

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
 Data File : VX012589.D
 Acq On : 21 Sep 2019 04:26
 Operator : JC/SP
 Sample : K4978-04
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 Z2-0163

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\82X091719W.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	43	rBV	889760	1043260	15.54%	2.133%
2	1.265	58	62	65	rBV	61713	73417	1.09%	0.150%
3	1.783	141	147	159	rVB	446338	649535	9.68%	1.328%
4	2.594	274	280	288	rBV	35557	67520	1.01%	0.138%
5	2.832	310	319	326	rBV	362690	840517	12.52%	1.718%
6	2.923	331	334	343	rVB	39971	73319	1.09%	0.150%
7	3.161	364	373	390	rVB	273204	630083	9.39%	1.288%
8	4.301	546	560	568	rBV	84747	263714	3.93%	0.539%
9	4.393	568	575	588	rVV2	52981	156029	2.32%	0.319%
10	5.234	701	713	730	rVB5	18988	75239	1.12%	0.154%
11	5.490	743	755	761	rBV2	99235	287477	4.28%	0.588%
12	5.575	761	769	775	rVV2	119614	390637	5.82%	0.799%
13	5.655	775	782	786	rVV	197572	553169	8.24%	1.131%
14	5.716	786	792	807	rVB	270469	836178	12.46%	1.709%
15	5.941	815	829	839	rBV4	128718	433051	6.45%	0.885%
16	6.051	839	847	856	rBV2	116808	297877	4.44%	0.609%
17	6.252	869	880	888	rBV2	227545	719108	10.71%	1.470%
18	6.343	888	895	905	rVV3	340504	1026053	15.29%	2.098%
19	6.447	905	912	924	rVB3	49562	137545	2.05%	0.281%
20	6.849	968	978	990	rBV	283062	685826	10.22%	1.402%
21	7.447	1066	1076	1089	rBV3	168864	440139	6.56%	0.900%
22	7.843	1133	1141	1149	rVB2	93998	192510	2.87%	0.394%
23	8.050	1164	1175	1185	rVB2	200054	573797	8.55%	1.173%
24	8.172	1186	1195	1204	rBV	314037	640895	9.55%	1.310%
25	8.386	1224	1230	1236	rBV3	101517	186422	2.78%	0.381%
26	8.666	1268	1276	1279	rBV3	127953	250623	3.73%	0.512%
27	8.709	1279	1283	1297	rVB	577133	939256	13.99%	1.920%
28	8.837	1297	1304	1308	rBV	260534	443292	6.60%	0.906%
29	9.038	1331	1337	1345	rVB	398286	643040	9.58%	1.315%
30	9.160	1348	1357	1363	rBV	189977	312554	4.66%	0.639%
31	9.569	1418	1424	1428	rBV2	123130	194623	2.90%	0.398%
32	9.617	1428	1432	1436	rVB	58889	76058	1.13%	0.155%
33	9.672	1436	1441	1446	rBV	303086	451583	6.73%	0.923%
34	10.111	1508	1513	1518	rBV	530252	725210	10.80%	1.483%

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35	10.184	1518	1525	1529	rBV	156414	220804	3.29%	0.451%
36	10.251	1529	1536	1545	rBV	4907454	6712066	100.00%	13.722%
37	10.355	1545	1553	1559	rVV	3329990	4583555	68.29%	9.370%
38	10.641	1590	1600	1607	rBV3	54307	150678	2.24%	0.308%
39	10.830	1620	1631	1639	rBV3	83186	152543	2.27%	0.312%
40	10.910	1639	1644	1648	rBV3	45656	79219	1.18%	0.162%
41	11.013	1656	1661	1667	rBV	1349978	1693048	25.22%	3.461%
42	11.135	1675	1681	1685	rBV	440259	590608	8.80%	1.207%
43	11.355	1712	1717	1727	rVB	966510	1164243	17.35%	2.380%
44	11.452	1727	1733	1737	rBV	990616	1243149	18.52%	2.541%
45	11.666	1757	1768	1777	rBV	1291688	1819974	27.11%	3.721%
46	11.763	1777	1784	1786	rVV2	45440	97524	1.45%	0.199%
47	11.800	1786	1790	1796	rVB	1092712	1355128	20.19%	2.770%
48	11.916	1801	1809	1810	rBV2	78436	125080	1.86%	0.256%
49	11.940	1810	1813	1821	rVB	268230	369421	5.50%	0.755%
50	12.074	1829	1835	1840	rVB2	597267	854673	12.73%	1.747%
51	12.135	1841	1845	1850	rVB	581008	733824	10.93%	1.500%
52	12.227	1856	1860	1865	rVB	118795	144319	2.15%	0.295%
53	12.294	1866	1871	1876	rBV	1202749	1488617	22.18%	3.043%
54	12.361	1876	1882	1892	rVB	238836	364474	5.43%	0.745%
55	12.458	1892	1898	1902	rBV	209662	266413	3.97%	0.545%
56	12.513	1902	1907	1914	rBV	545097	652562	9.72%	1.334%
57	12.580	1914	1918	1921	rBV	211207	285961	4.26%	0.585%
58	12.666	1926	1932	1935	rVV	377885	477245	7.11%	0.976%
59	12.696	1935	1937	1942	rVV	234155	272986	4.07%	0.558%
60	12.751	1942	1946	1953	rVB2	650453	987735	14.72%	2.019%
61	12.891	1965	1969	1975	rVB2	98322	150573	2.24%	0.308%
62	12.970	1975	1982	1986	rBV	363336	502871	7.49%	1.028%
63	13.013	1986	1989	1994	rVB	251073	308660	4.60%	0.631%
64	13.080	1995	2000	2006	rBV2	70883	103773	1.55%	0.212%
65	13.190	2014	2018	2021	rBV2	78418	95125	1.42%	0.194%
66	13.220	2021	2023	2026	rVV	102379	99208	1.48%	0.203%
67	13.306	2033	2037	2038	rBV2	65343	80721	1.20%	0.165%
68	13.342	2038	2043	2048	rVB2	1033830	1435297	21.38%	2.934%
69	13.476	2060	2065	2071	rVB	183607	242330	3.61%	0.495%
70	13.556	2074	2078	2081	rVV2	49910	68008	1.01%	0.139%
71	13.598	2081	2085	2087	rVV	80873	114132	1.70%	0.233%

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72	13.635	2087	2091	2097	rVV3	146664	293520	4.37%	0.600%
73	13.696	2097	2101	2102	rVV2	84642	119512	1.78%	0.244%
74	13.714	2102	2104	2113	rVB3	134636	242805	3.62%	0.496%
75	13.830	2114	2123	2131	rVB	1011863	1336822	19.92%	2.733%
76	13.921	2131	2138	2142	rBV2	57073	103829	1.55%	0.212%
77	13.982	2142	2148	2152	rVB3	58280	84975	1.27%	0.174%
78	14.269	2190	2195	2202	rVB2	70925	120948	1.80%	0.247%
79	14.537	2234	2239	2244	rBV2	75276	106333	1.58%	0.217%
80	14.690	2251	2264	2269	rBV	284703	404856	6.03%	0.828%
81	14.836	2282	2288	2296	rBV	262020	351168	5.23%	0.718%
82	15.269	2348	2359	2363	rBV2	45364	90396	1.35%	0.185%
83	15.543	2399	2404	2408	rBV	49792	73971	1.10%	0.151%
84	15.683	2418	2427	2430	rBV	65224	115133	1.72%	0.235%
85	15.720	2430	2433	2439	rVB	49670	75816	1.13%	0.155%

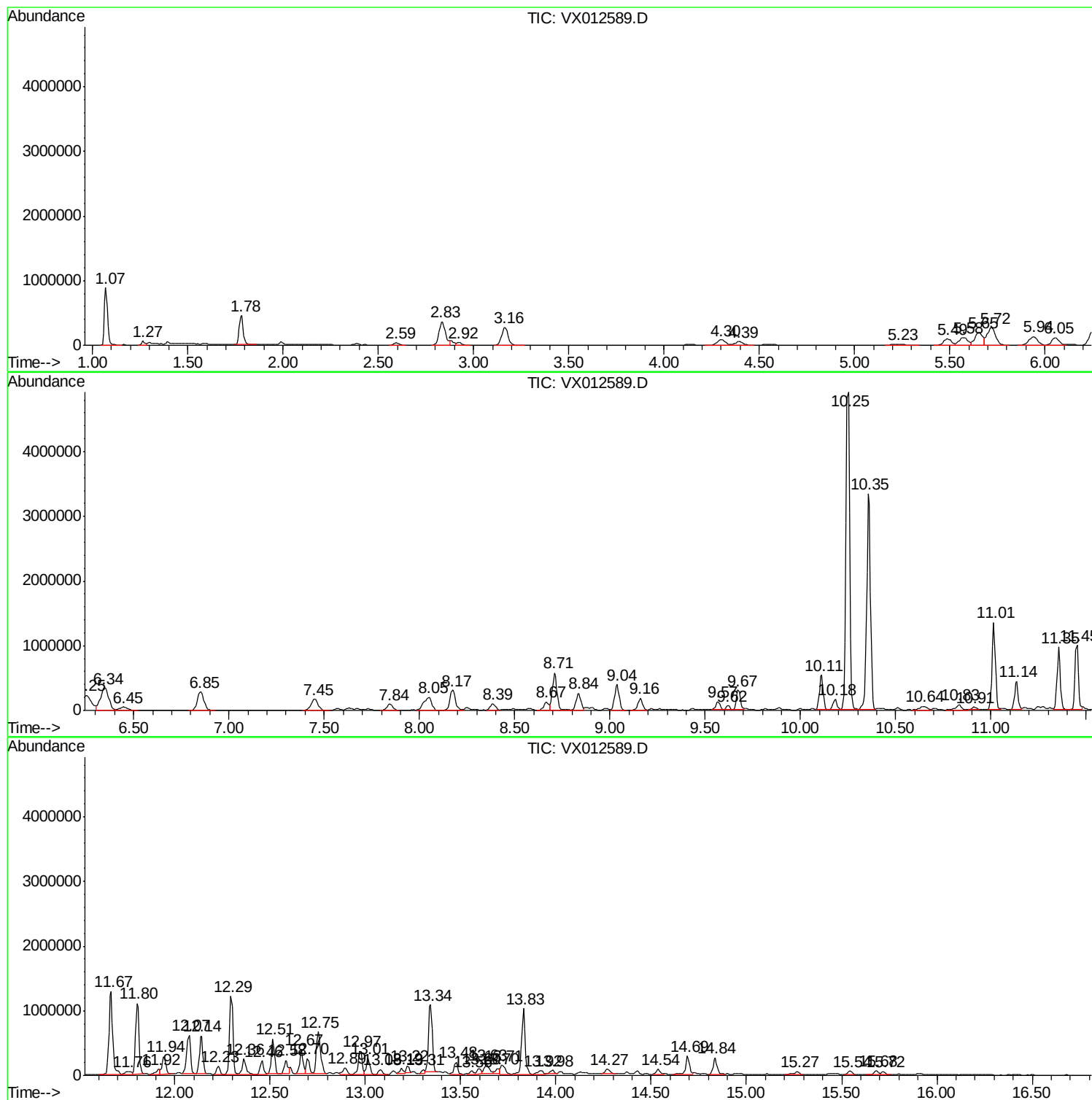
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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



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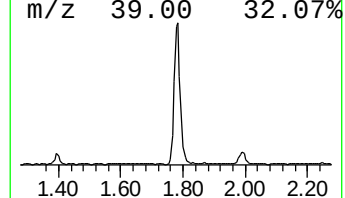
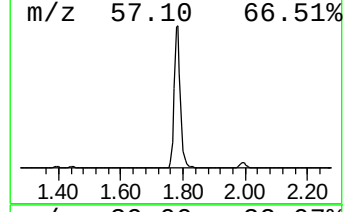
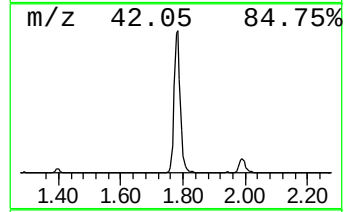
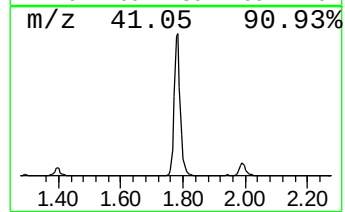
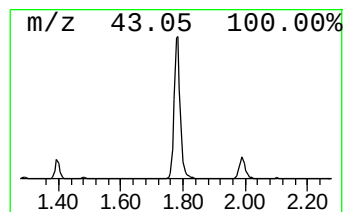
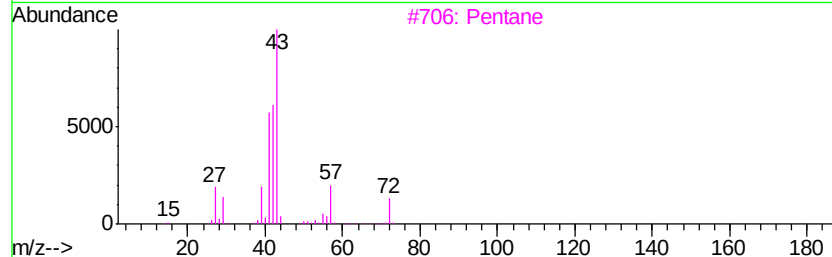
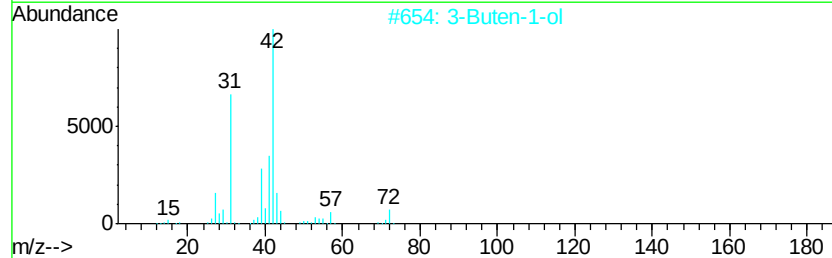
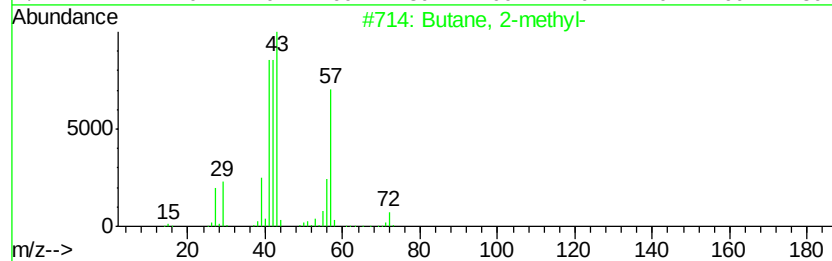
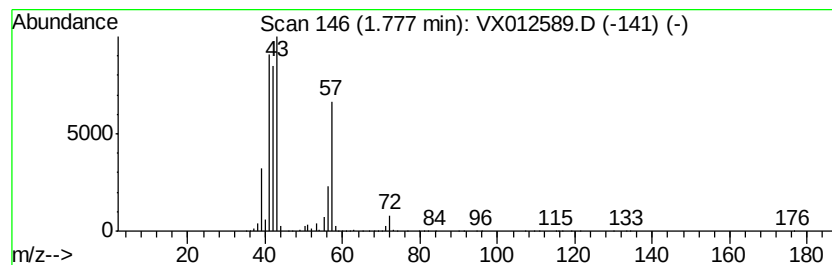
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	58.71 ug/l	649535	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Pentane	72	C5H12	000109-66-0	36
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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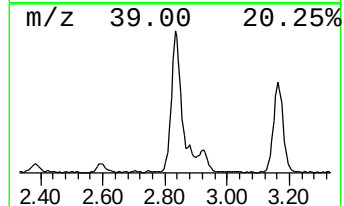
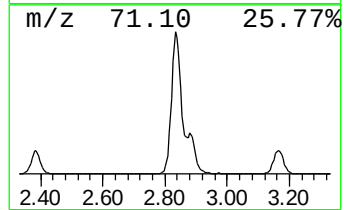
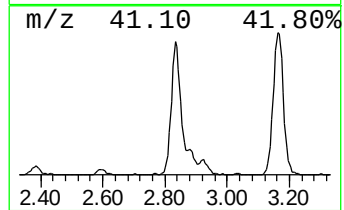
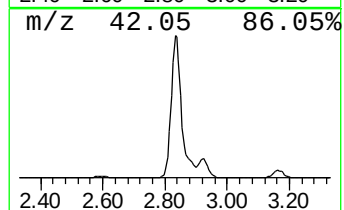
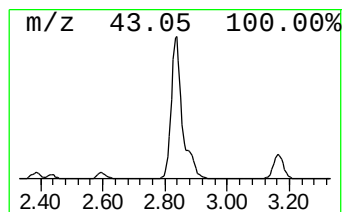
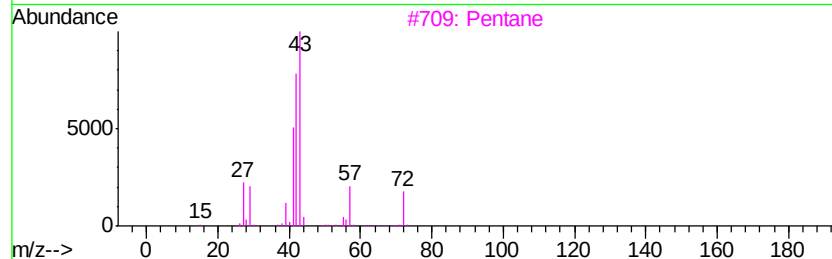
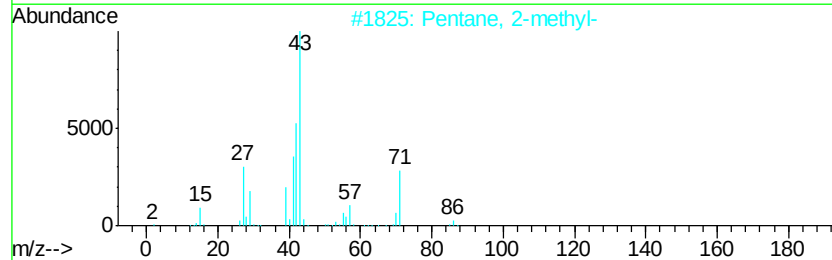
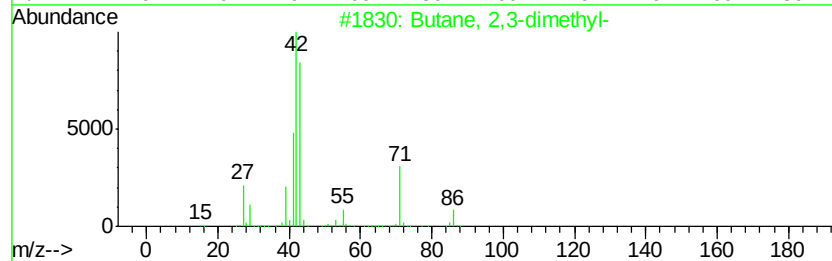
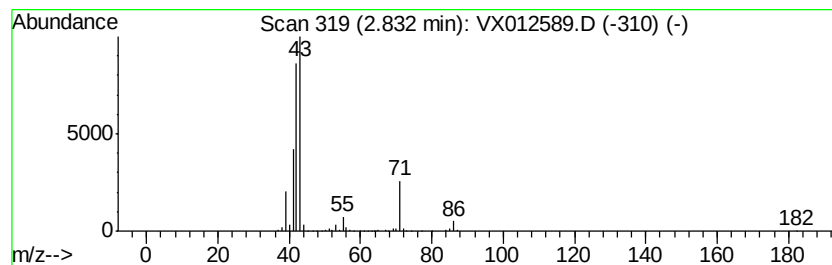
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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	75.97 ug/l	840517	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Pentane	72	C5H12	000109-66-0	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	36
5		1-Pentene	70	C5H10	000109-67-1	28



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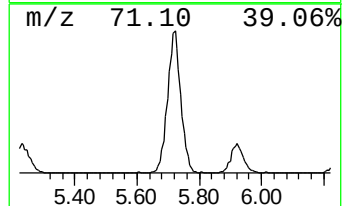
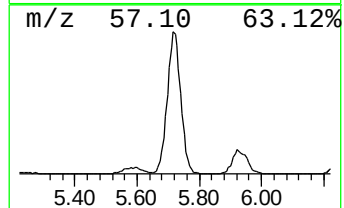
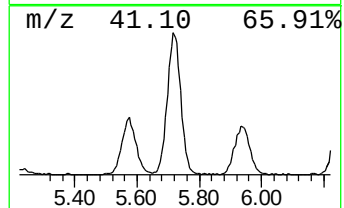
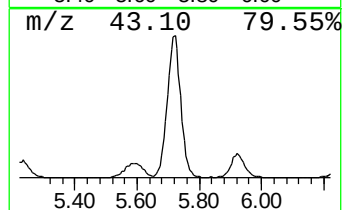
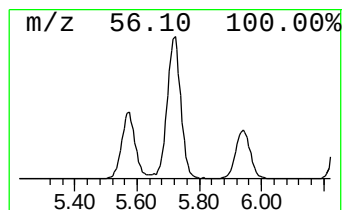
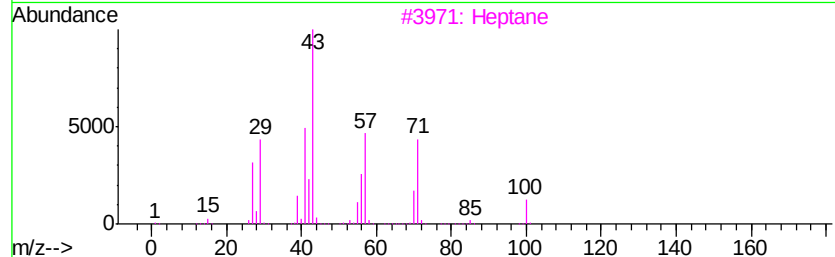
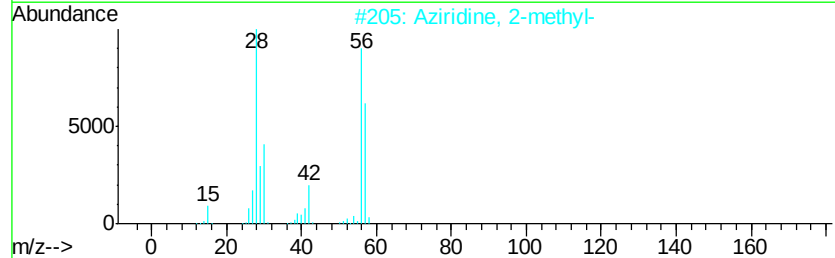
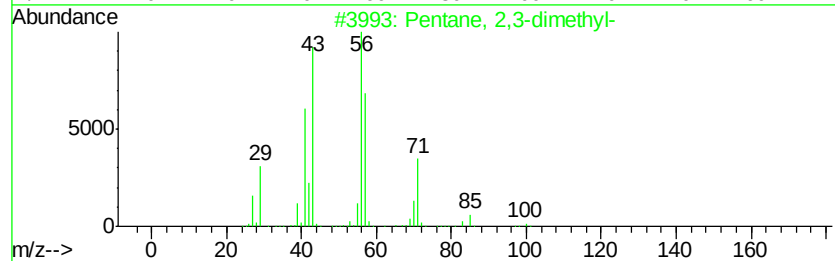
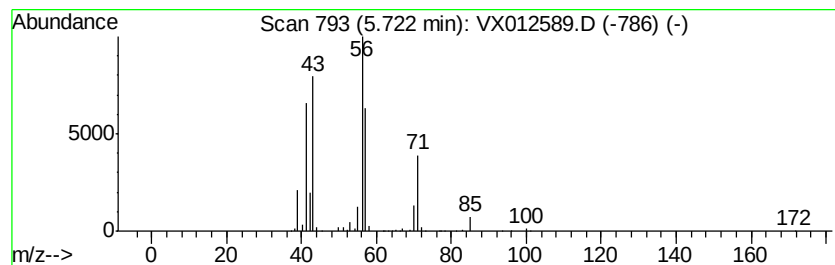
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	75.58 ug/l	836178	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
3		Heptane	100	C7H16	000142-82-5	40
4		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	36



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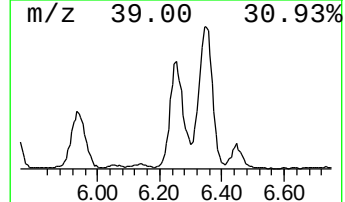
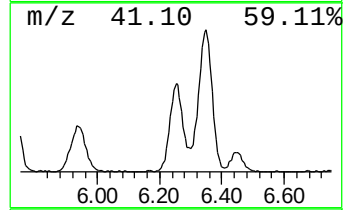
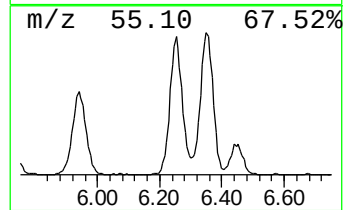
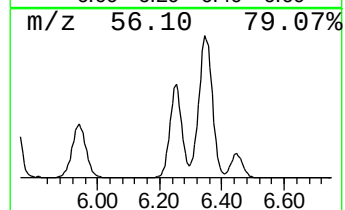
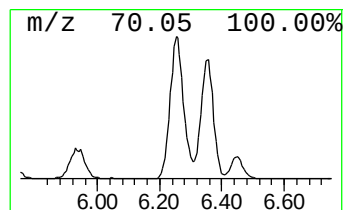
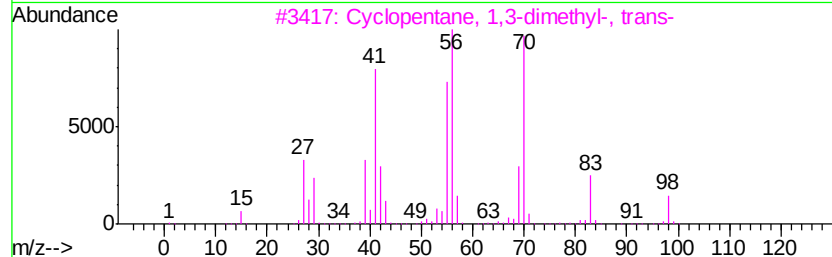
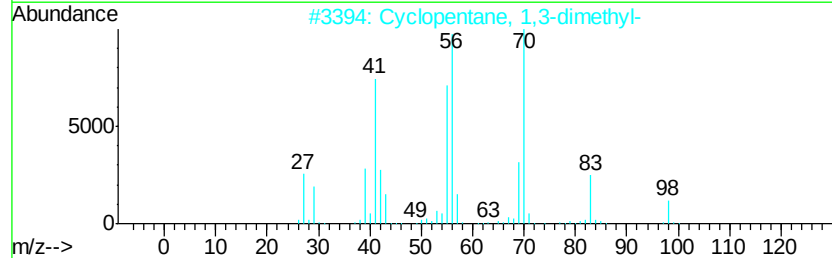
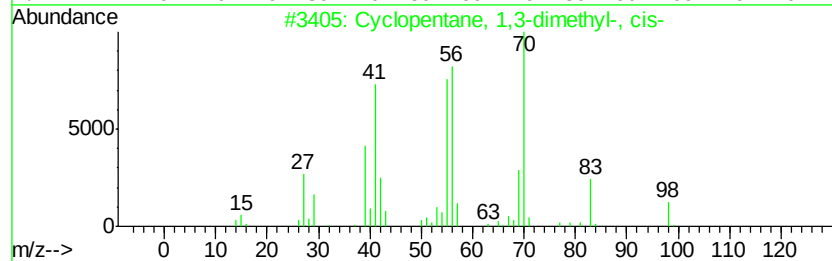
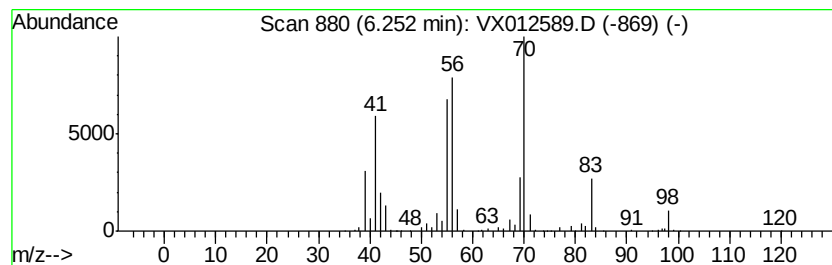
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1,3-dimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	65.00 ug/l	719108	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	94
2		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	94
3		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	91
4		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	90
5		2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012589.D
Acq On : 21 Sep 2019 04:26
Operator : JC/SP
Sample : K4978-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0163

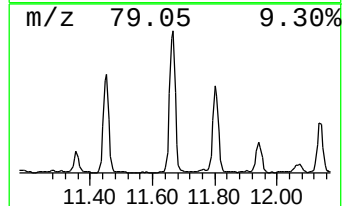
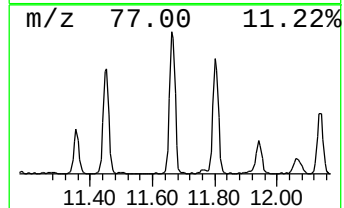
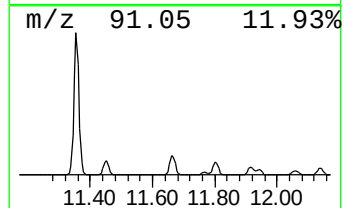
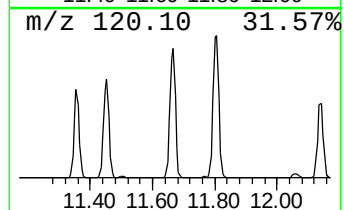
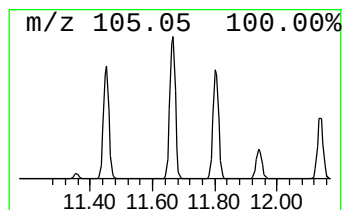
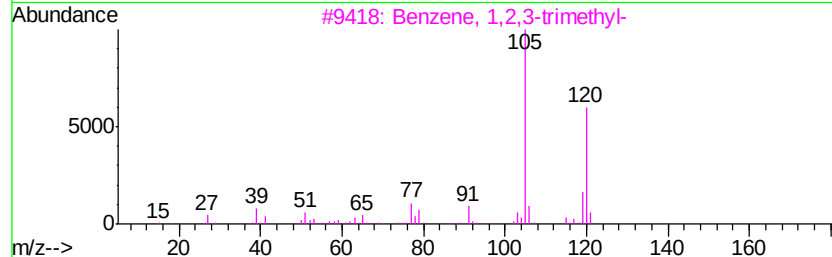
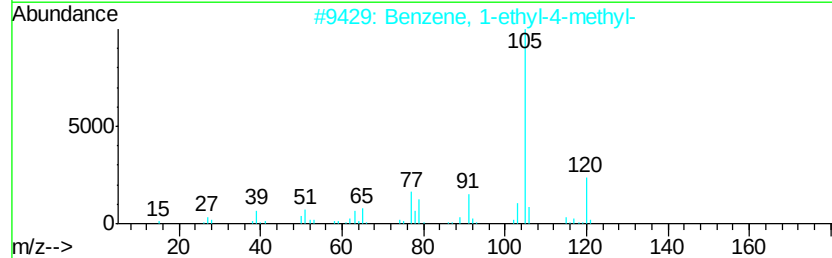
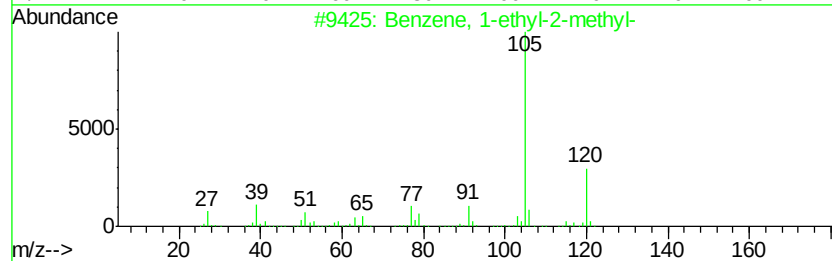
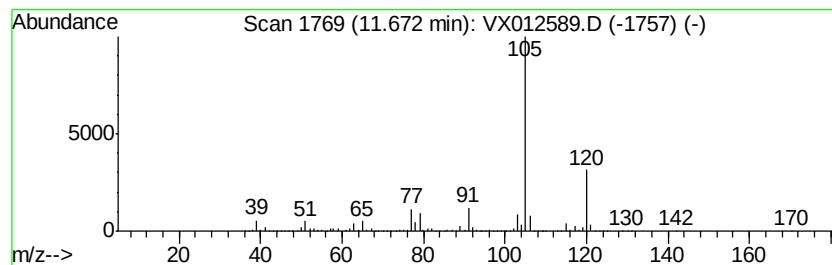
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	106.47 ug/l	1819970	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012589.D
Acq On : 21 Sep 2019 04:26
Operator : JC/SP
Sample : K4978-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0163

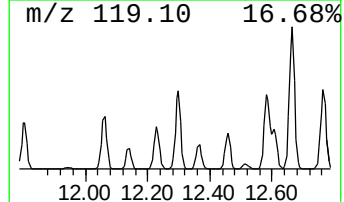
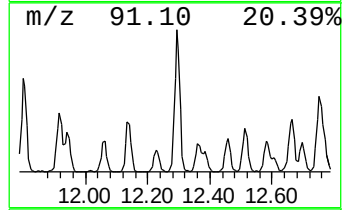
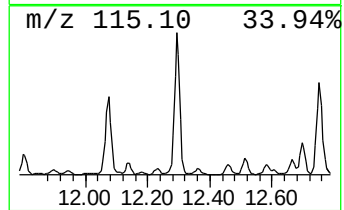
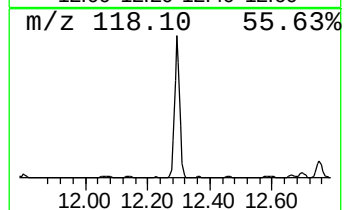
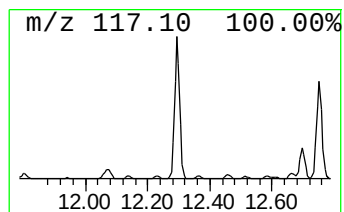
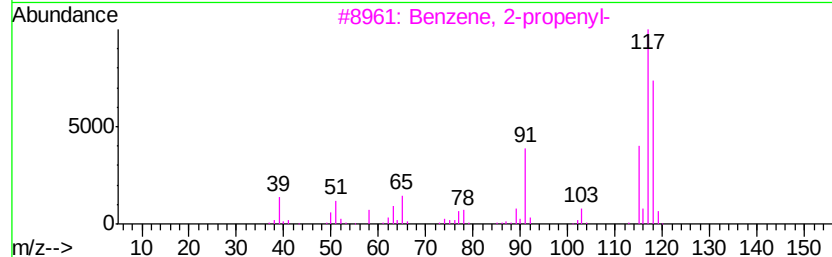
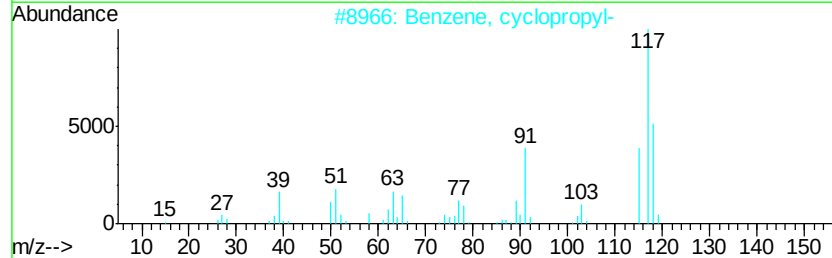
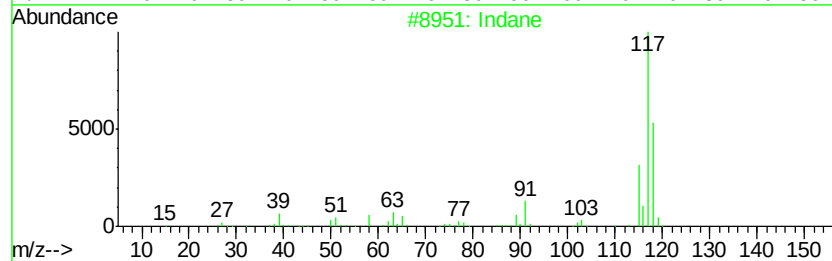
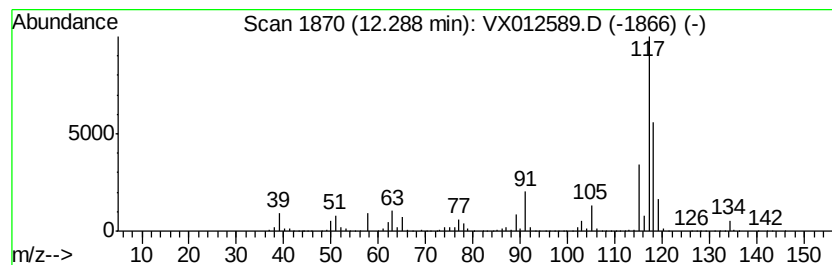
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Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	87.09 ug/l	1488620	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	70
2		Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3		Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4		Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5		(Z)-1-Phenylpropene	118	C9H10	000766-90-5	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012589.D
Acq On : 21 Sep 2019 04:26
Operator : JC/SP
Sample : K4978-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
Z2-0163

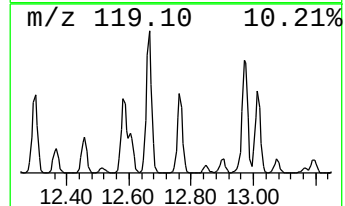
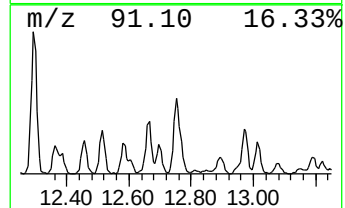
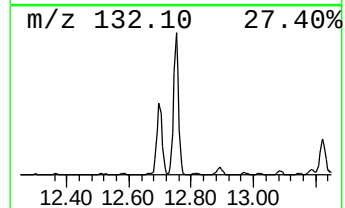
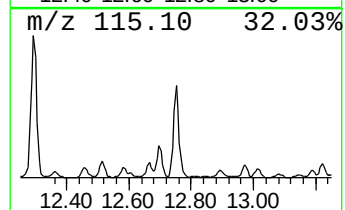
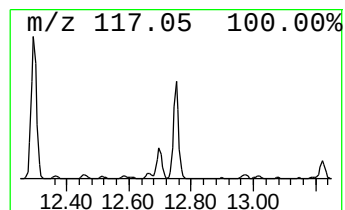
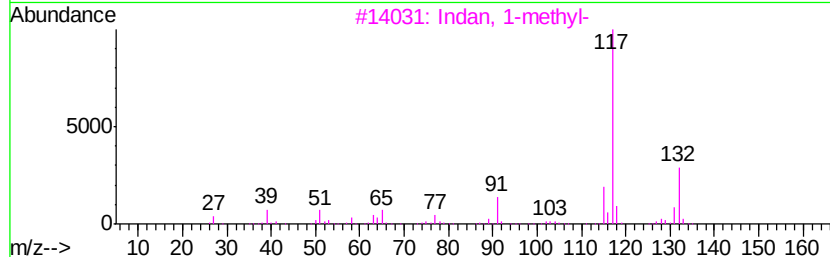
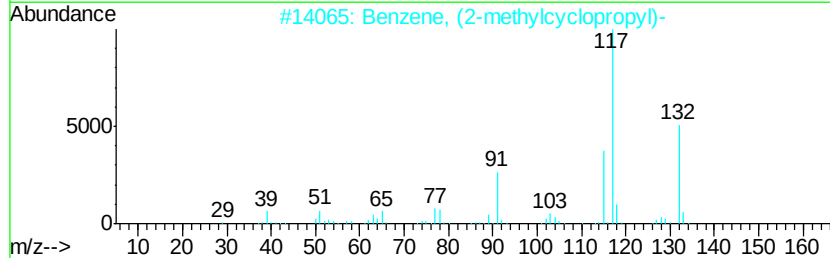
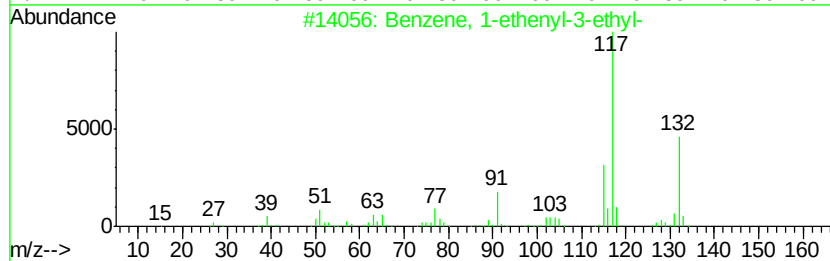
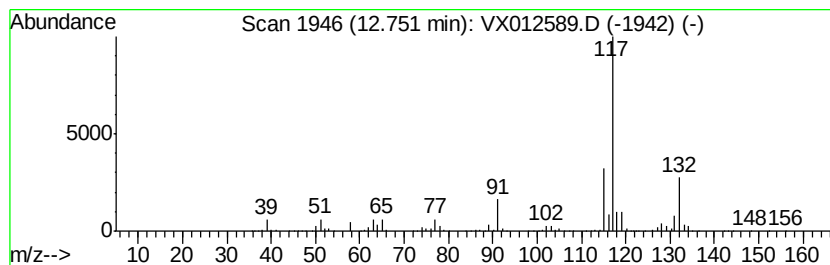
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	57.78 ug/l	987735	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2		Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	87
3		Indan, 1-methyl-	132	C10H12	000767-58-8	87
4		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012589.D
Acq On : 21 Sep 2019 04:26
Operator : JC/SP
Sample : K4978-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0163

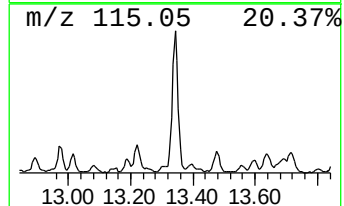
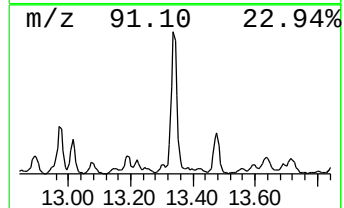
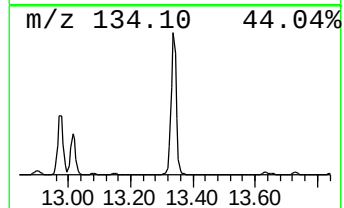
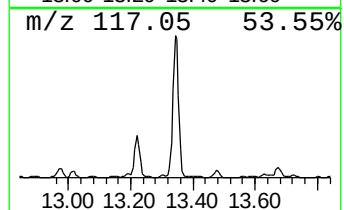
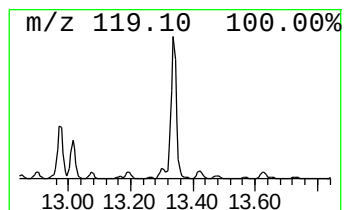
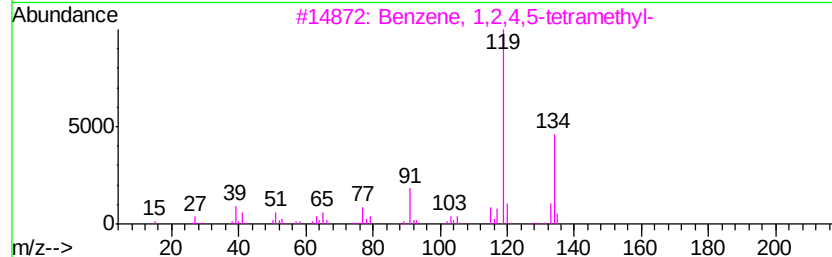
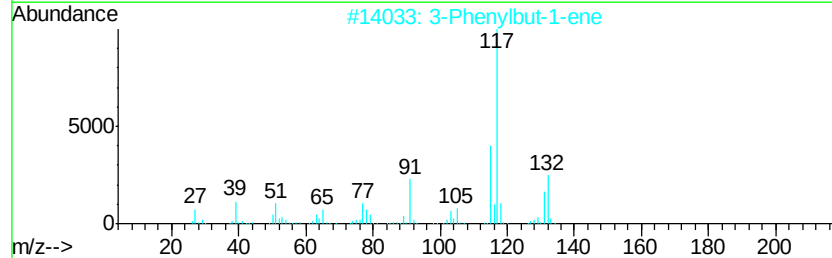
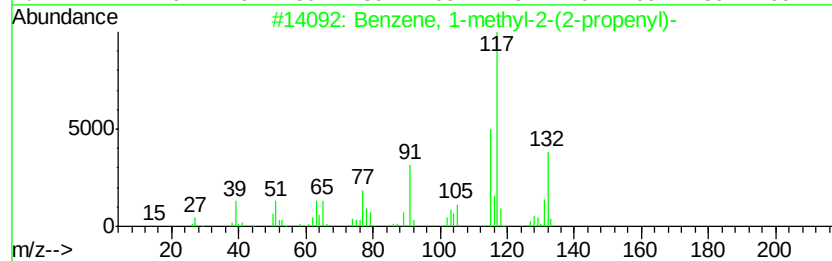
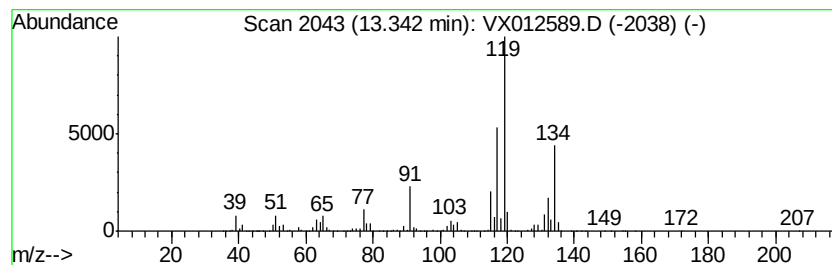
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-methyl-2-(2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	83.97 ug/l	1435300	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
4		o-Cymene	134	C10H14	000527-84-4	64
5		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX092019\
Data File : VX012589.D
Acq On : 21 Sep 2019 04:26
Operator : JC/SP
Sample : K4978-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0163

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.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	58.7	ug/l	649535	1	5.65	553169	50.0
Butane, 2,3-dimet...	2.83	76.0	ug/l	840517	1	5.65	553169	50.0
Pentane, 2,3-dime...	5.72	75.6	ug/l	836178	1	5.65	553169	50.0
Cyclopentane, 1,3...	6.25	65.0	ug/l	719108	1	5.65	553169	50.0
Benzene, 1-ethyl-...	11.67	106.5	ug/l	1819970	4	12.07	854673	50.0
Indane	12.29	87.1	ug/l	1488620	4	12.07	854673	50.0
Benzene, 1-etheny...	12.75	57.8	ug/l	987735	4	12.07	854673	50.0
Benzene, 1-methyl...	13.34	84.0	ug/l	1435300	4	12.07	854673	50.0