

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091819\
 Data File : VX012510.D
 Acq On : 19 Sep 2019 06:11
 Operator : JC/SP
 Sample : K4887-05
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 Z2-0158

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	38	rBV	564342	659925	66.60%	7.415%
2	1.265	58	62	69	rBV	31558	43257	4.37%	0.486%
3	1.393	80	83	89	rVB	23662	24188	2.44%	0.272%
4	1.588	107	115	118	rBV10	6593	13418	1.35%	0.151%
5	1.783	142	147	156	rVB	198888	269858	27.23%	3.032%
6	1.991	177	181	187	rVB	18947	25251	2.55%	0.284%
7	2.387	239	246	250	rBV4	5873	12373	1.25%	0.139%
8	2.594	275	280	289	rVB	21609	39114	3.95%	0.440%
9	2.838	311	320	330	rBV	71155	167068	16.86%	1.877%
10	2.923	330	334	341	rVB	10693	22018	2.22%	0.247%
11	3.167	362	374	385	rVB	38582	88636	8.94%	0.996%
12	4.295	550	559	567	rBV5	6217	19265	1.94%	0.216%
13	4.393	567	575	585	rVB5	7010	22046	2.22%	0.248%
14	4.545	588	600	603	rBV10	4011	11522	1.16%	0.129%
15	5.490	743	755	763	rBV	105853	310230	31.31%	3.486%
16	5.655	772	782	789	rBV	206710	582063	58.74%	6.540%
17	5.941	820	829	838	rBV2	16735	51359	5.18%	0.577%
18	6.051	838	847	856	rVV	127082	343164	34.63%	3.856%
19	6.136	856	861	869	rVV3	14946	40925	4.13%	0.460%
20	6.252	871	880	887	rVV3	24397	77678	7.84%	0.873%
21	6.344	887	895	906	rVV4	41199	127854	12.90%	1.437%
22	6.453	906	913	922	rVB4	4228	10742	1.08%	0.121%
23	6.850	968	978	992	rBV	307105	737820	74.46%	8.290%
24	7.447	1067	1076	1087	rVB4	13414	36387	3.67%	0.409%
25	7.843	1136	1141	1148	rVB3	9379	18847	1.90%	0.212%
26	8.051	1165	1175	1182	rVB5	23170	63115	6.37%	0.709%
27	8.173	1188	1195	1204	rBV2	38809	84013	8.48%	0.944%
28	8.386	1223	1230	1235	rBV4	12445	24789	2.50%	0.279%
29	8.490	1235	1247	1255	rVV	16628	31458	3.17%	0.353%
30	8.575	1255	1261	1267	rVB9	4214	10301	1.04%	0.116%
31	8.709	1271	1283	1298	rBV	612604	990901	100.00%	11.134%
32	8.837	1298	1304	1314	rVV2	26458	46569	4.70%	0.523%
33	9.038	1331	1337	1343	rVB	38571	62473	6.30%	0.702%
34	9.160	1349	1357	1363	rBV2	16918	28539	2.88%	0.321%

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35	9.514	1407	1415	1419	rBV2	7423	14945	1.51%	0.168%
36	9.569	1419	1424	1429	rVB3	11851	19572	1.98%	0.220%
37	9.672	1435	1441	1446	rBV2	23076	37667	3.80%	0.423%
38	10.111	1507	1513	1519	rVV	572654	798400	80.57%	8.971%
39	10.178	1521	1524	1530	rVV	18291	29153	2.94%	0.328%
40	10.245	1530	1535	1540	rVB2	11270	18270	1.84%	0.205%
41	10.331	1545	1549	1558	rVB4	18573	42386	4.28%	0.476%
42	10.654	1598	1602	1608	rVB7	6070	11969	1.21%	0.134%
43	10.831	1628	1631	1639	rVB7	8369	13891	1.40%	0.156%
44	11.013	1656	1661	1667	rBV	212099	268454	27.09%	3.016%
45	11.135	1674	1681	1686	rBV	460326	595064	60.05%	6.686%
46	11.355	1712	1717	1727	rVB	109334	140526	14.18%	1.579%
47	11.440	1727	1731	1735	rVV6	5562	11351	1.15%	0.128%
48	11.483	1735	1738	1749	rVB9	7440	14645	1.48%	0.165%
49	11.684	1764	1771	1777	rBV7	10723	28063	2.83%	0.315%
50	11.757	1777	1783	1788	rVB4	12976	28144	2.84%	0.316%
51	11.940	1801	1813	1821	rBV2	47430	88665	8.95%	0.996%
52	12.019	1821	1826	1830	rVV7	7131	13365	1.35%	0.150%
53	12.074	1830	1835	1847	rVB	540132	675098	68.13%	7.586%
54	12.227	1856	1860	1865	rVB	25506	30858	3.11%	0.347%
55	12.294	1865	1871	1876	rBV	213250	269924	27.24%	3.033%
56	12.367	1876	1883	1892	rVB7	15344	41228	4.16%	0.463%
57	12.458	1892	1898	1902	rBV	18724	25839	2.61%	0.290%
58	12.513	1902	1907	1910	rBV6	6277	9940	1.00%	0.112%
59	12.696	1934	1937	1942	rVV	43407	60269	6.08%	0.677%
60	12.751	1942	1946	1953	rVV	99503	129723	13.09%	1.458%
61	12.891	1960	1969	1974	rVB3	18469	31910	3.22%	0.359%
62	12.970	1975	1982	1988	rBV	27081	45193	4.56%	0.508%
63	13.086	1995	2001	2006	rBV6	6699	11975	1.21%	0.135%
64	13.190	2014	2018	2020	rVV2	9044	12426	1.25%	0.140%
65	13.220	2020	2023	2032	rVB3	14335	26700	2.69%	0.300%
66	13.342	2037	2043	2048	rVV2	100331	146805	14.82%	1.650%
67	13.397	2048	2052	2059	rVV8	6993	14946	1.51%	0.168%
68	13.641	2088	2092	2095	rVV5	9564	14503	1.46%	0.163%
69	13.696	2095	2101	2102	rVV2	10715	17603	1.78%	0.198%
70	13.714	2102	2104	2113	rVB4	15082	26125	2.64%	0.294%
71	13.976	2143	2147	2152	rVV8	6020	10214	1.03%	0.115%

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Integration Parameters: RTEINT.P

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72	14.537	2235	2239	2243	rBV4	8159	12427	1.25%	0.140%
73	14.836	2282	2288	2293	rBV4	7852	14230	1.44%	0.160%

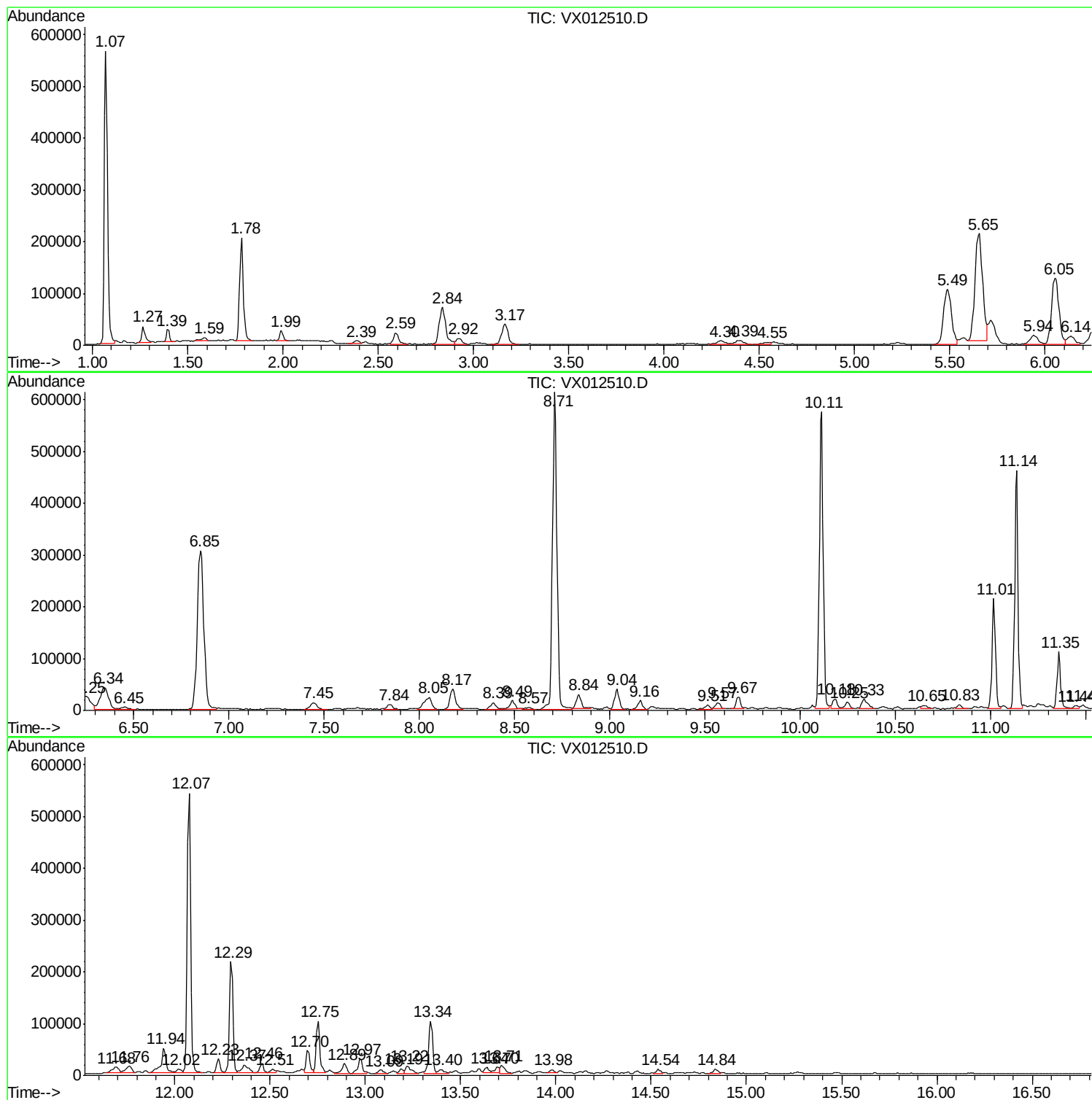
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
Z2-0158

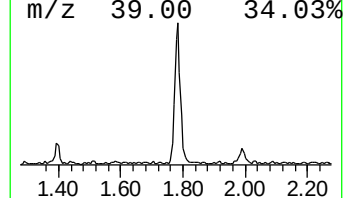
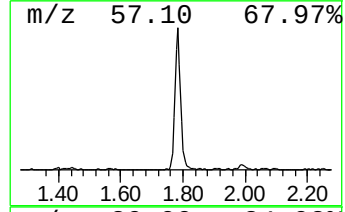
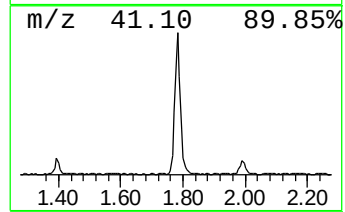
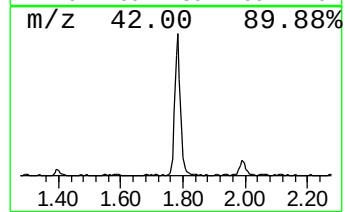
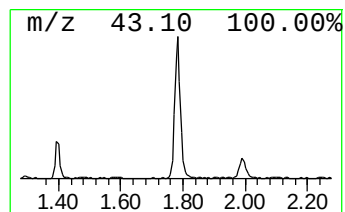
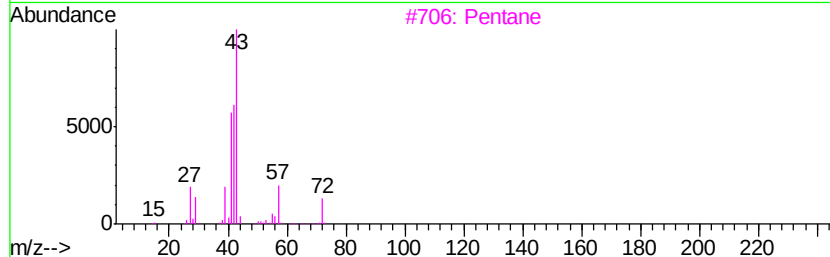
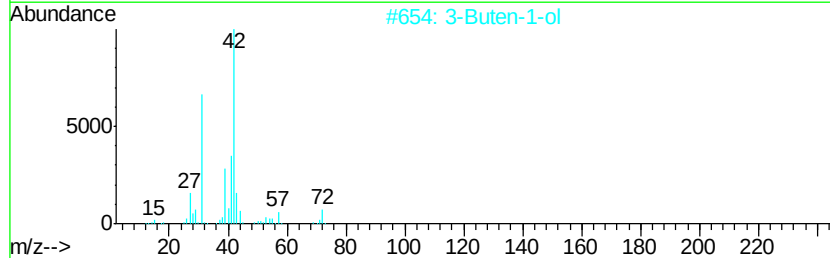
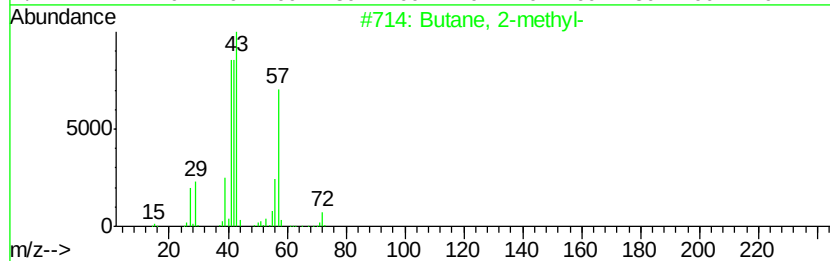
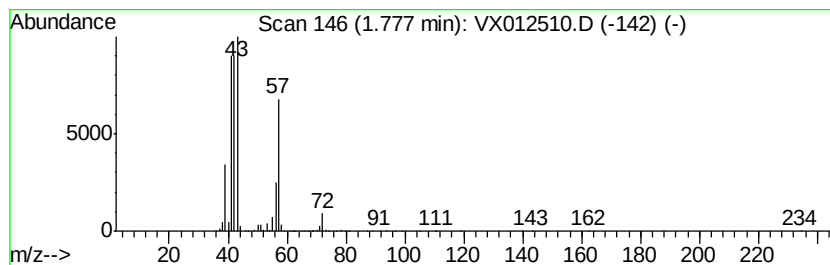
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	23.18 ug/l	269858	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		1-Butene	56	C4H8	000106-98-9	14
5		Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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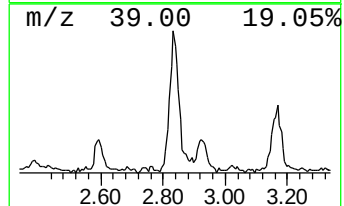
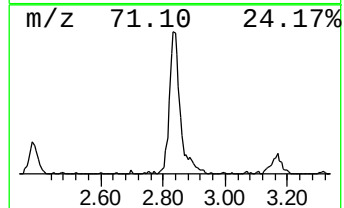
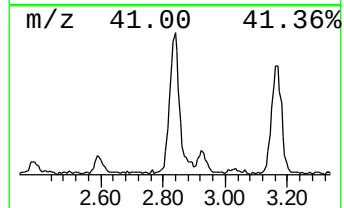
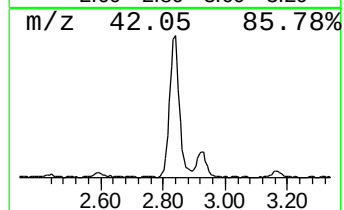
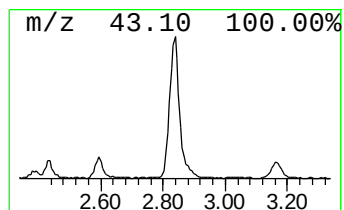
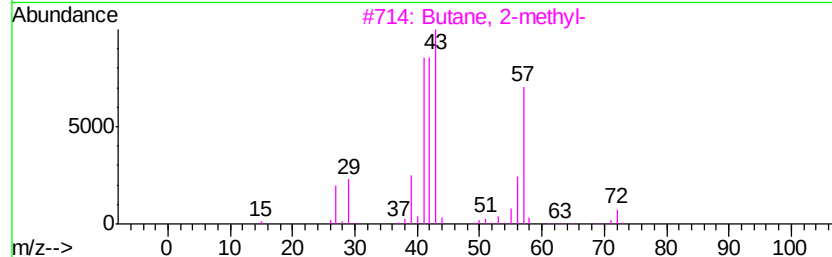
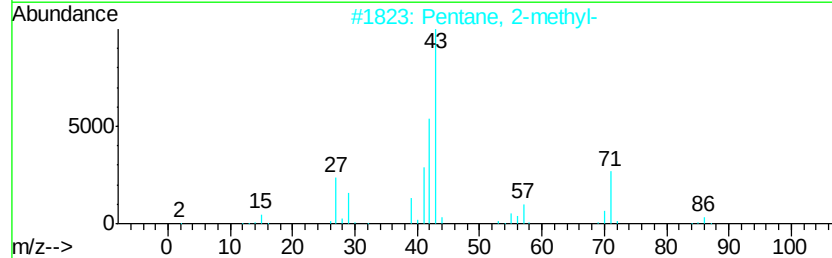
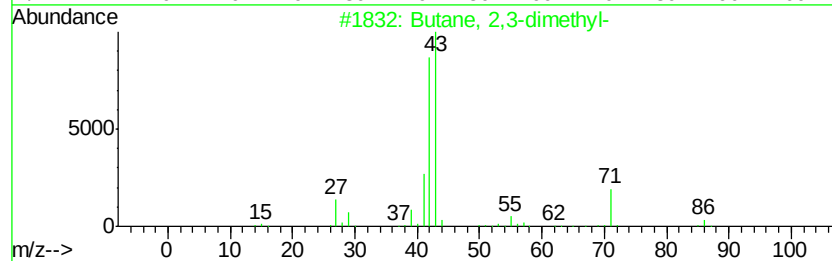
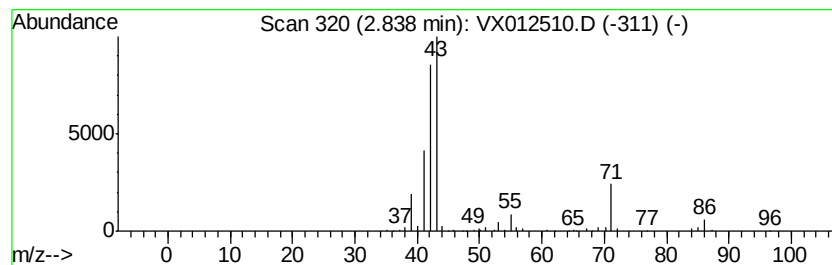
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	14.35 ug/l	167068	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3		Butane, 2-methyl-	72	C5H12	000078-78-4	38
4		Tetrahydrofuran	72	C4H8O	000109-99-9	36
5		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	22



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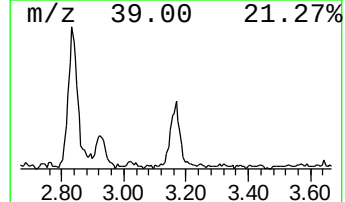
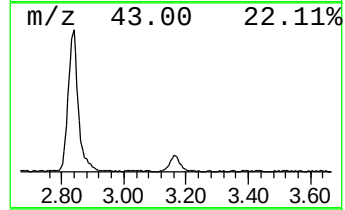
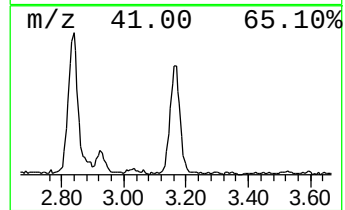
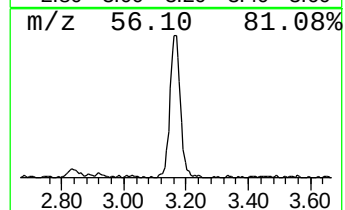
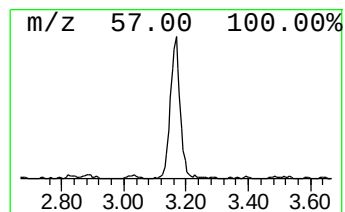
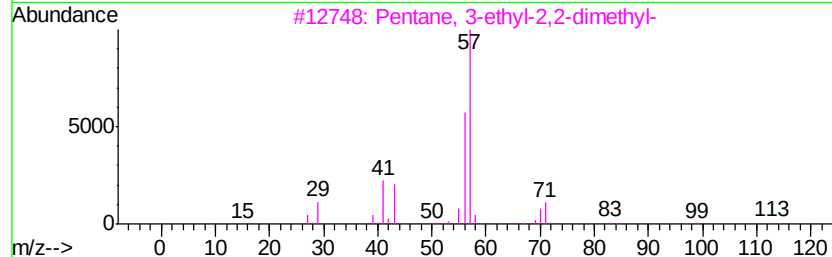
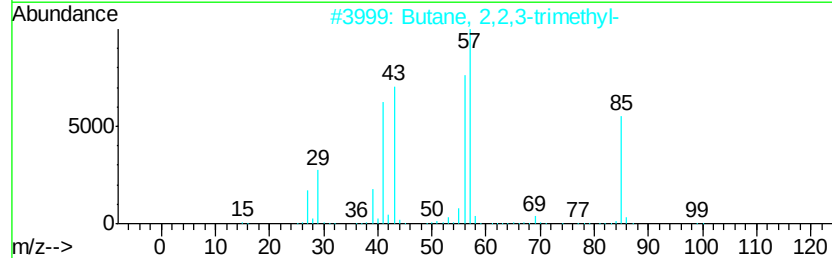
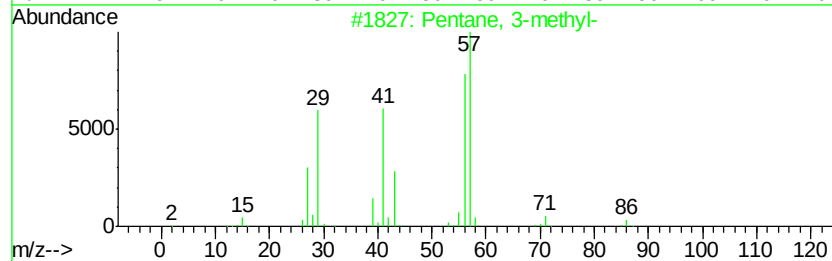
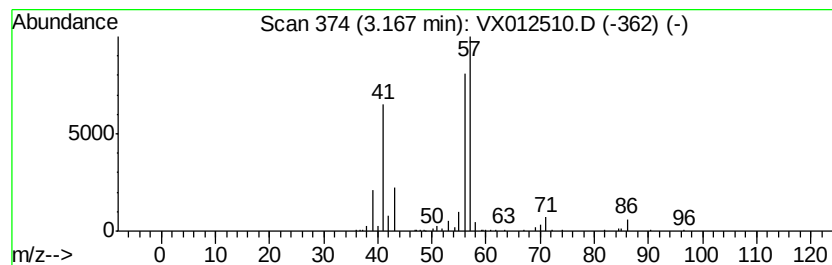
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	7.61 ug/l	88636	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	72
3		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	56
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	52



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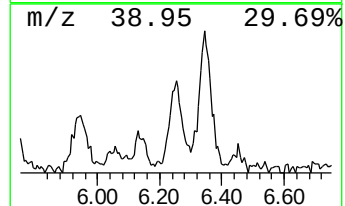
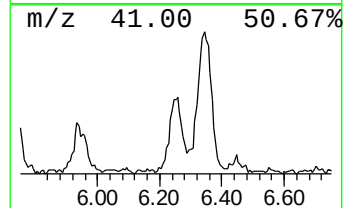
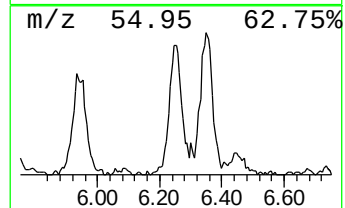
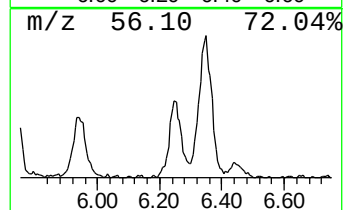
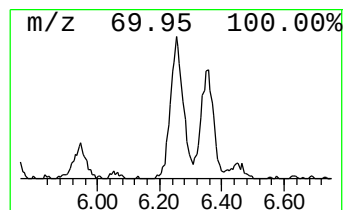
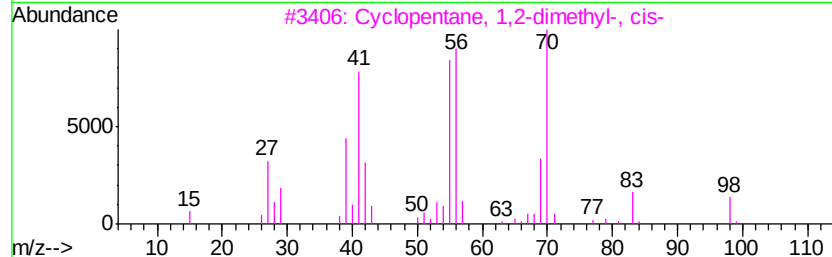
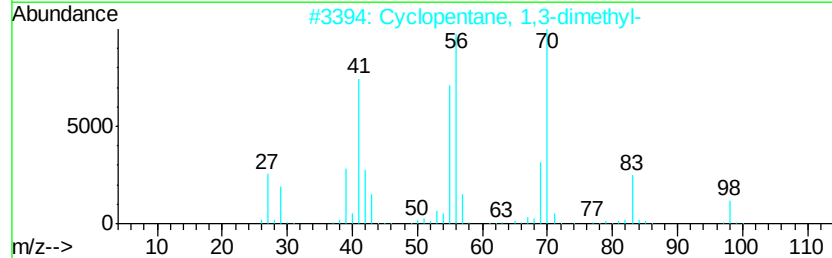
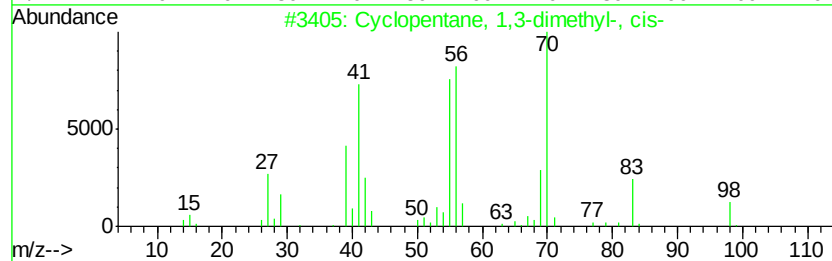
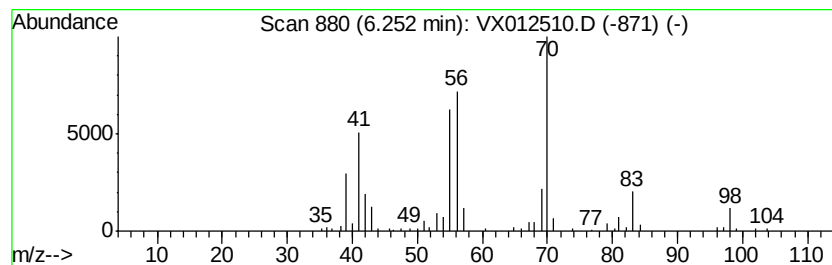
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1,3-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	6.67 ug/l	77678	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	97
2		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	94
3		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	70
4		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	70
5		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012510.D
Acq On : 19 Sep 2019 06:11
Operator : JC/SP
Sample : K4887-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 52 Sample Multiplier: 1

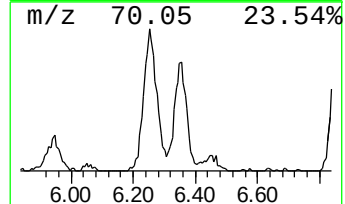
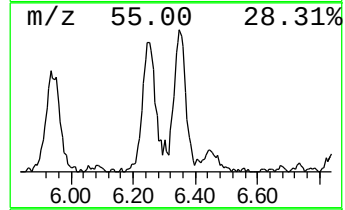
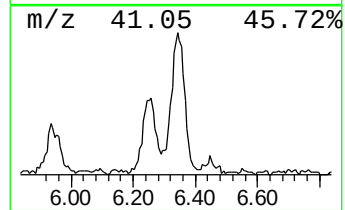
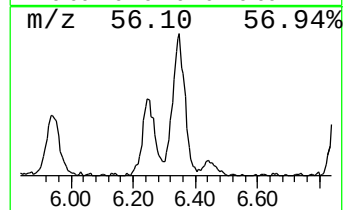
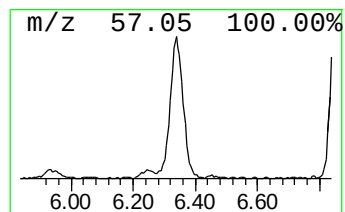
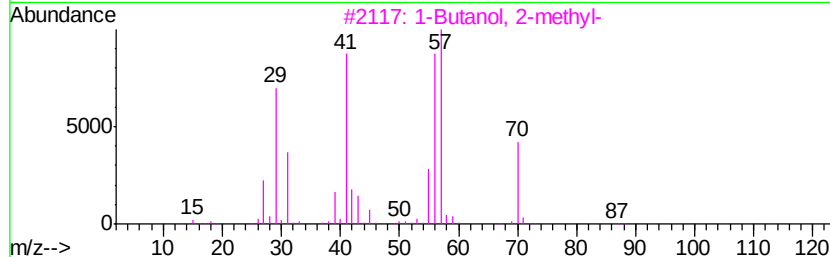
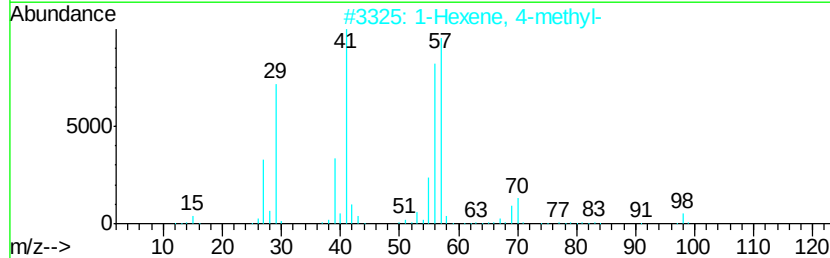
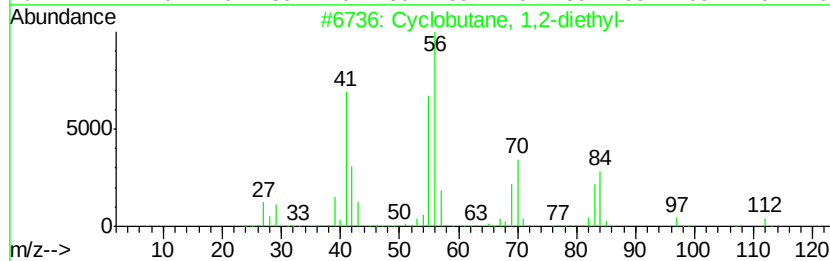
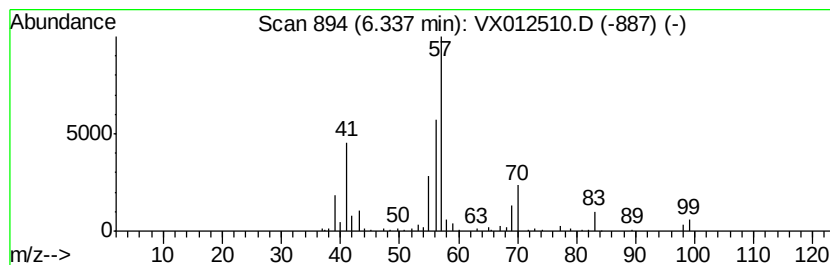
Instrument :
MSVOA_X
ClientSampled :
Z2-0158

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 6 Cyclobutane, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	8.66 ug/l	127854	1,4-Difluorobenzene	6.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclobutane, 1,2-diethyl-	112 C8H16	061141-83-1 64
2		1-Hexene, 4-methyl-	98 C7H14	003769-23-1 59
3		1-Butanol, 2-methyl-	88 C5H12O	000137-32-6 53
4		1-Hexene, 5-methyl-	98 C7H14	003524-73-0 50
5		2-Ethyl-1-hexanol, trifluoroacetate	226 C10H17F3O2	1000365-19-6 47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012510.D
Acq On : 19 Sep 2019 06:11
Operator : JC/SP
Sample : K4887-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0158

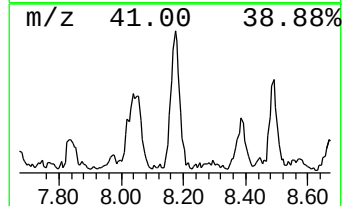
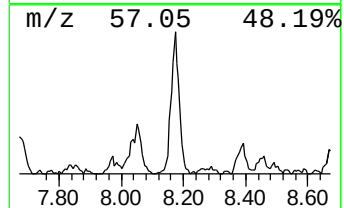
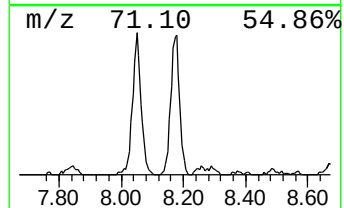
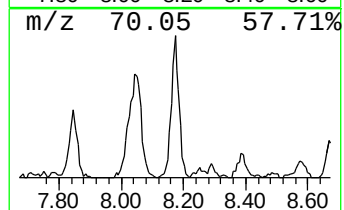
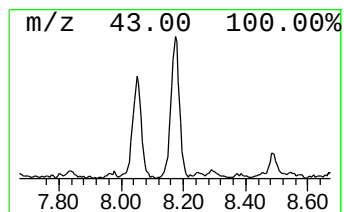
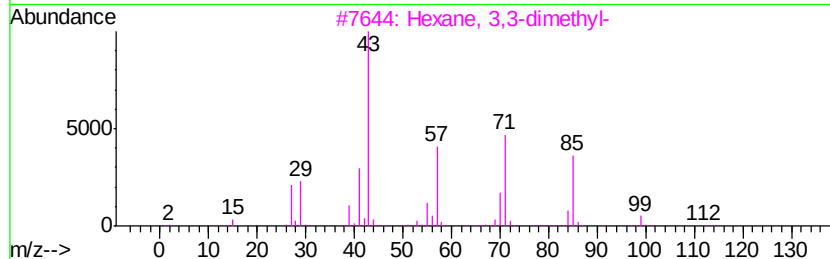
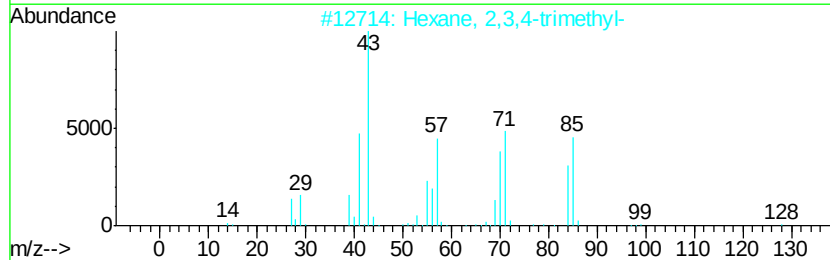
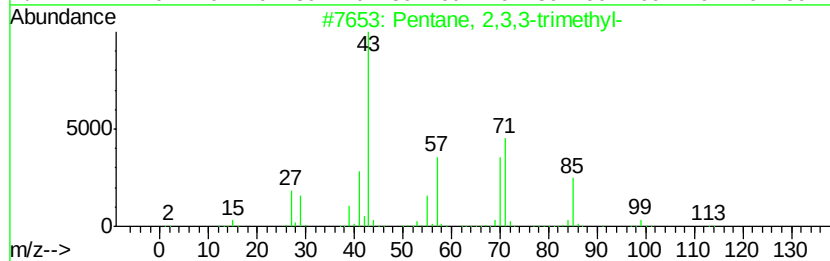
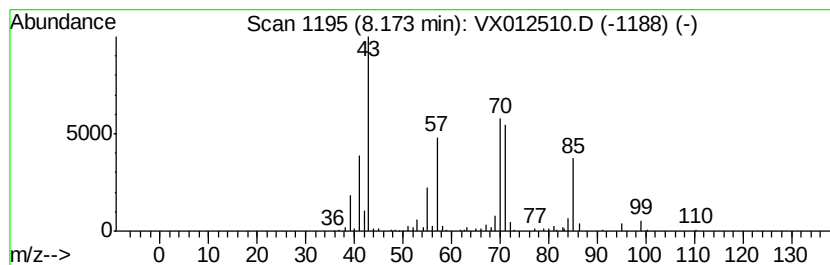
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	5.69 ug/l	84013	1,4-Difluorobenzene	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	72
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012510.D
Acq On : 19 Sep 2019 06:11
Operator : JC/SP
Sample : K4887-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 52 Sample Multiplier: 1

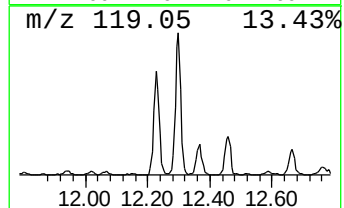
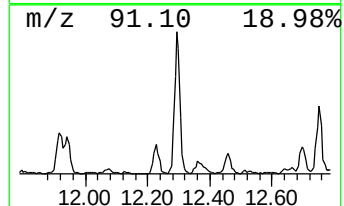
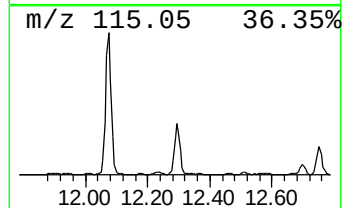
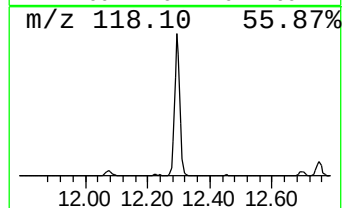
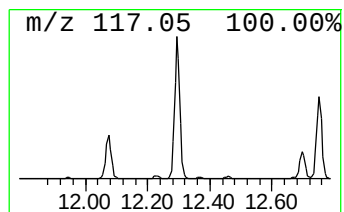
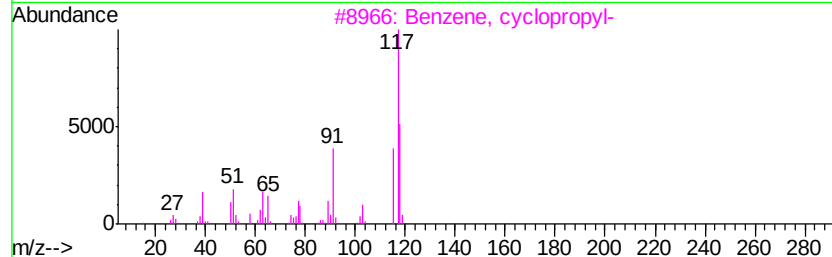
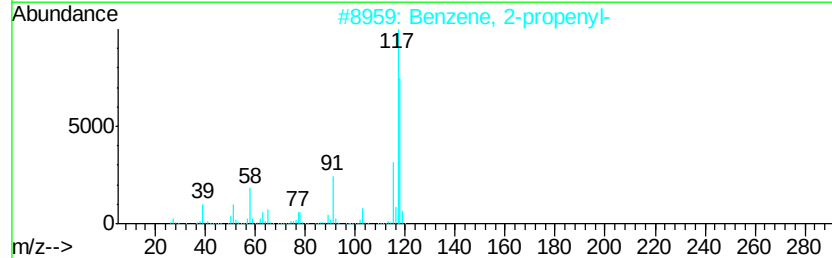
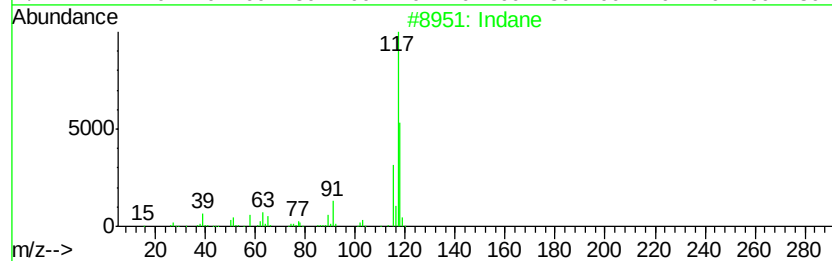
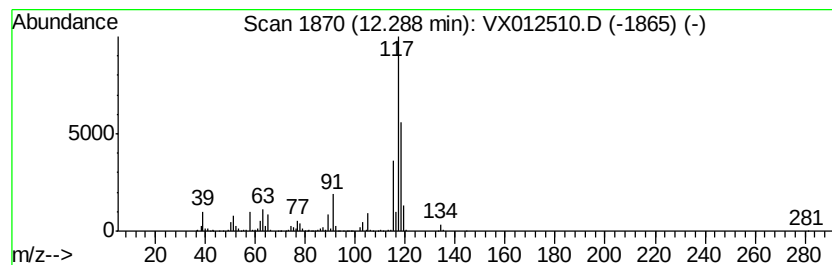
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	19.99 ug/l	269924	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indane		118 C9H10	000496-11-7 81
2	Benzene, 2-propenyl-		118 C9H10	000300-57-2 81
3	Benzene, cyclopropyl-		118 C9H10	000873-49-4 76
4	(Z)-1-Phenylpropene		118 C9H10	000766-90-5 76
5	Deltacyclene		118 C9H10	007785-10-6 64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012510.D
Acq On : 19 Sep 2019 06:11
Operator : JC/SP
Sample : K4887-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0158

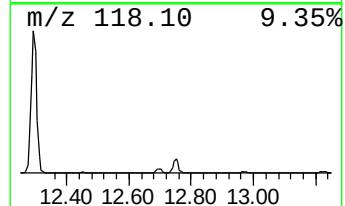
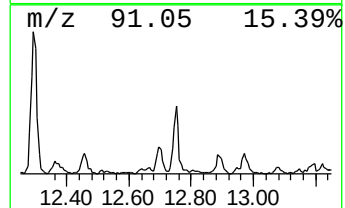
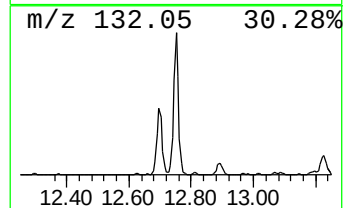
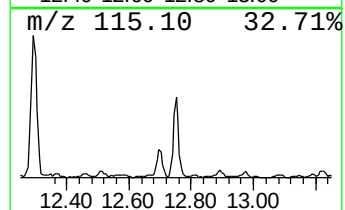
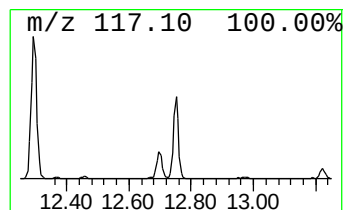
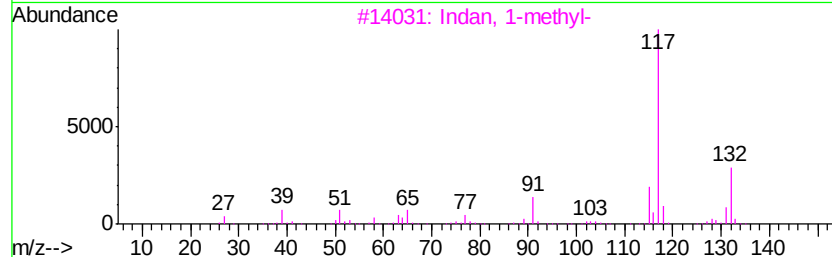
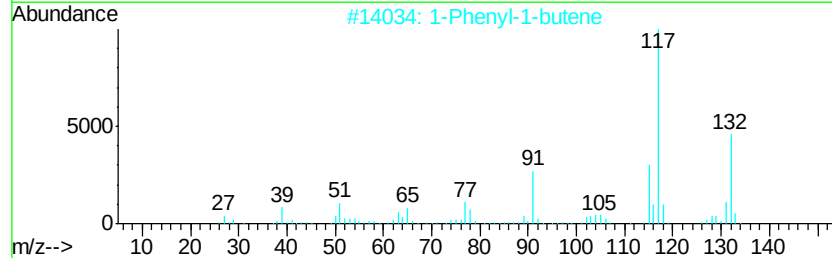
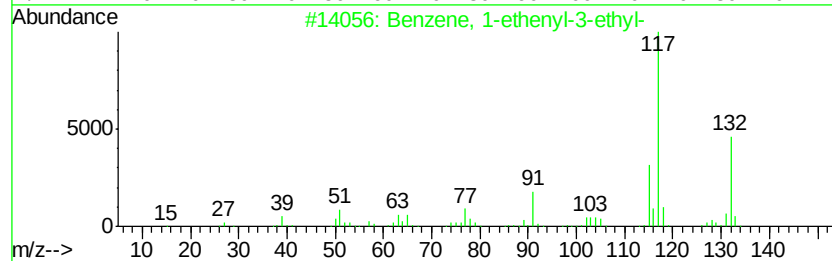
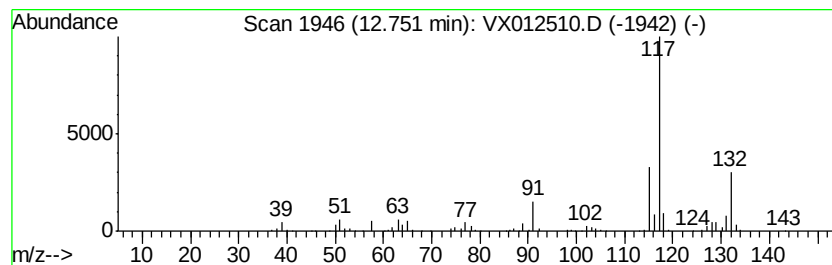
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	9.61 ug/l	129723	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	91
2		1-Phenyl-1-butene	132	C10H12	000824-90-8	90
3		Indan, 1-methyl-	132	C10H12	000767-58-8	90
4		Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	90
5		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091819\
Data File : VX012510.D
Acq On : 19 Sep 2019 06:11
Operator : JC/SP
Sample : K4887-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
Z2-0158

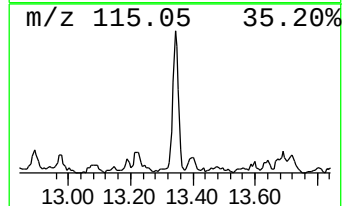
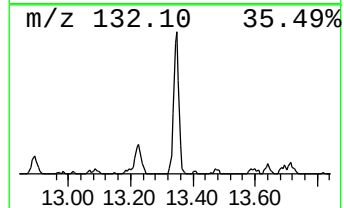
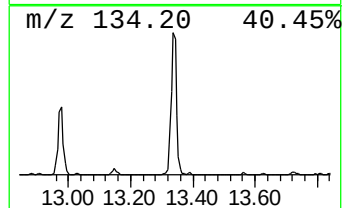
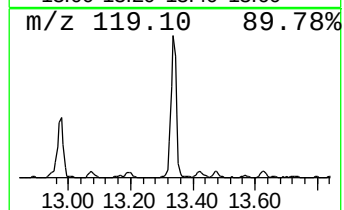
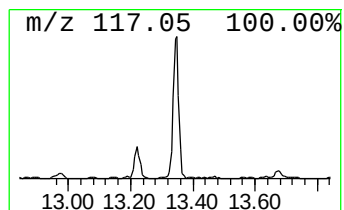
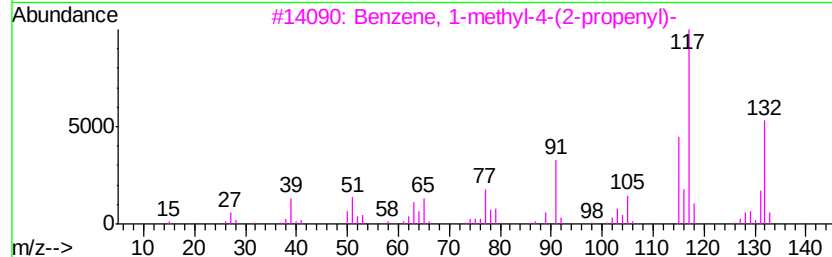
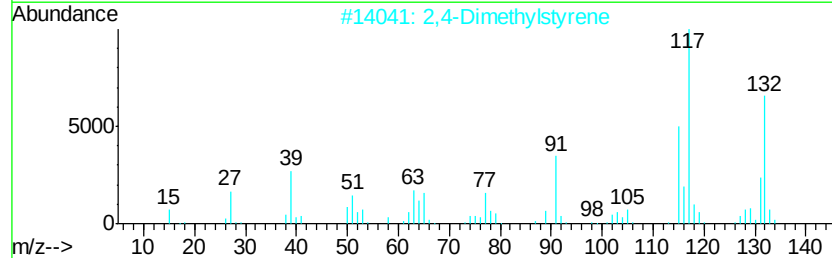
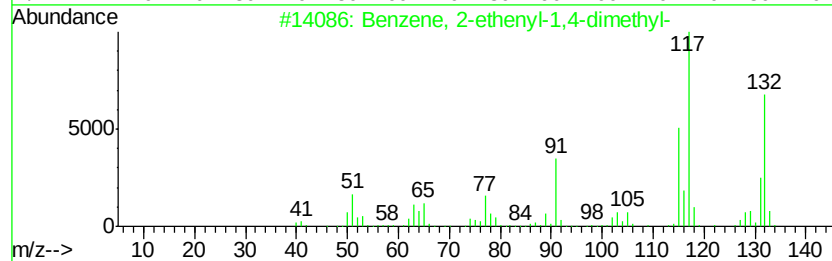
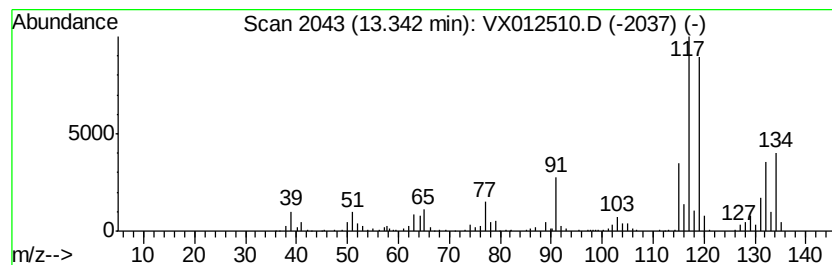
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	10.87 ug/l	146805	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
2		2,4-Dimethylstyrene	132	C10H12	002234-20-0	83
3		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
5		Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	55



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091819\
Data File : VX012510.D
Acq On : 19 Sep 2019 06:11
Operator : JC/SP
Sample : K4887-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0158

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
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Butane, 2,3-dimet...	2.84	14.4	ug/l	167068	1	5.65	582063	50.0
Pentane, 3-methyl-	3.17	7.6	ug/l	88636	1	5.65	582063	50.0
Cyclopentane, 1,3...	6.25	6.7	ug/l	77678	1	5.65	582063	50.0
Cyclobutane, 1,2-...	6.34	8.7	ug/l	127854	2	6.85	737820	50.0
Pentane, 2,3,3-tr...	8.17	5.7	ug/l	84013	2	6.85	737820	50.0
Indane	12.29	20.0	ug/l	269924	4	12.07	675098	50.0
Benzene, 1-etheny...	12.75	9.6	ug/l	129723	4	12.07	675098	50.0
Benzene, 2-etheny...	13.34	10.9	ug/l	146805	4	12.07	675098	50.0