.18%	0.123%
44	8.909	1270	1272	1278	rVB2	9874	14033	1.47%	0.153%
45	9.037	1288	1293	1299	rVB2	12106	21921	2.29%	0.239%
46	9.165	1306	1314	1319	rVB2	25049	46525	4.87%	0.506%
47	9.220	1319	1323	1327	rBV	13682	21517	2.25%	0.234%
48	9.439	1354	1359	1363	rBV2	10142	15418	1.61%	0.168%
49	9.518	1363	1372	1377	rVV	133693	206677	21.61%	2.249%
50	9.567	1377	1380	1386	rVB4	12978	22347	2.34%	0.243%
51	9.719	1401	1405	1415	rVB3	5103	12041	1.26%	0.131%
52	9.823	1415	1422	1425	rBV2	6497	11362	1.19%	0.124%
53	10.116	1464	1470	1477	rVV	397503	532048	55.64%	5.790%
54	10.311	1496	1502	1504	rBV4	5776	11430	1.20%	0.124%
55	10.841	1581	1589	1596	rBV7	5593	14159	1.48%	0.154%
56	11.018	1612	1618	1622	rBV	6892	10355	1.08%	0.113%
57	11.073	1622	1627	1632	rBV	10150	13985	1.46%	0.152%
58	11.140	1632	1638	1643	rBV	303785	396934	41.51%	4.319%
59	11.670	1721	1725	1733	rVB	9939	14695	1.54%	0.160%
60	11.768	1733	1741	1745	rBV4	7381	12392	1.30%	0.135%
61	11.945	1767	1770	1774	rVB	10594	12703	1.33%	0.138%
62	12.079	1787	1792	1799	rBV	403674	492965	51.55%	5.365%
63	12.231	1813	1817	1821	rBV	9141	10303	1.08%	0.112%
64	12.298	1821	1828	1835	rVV	782504	956229	100.00%	10.406%
65	12.371	1835	1840	1848	rVB	44792	62772	6.56%	0.683%
66	12.463	1848	1855	1859	rBV	14649	20515	2.15%	0.223%
67	12.530	1859	1866	1870	rVB2	25525	34996	3.66%	0.381%
68	12.670	1882	1889	1891	rBV	34606	46332	4.85%	0.504%
69	12.701	1891	1894	1899	rVV	53328	66030	6.91%	0.719%
70	12.755	1899	1903	1910	rVB	129781	172976	18.09%	1.882%
71	12.896	1919	1926	1932	rVB2	13150	20243	2.12%	0.220%

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Integration Parameters: RTEINT.P

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 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
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72	12.975	1932	1939	1944	rBV	21395	38172	3.99%	0.415%
73	13.079	1952	1956	1964	rBV3	22613	36156	3.78%	0.393%
74	13.194	1964	1975	1977	rBV3	12933	23815	2.49%	0.259%
75	13.225	1977	1980	1983	rBV	41199	46034	4.81%	0.501%
76	13.353	1996	2001	2006	rVB	243609	295230	30.87%	3.213%
77	13.481	2018	2022	2027	rVB3	12895	18126	1.90%	0.197%
78	13.603	2038	2042	2045	rVV	12827	19277	2.02%	0.210%
79	13.646	2045	2049	2052	rVV2	27287	39925	4.18%	0.434%
80	13.700	2052	2058	2059	rVV2	22882	37759	3.95%	0.411%
81	13.719	2059	2061	2069	rVB2	40727	53374	5.58%	0.581%
82	13.914	2089	2093	2099	rVB2	6843	10266	1.07%	0.112%
83	13.981	2099	2104	2108	rBV2	17620	23502	2.46%	0.256%
84	14.030	2108	2112	2116	rBV	15846	21485	2.25%	0.234%
85	14.133	2125	2129	2140	rVB	15740	26368	2.76%	0.287%
86	14.273	2148	2152	2156	rBV	13682	17721	1.85%	0.193%
87	14.377	2166	2169	2172	rBV	9401	12173	1.27%	0.132%
88	14.432	2175	2178	2183	rVB2	12352	17377	1.82%	0.189%
89	14.542	2191	2196	2201	rBV2	12039	16728	1.75%	0.182%
90	14.664	2209	2216	2224	rBV4	6702	15930	1.67%	0.173%
91	14.840	2240	2245	2250	rBV2	14334	22758	2.38%	0.248%

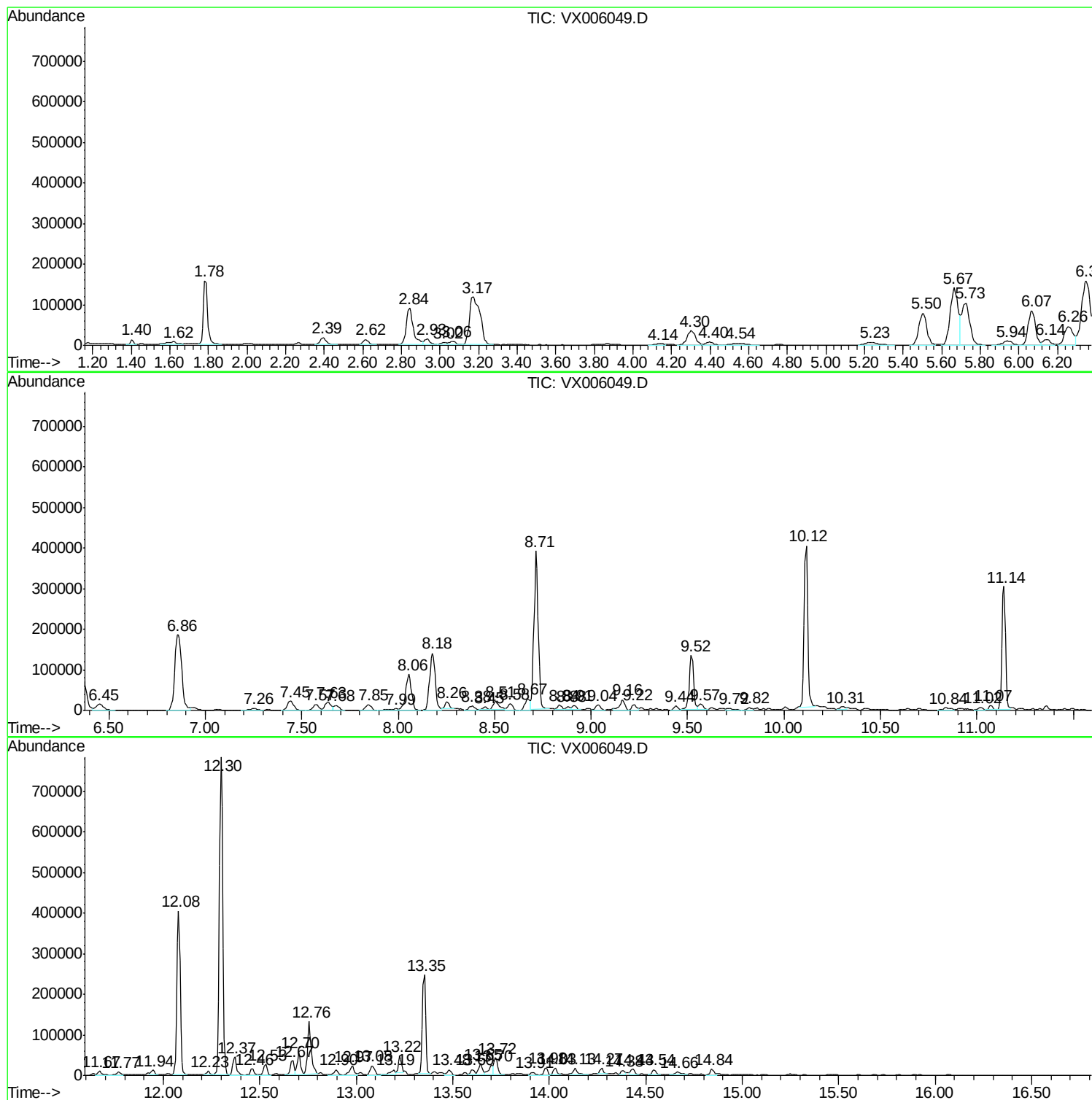
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Instrument :
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ClientSampleId :
MW-1R

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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



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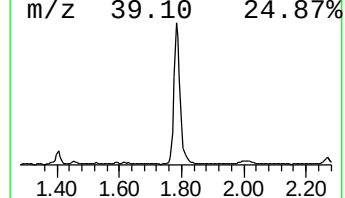
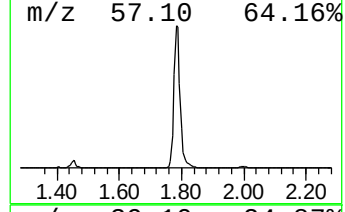
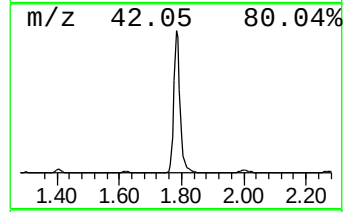
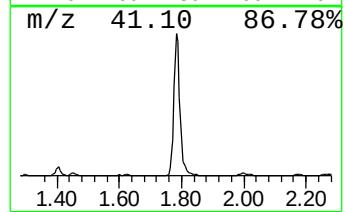
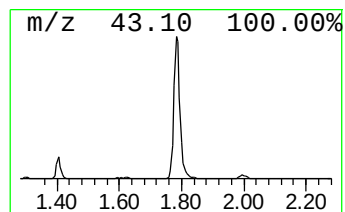
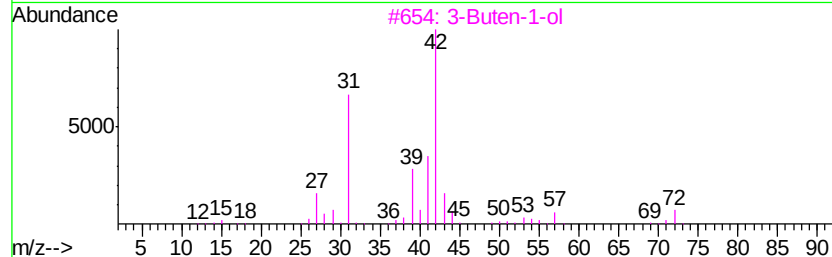
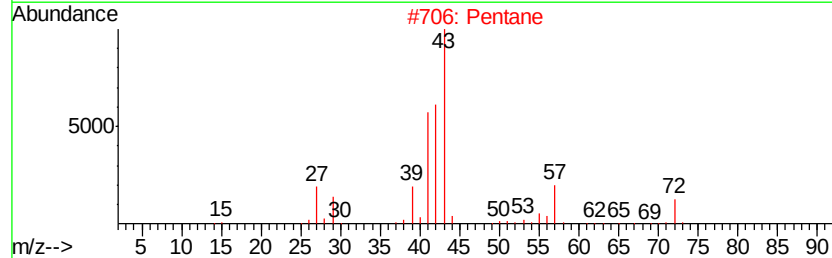
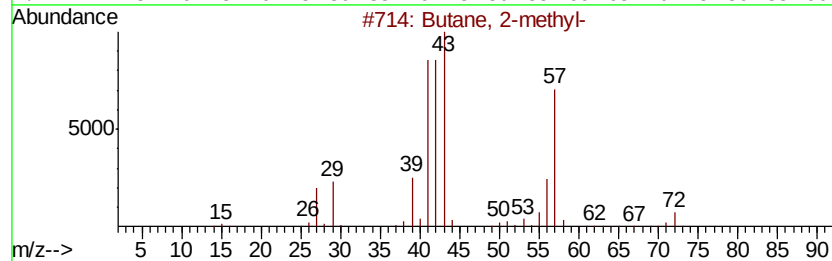
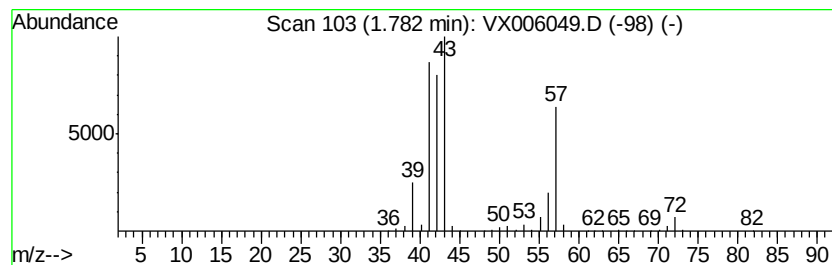
Instrument :
MSVOA_X
ClientSampled :
MW-1R

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	27.87 ug/l	229003	Pentafluorobenzene	5.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butane, 2-methyl-	72 C5H12	000078-78-4	94
2	Pentane	72 C5H12	000109-66-0	36
3	3-Buten-1-ol	72 C4H8O	000627-27-0	28
4	1-Butene	56 C4H8	000106-98-9	10
5	1-Propene, 2-methyl-	56 C4H8	000115-11-7	9



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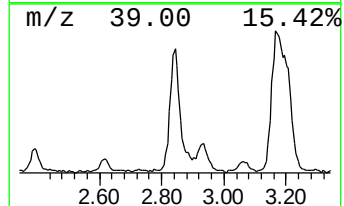
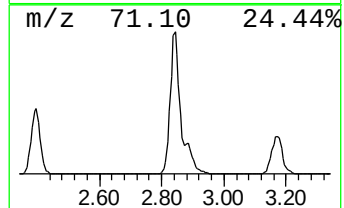
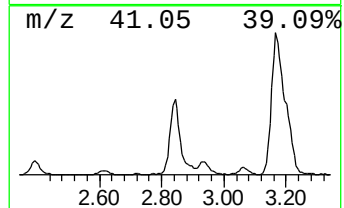
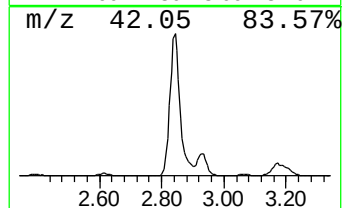
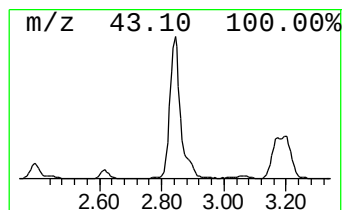
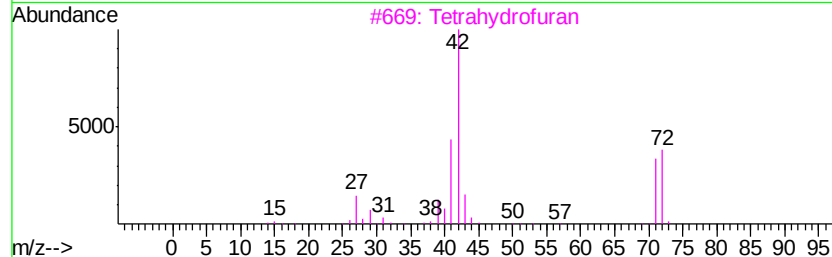
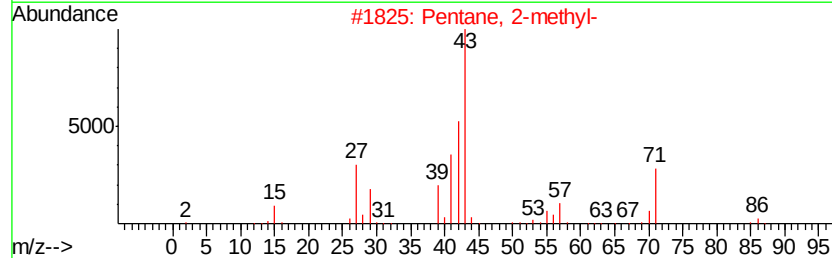
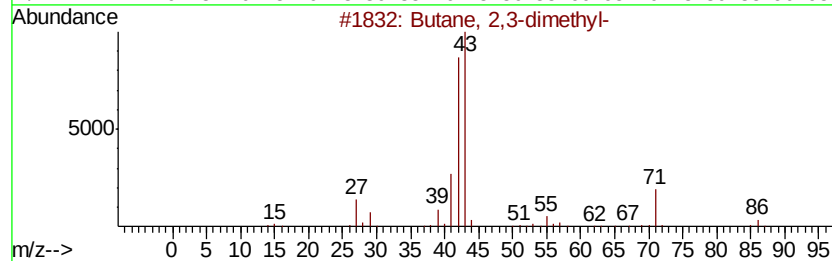
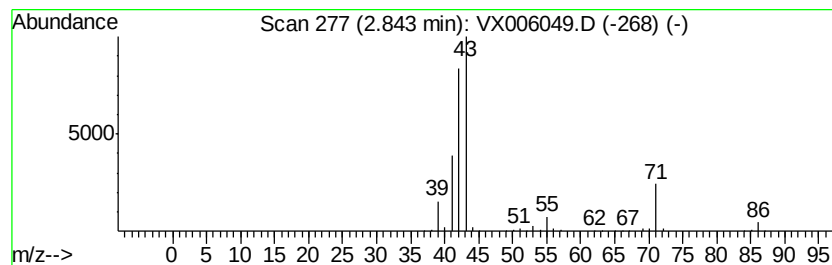
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	26.59 ug/l	218510	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
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	36
5			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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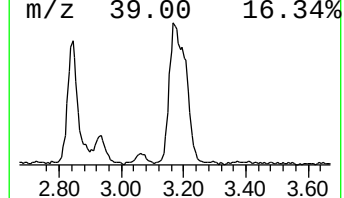
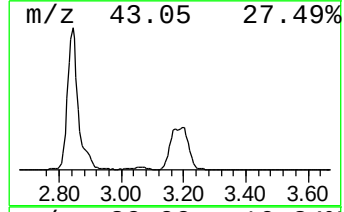
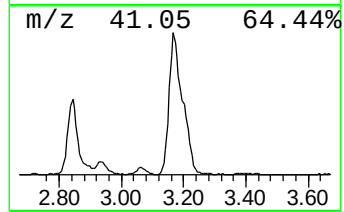
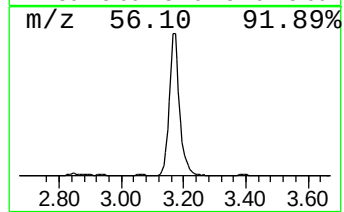
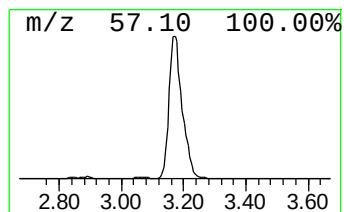
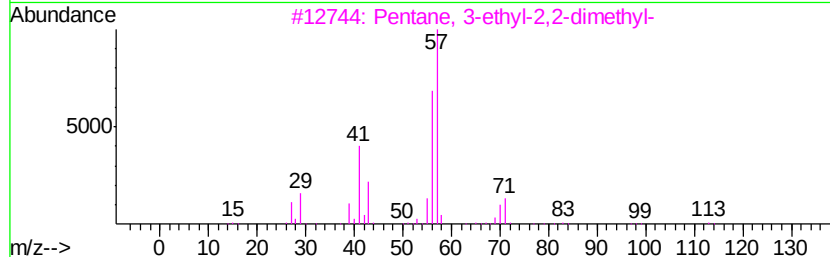
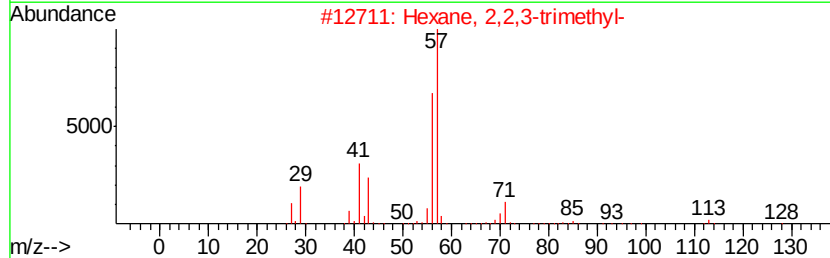
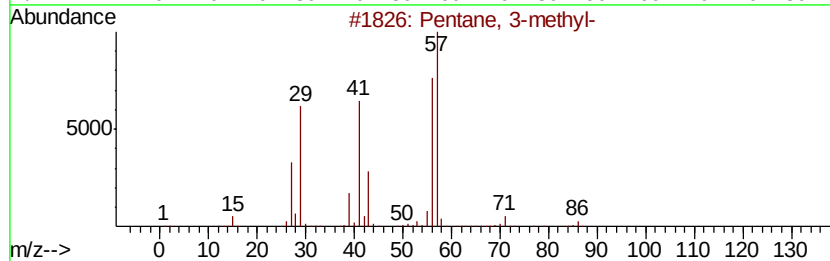
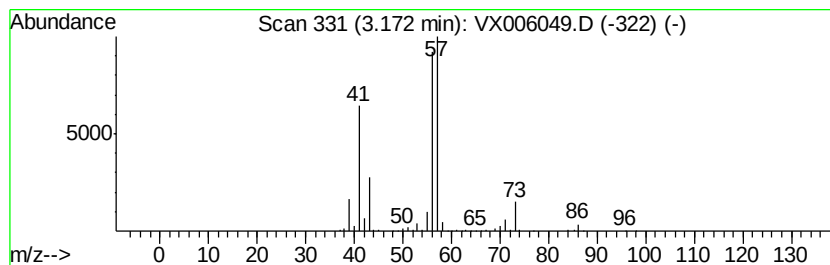
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	53.65 ug/l	440813	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
4		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
5		Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40



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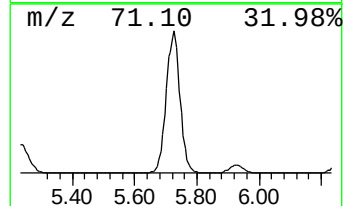
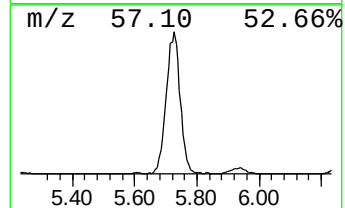
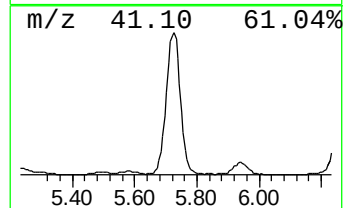
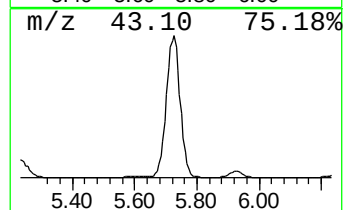
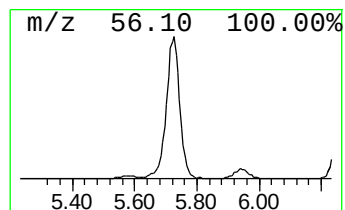
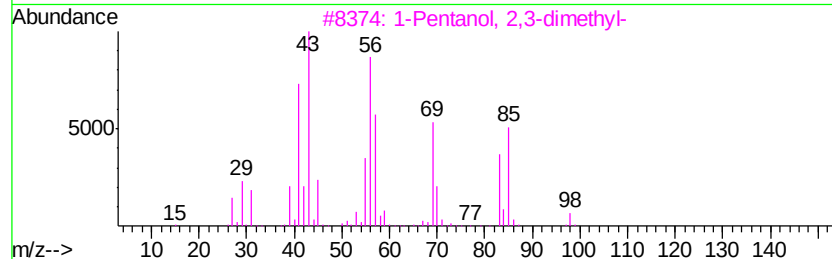
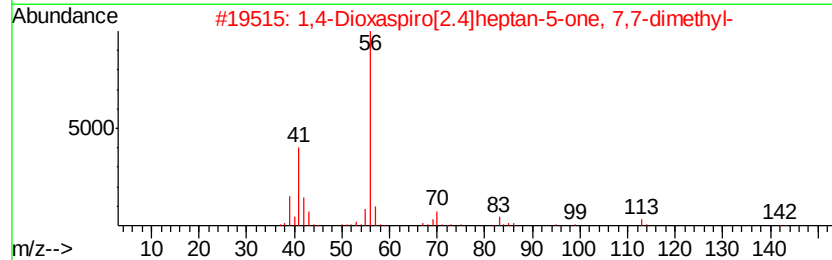
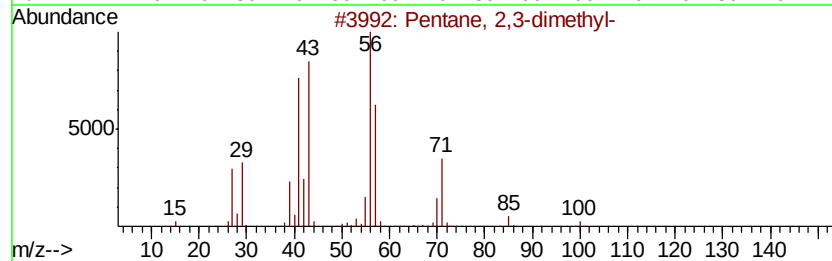
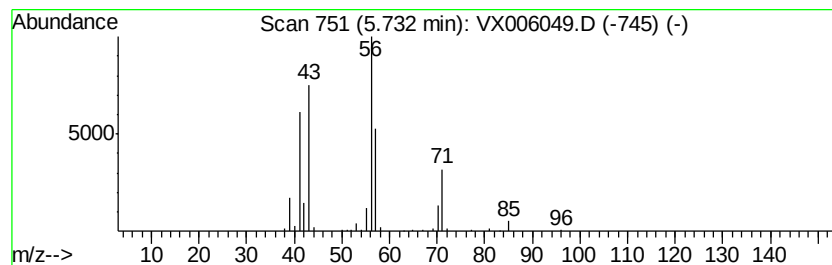
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Quant Title : SW846 8260

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.
5.73	36.31 ug/l	298356	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2		1,4-Dioxaspiro[2.4]heptan-5-one,...	142	C7H10O3	126091-79-0	45
3		1-Pentanol, 2,3-dimethyl-	116	C7H16O	010143-23-4	39
4		Cycloheptylamine	113	C7H15N	005452-35-7	36
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX111618\
Data File : VX006049.D
Acq On : 16 Nov 2018 14:55
Operator : JC/MD
Sample : J5965-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

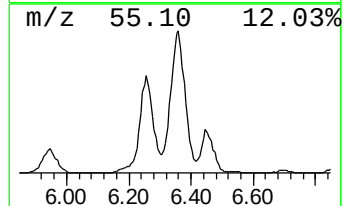
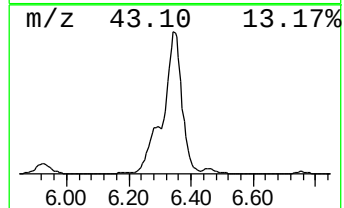
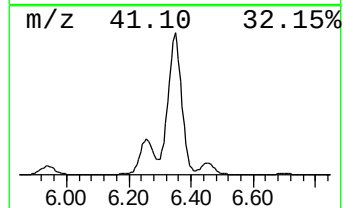
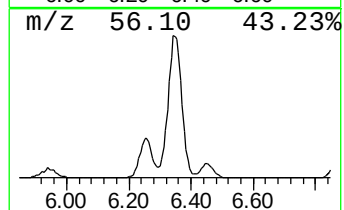
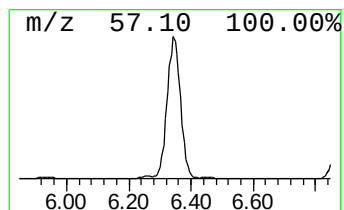
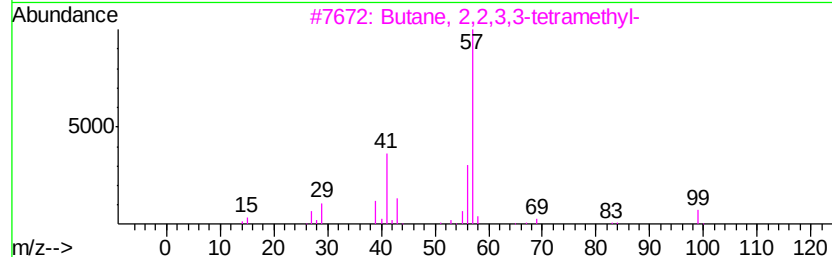
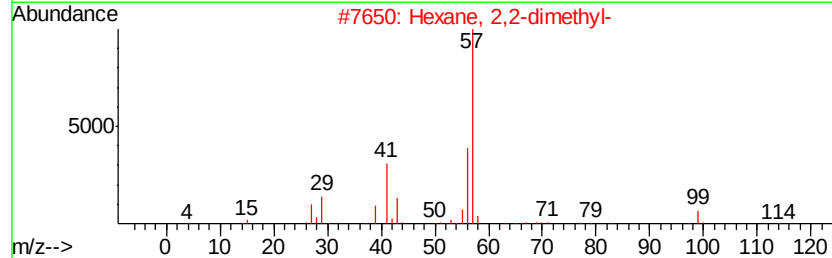
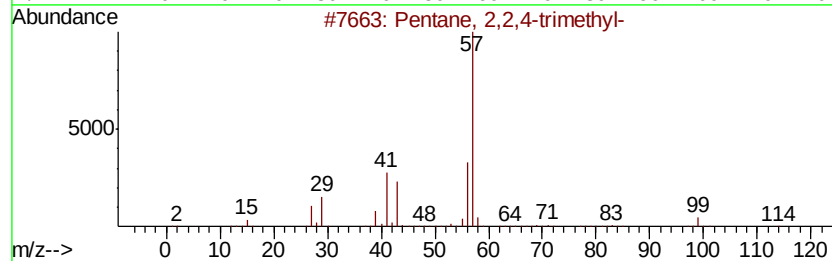
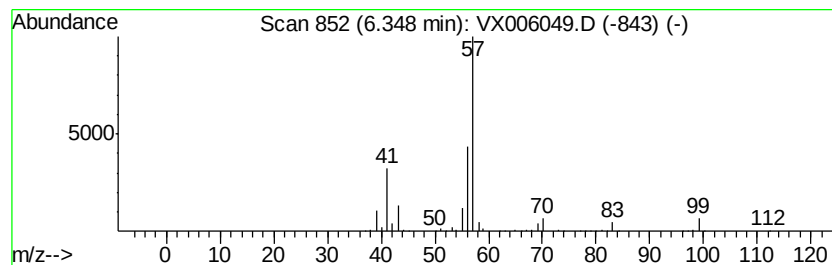
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	56.66 ug/l	528082	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	56
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA X\Data\VX111618\
Data File : VX006049.D
Acq On : 16 Nov 2018 14:55
Operator : JC/MD
Sample : J5965-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

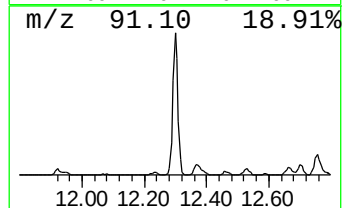
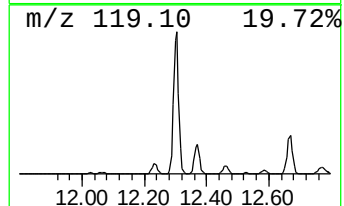
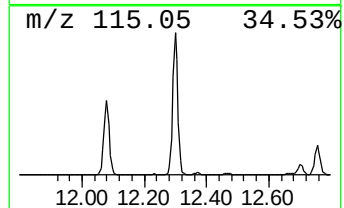
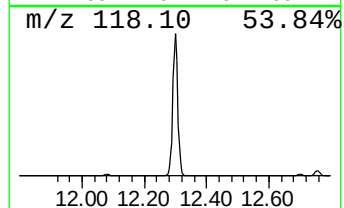
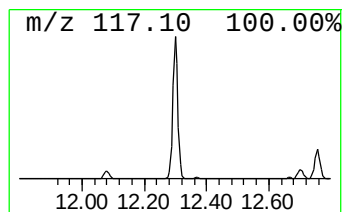
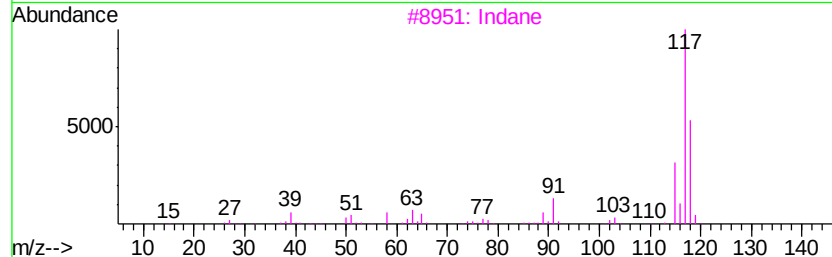
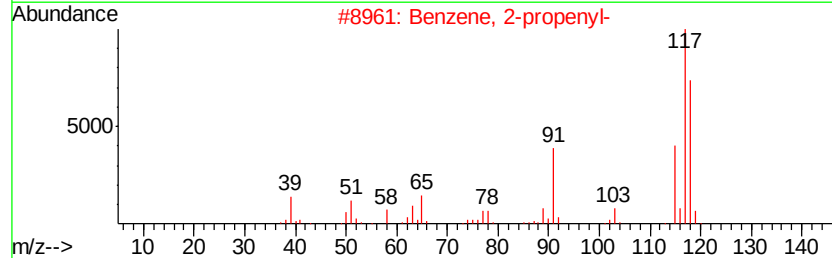
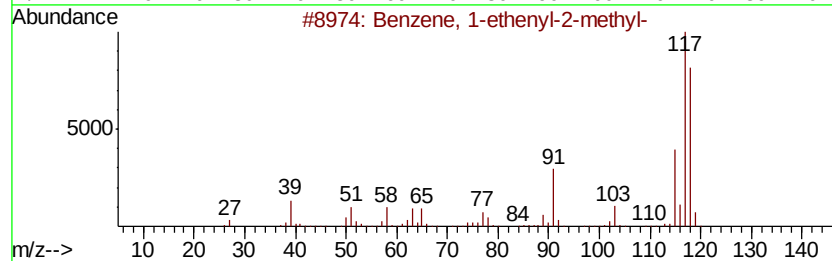
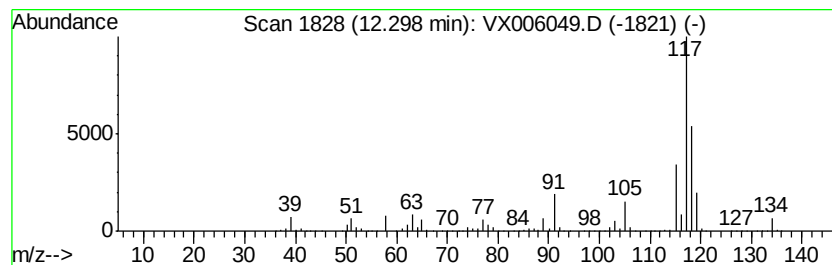
Instrument :
MSVOA_X
ClientSampleId :
MW-1R

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	96.99 ug/l	956229	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Benzene, 1-ethenyl-2-methyl-	118 C9H10	000611-15-4	87
2	Benzene, 2-propenyl-	118 C9H10	000300-57-2	76
3	Indane	118 C9H10	000496-11-7	76
4	Benzene, cyclopropyl-	118 C9H10	000873-49-4	76
5	Benzene, 1-propenyl-	118 C9H10	000637-50-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111618\
Data File : VX006049.D
Acq On : 16 Nov 2018 14:55
Operator : JC/MD
Sample : J5965-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.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-	1.78	27.9	ug/l	229003	1	5.67	410825	50.0
Butane, 2,3-dimet...	2.84	26.6	ug/l	218510	1	5.67	410825	50.0
Pentane, 3-methyl-	3.17	53.6	ug/l	440813	1	5.67	410825	50.0
Pentane, 2,3-dime...	5.73	36.3	ug/l	298356	1	5.67	410825	50.0
Pentane, 2,2,4-tr...	6.35	56.7	ug/l	528082	2	6.85	465980	50.0
Benzene, 1-etheny...	12.30	97.0	ug/l	956229	4	12.08	492965	50.0