

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX072619\
 Data File : VX011086.D
 Acq On : 26 Jul 2019 13:28
 Operator : JC/SP
 Sample : K4014-03 50X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

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\82X071619W.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	1.300	21	24	36	rVB	156126	154432	2.69%	0.614%
2	1.404	36	41	47	rBV	386254	410092	7.15%	1.630%
3	1.465	47	51	58	rVB	123918	125788	2.19%	0.500%
4	1.532	58	62	68	rBV	90287	90870	1.59%	0.361%
5	1.788	99	104	114	rBV	283385	418678	7.30%	1.664%
6	1.953	122	131	135	rBV	87067	120236	2.10%	0.478%
7	2.001	135	139	150	rVV	174965	249422	4.35%	0.991%
8	2.117	153	158	166	rVV	173417	250736	4.37%	0.997%
9	2.215	169	174	191	rVB	85817	142850	2.49%	0.568%
10	2.812	259	272	280	rBV	66710	163393	2.85%	0.649%
11	2.891	280	285	287	rVV	32104	58911	1.03%	0.234%
12	2.934	287	292	305	rVB	83576	187092	3.26%	0.744%
13	4.403	521	533	547	rBV2	73810	215781	3.76%	0.858%
14	5.501	701	713	720	rBV2	120353	353278	6.16%	1.404%
15	5.580	720	726	732	rVV2	75445	225716	3.94%	0.897%
16	5.659	732	739	755	rVB	200905	576023	10.05%	2.290%
17	6.062	795	805	810	rBV	116135	300847	5.25%	1.196%
18	6.141	810	818	831	rVB	1045471	2734670	47.71%	10.871%
19	6.336	838	850	862	rVB2	57831	190805	3.33%	0.758%
20	6.860	925	936	946	rBV	307476	734778	12.82%	2.921%
21	7.464	1023	1035	1044	rBV2	47932	114211	1.99%	0.454%
22	8.494	1197	1204	1210	rBV	49333	86700	1.51%	0.345%
23	8.567	1210	1216	1224	rVV	152402	240250	4.19%	0.955%
24	8.714	1233	1240	1245	rBV	662723	1018772	17.77%	4.050%
25	8.787	1245	1252	1264	rVV	3694542	5731722	100.00%	22.784%
26	8.903	1265	1271	1281	rVB	174050	275035	4.80%	1.093%
27	9.500	1363	1369	1376	rBV	71948	113600	1.98%	0.452%
28	10.079	1456	1464	1466	rBV	137284	238646	4.16%	0.949%
29	10.110	1466	1469	1474	rVV	680079	893334	15.59%	3.551%
30	10.158	1474	1477	1480	rVV	55097	75797	1.32%	0.301%
31	10.201	1480	1484	1487	rVV	156911	207706	3.62%	0.826%
32	10.250	1487	1492	1497	rVV	848897	1048360	18.29%	4.167%
33	10.354	1504	1509	1515	rVB	1988225	2669671	46.58%	10.612%
34	10.695	1560	1565	1575	rVB	889703	1119780	19.54%	4.451%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

35	10.841	1582	1589	1596	rBV	57771	102882	1.79%	0.409%
36	11.134	1630	1637	1642	rBV	622762	777642	13.57%	3.091%
37	11.225	1646	1652	1659	rVV2	73090	120572	2.10%	0.479%
38	11.323	1663	1668	1671	rVV	59021	82868	1.45%	0.329%
39	11.359	1671	1674	1678	rVV	63312	84267	1.47%	0.335%
40	11.433	1681	1686	1693	rVV	214029	366831	6.40%	1.458%
41	11.506	1693	1698	1707	rVB	103960	143222	2.50%	0.569%
42	11.664	1718	1724	1731	rBV	95016	122950	2.15%	0.489%
43	11.804	1742	1747	1751	rBV	329282	396439	6.92%	1.576%
44	11.933	1762	1768	1776	rBV4	49202	98086	1.71%	0.390%
45	12.073	1786	1791	1797	rBV	711366	925684	16.15%	3.680%
46	12.140	1797	1802	1808	rVV	115407	162513	2.84%	0.646%
47	12.298	1821	1828	1835	rBV2	95980	157300	2.74%	0.625%
48	13.829	2074	2079	2085	rVB	58932	77499	1.35%	0.308%

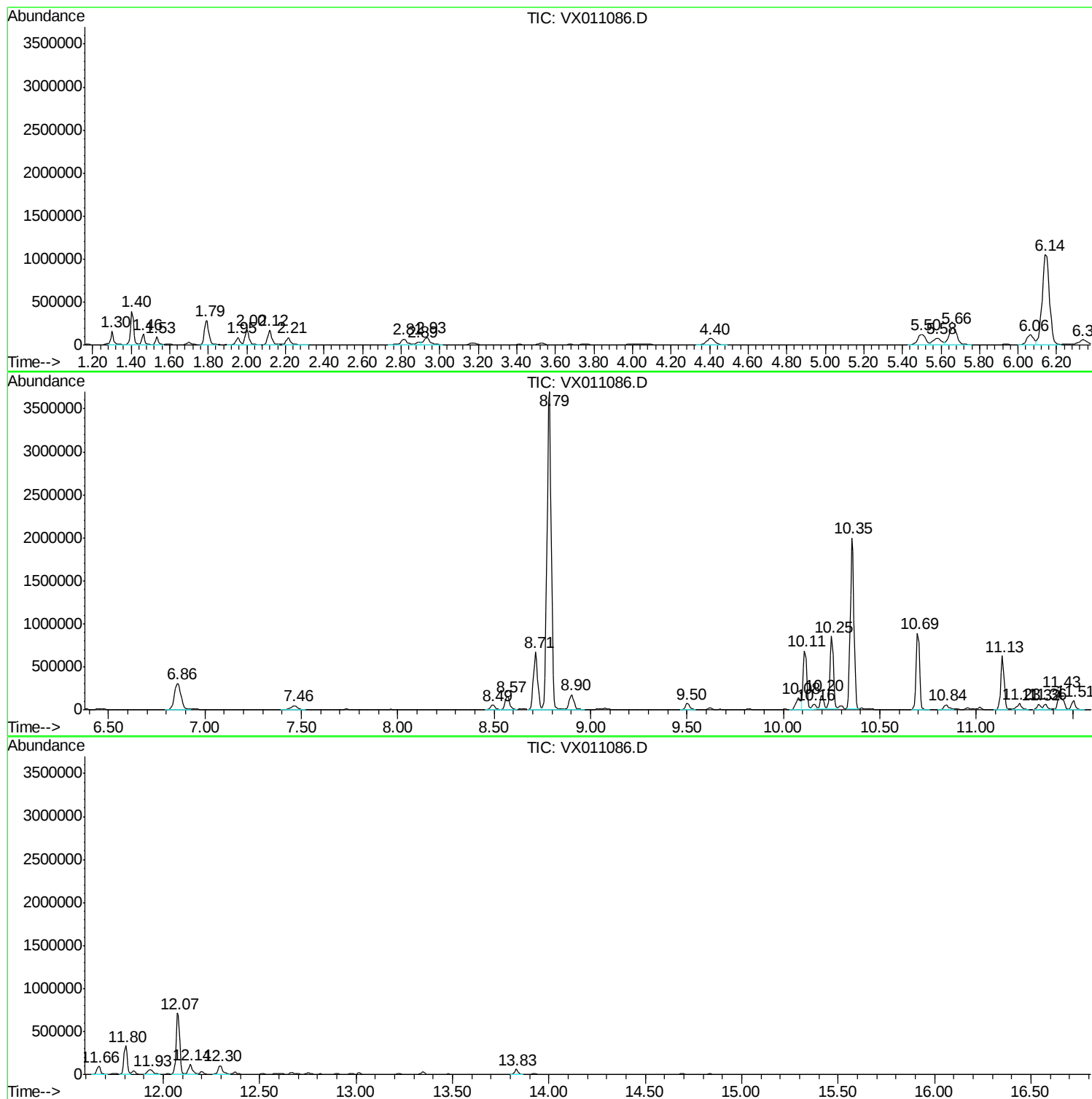
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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



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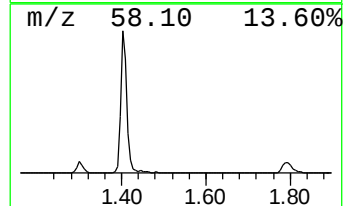
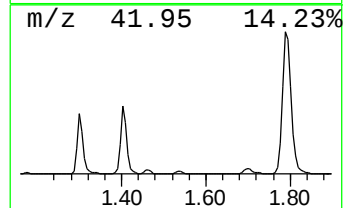
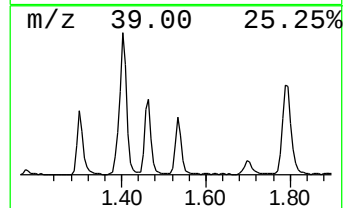
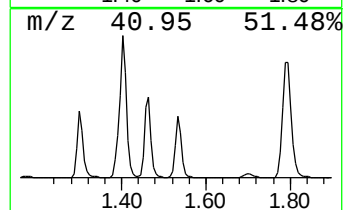
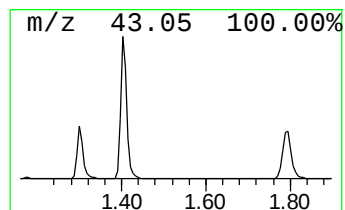
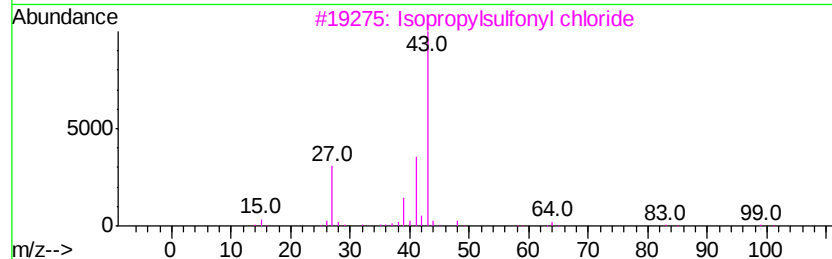
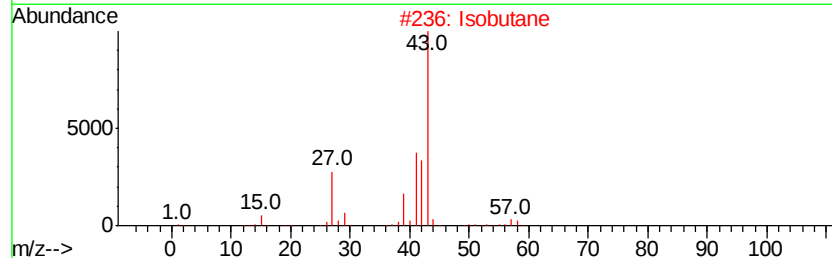
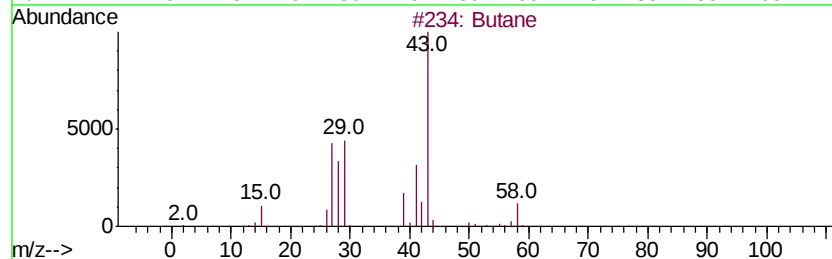
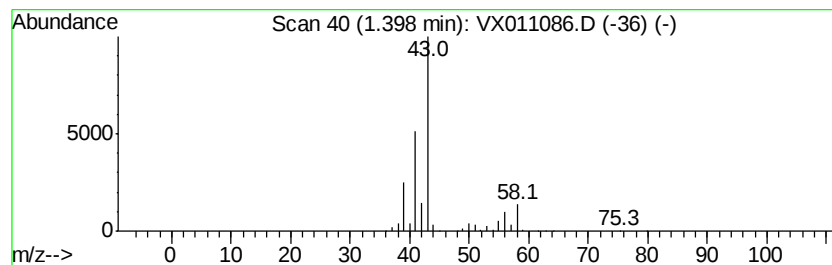
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	35.60 ug/l	410092	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane	58	C4H10	000106-97-8	64
2		Isobutane	58	C4H10	000075-28-5	9
3		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5		Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



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Instrument :
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ClientSampled :
MW-3

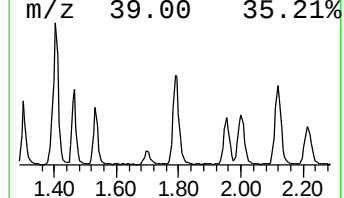
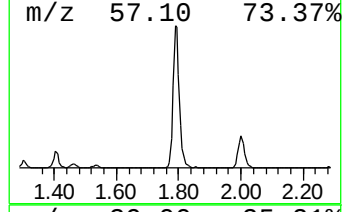
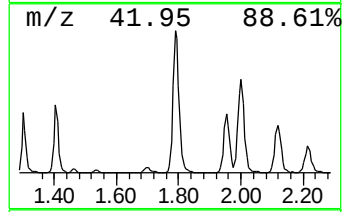
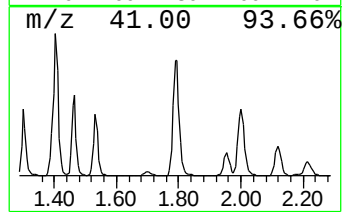
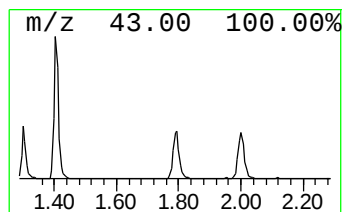
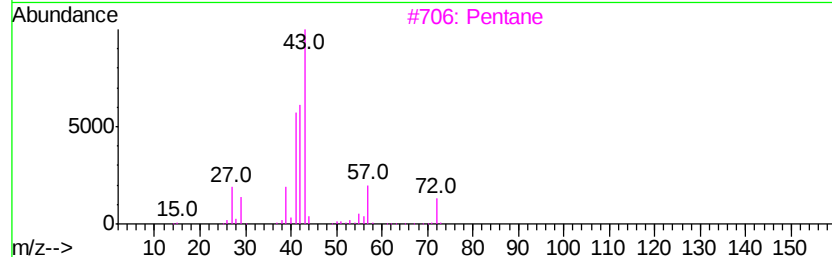
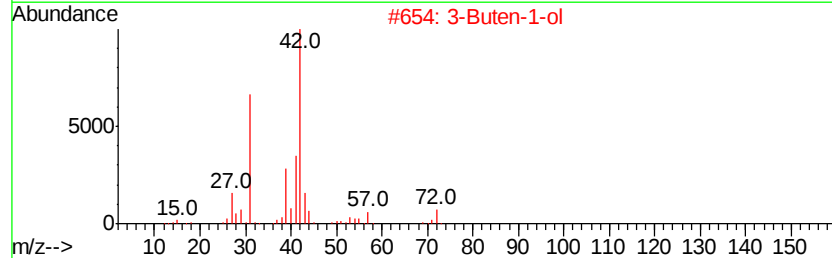
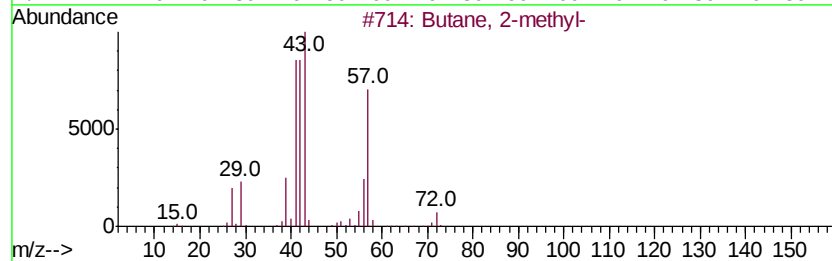
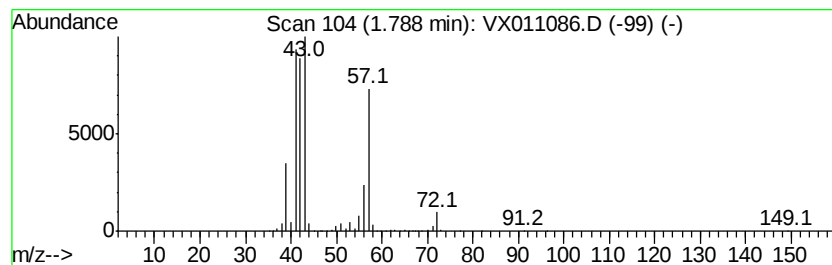
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	36.34 ug/l	418678	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	43
3		Pentane	72	C5H12	000109-66-0	36
4		2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	17
5		1-Butene	56	C4H8	000106-98-9	10



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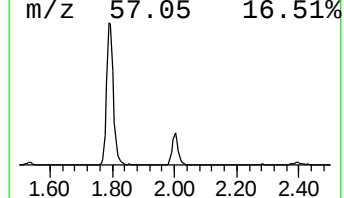
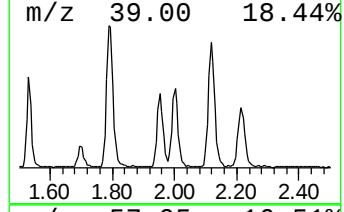
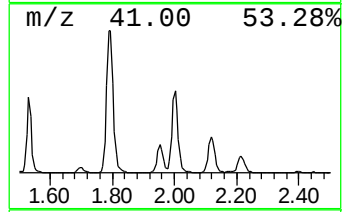
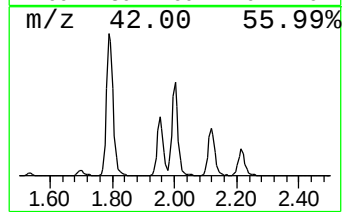
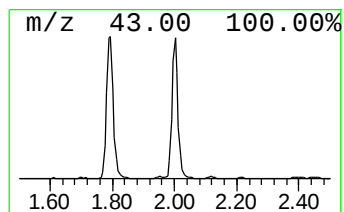
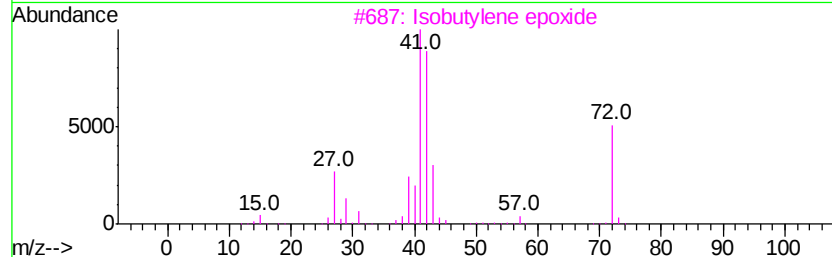
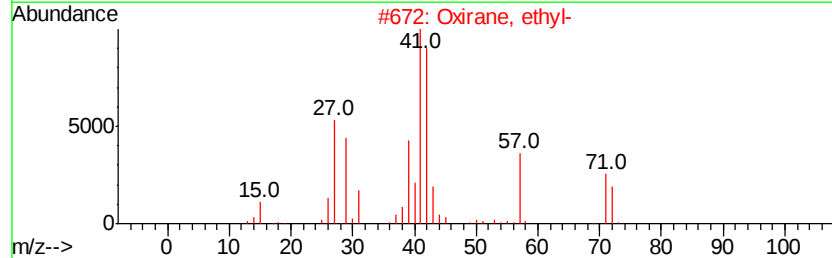
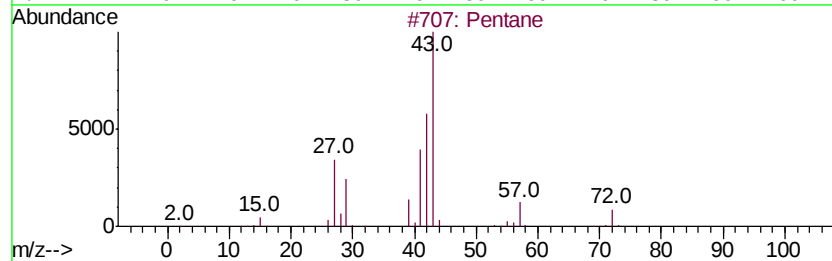
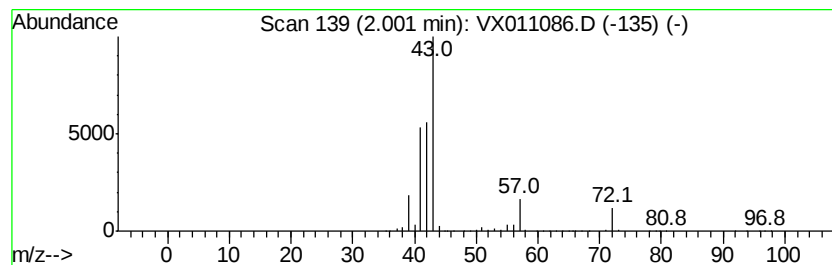
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	21.65 ug/l	249422	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Isobutylene epoxide	72	C4H8O	000558-30-5	40
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	25
5			Tetrahydrofuran	72	C4H8O	000109-99-9	9



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Instrument :
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ClientSampled :
MW-3

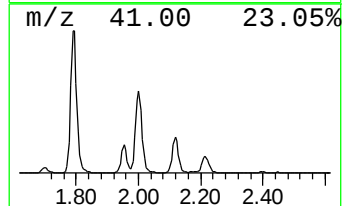
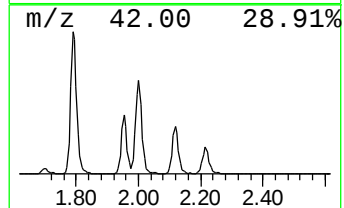
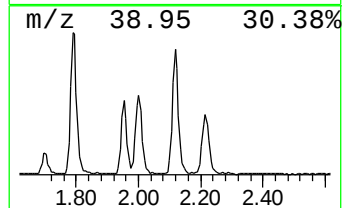
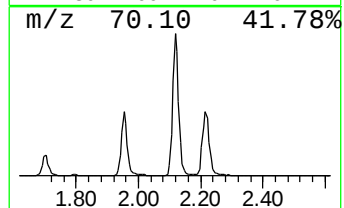
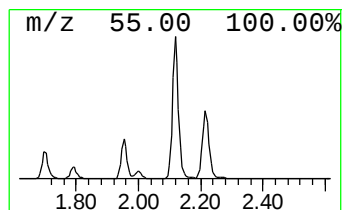
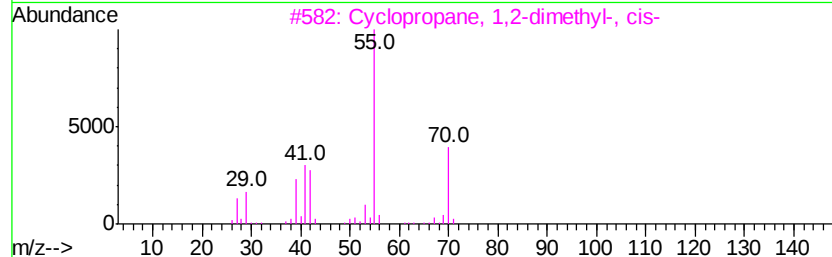
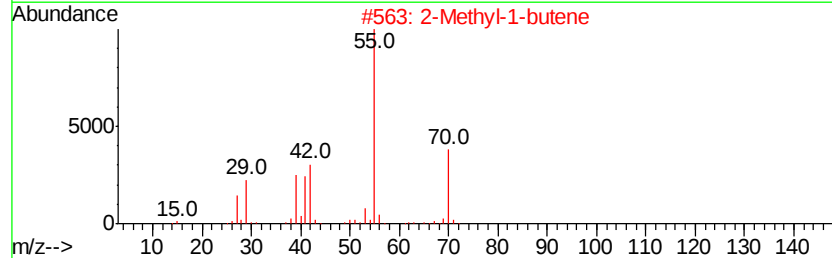
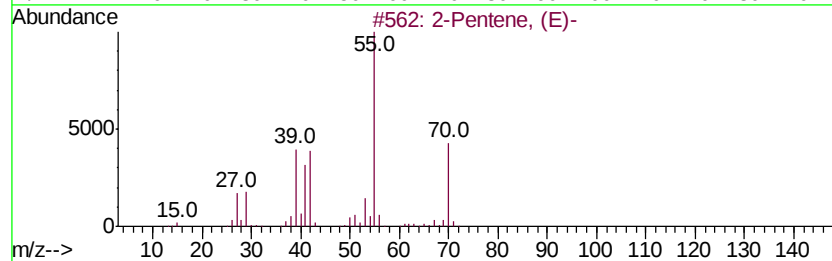
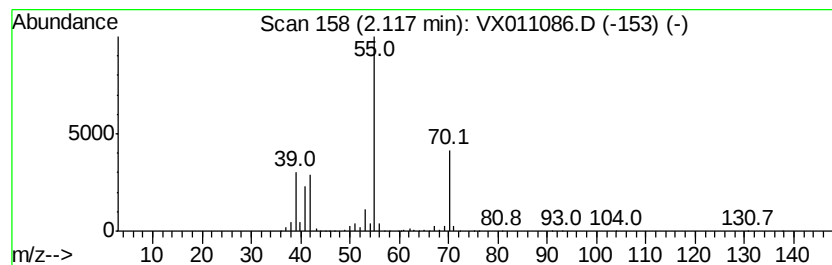
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Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	21.76 ug/l	250736	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentene, (E)-	70	C5H10	000646-04-8	94
2		2-Methyl-1-butene	70	C5H10	000563-46-2	91
3		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
4		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
5		2-Butene, 2-methyl-	70	C5H10	000513-35-9	86



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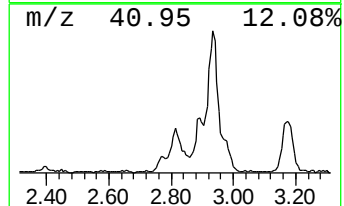
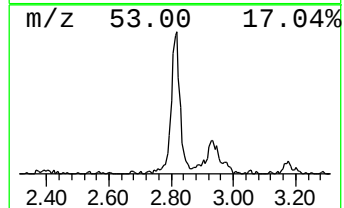
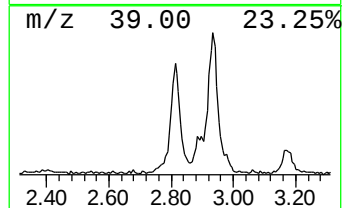
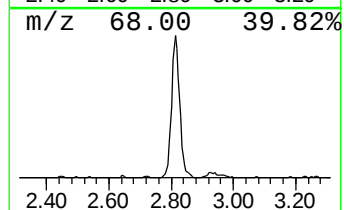
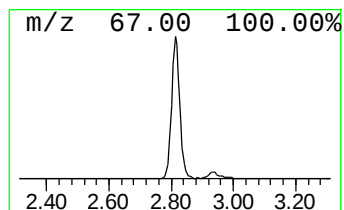
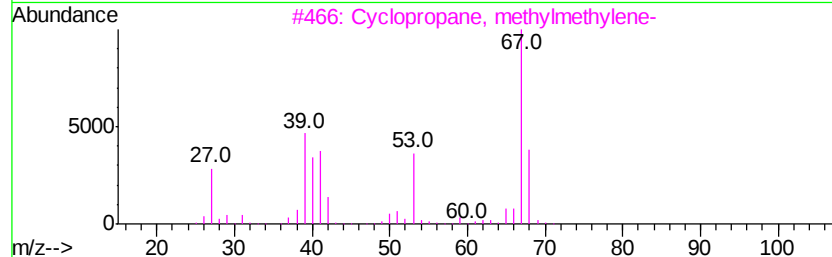
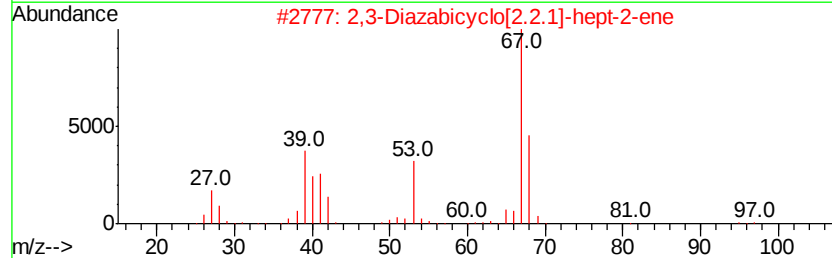
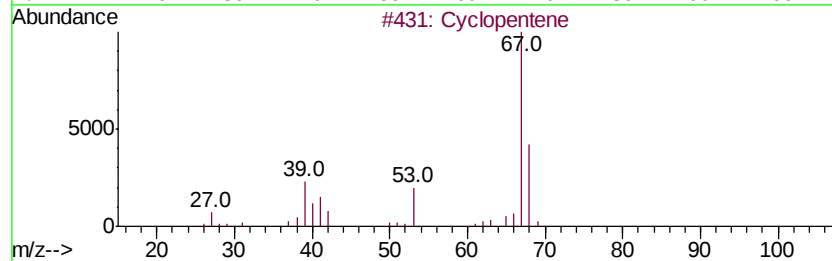
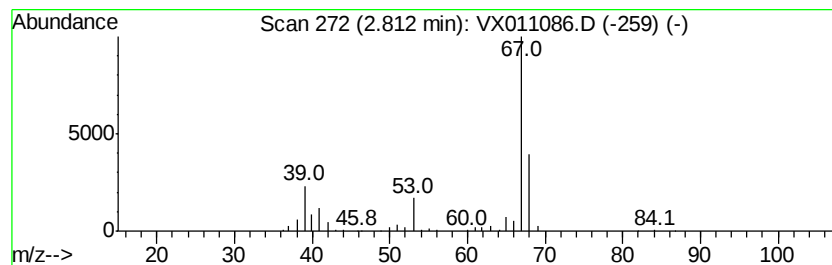
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	14.18 ug/l	163393	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentene	68	C5H8	000142-29-0	91
2		2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	83
3		Cyclopropane, methylmethylen-	68	C5H8	018631-84-0	83
4		1-Butyne, 3-methyl-	68	C5H8	000598-23-2	59
5		1,4-Pentadiene	68	C5H8	000591-93-5	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX072619\
Data File : VX011086.D
Acq On : 26 Jul 2019 13:28
Operator : JC/SP
Sample : K4014-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-3

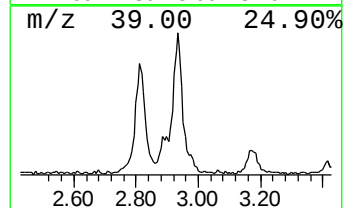
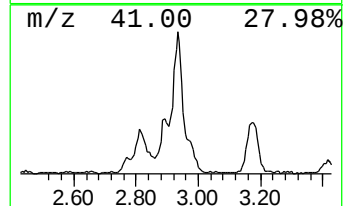
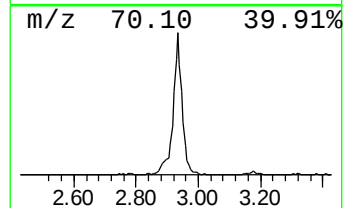
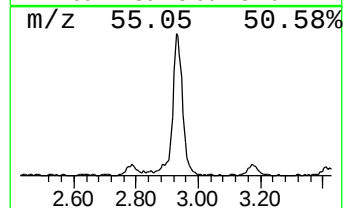
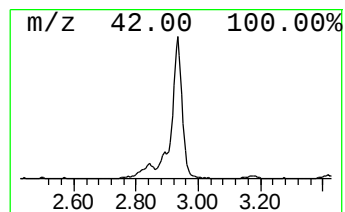
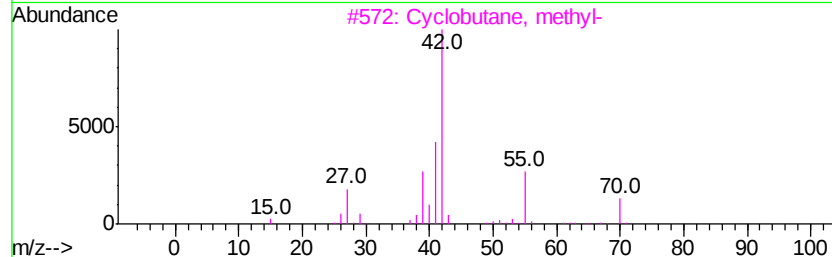
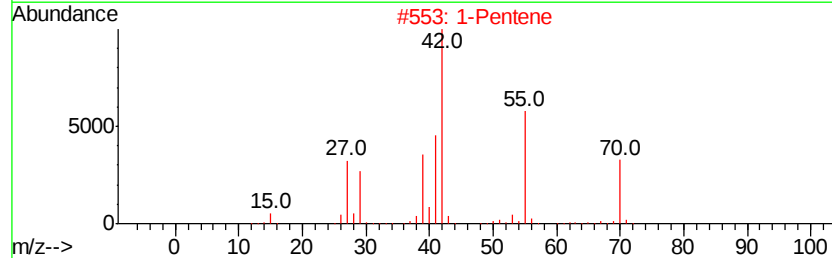
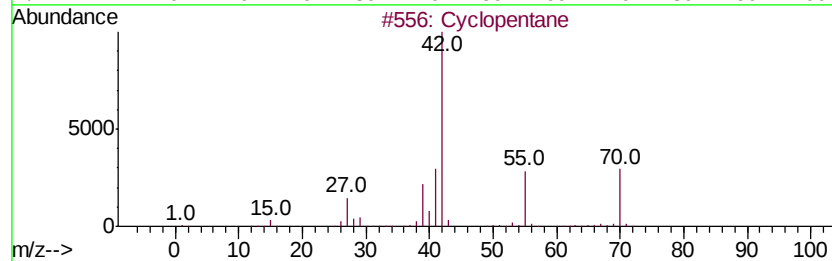
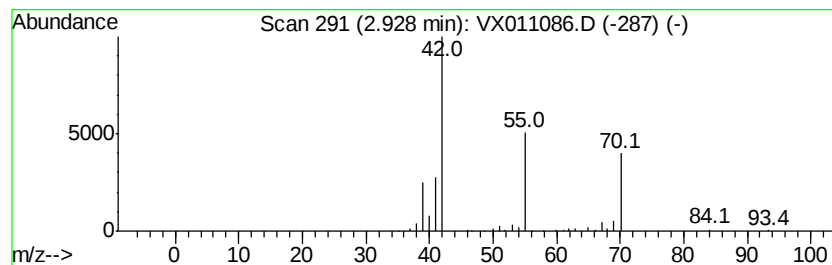
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	16.24 ug/l	187092	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane	70	C5H10	000287-92-3	86
2		1-Pentene	70	C5H10	000109-67-1	50
3		Cyclobutane, methyl-	70	C5H10	000598-61-8	47
4		Cyclopropane, ethyl-	70	C5H10	001191-96-4	33
5		n-Propyl chloride	78	C3H7Cl	000540-54-5	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX072619\
Data File : VX011086.D
Acq On : 26 Jul 2019 13:28
Operator : JC/SP
Sample : K4014-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

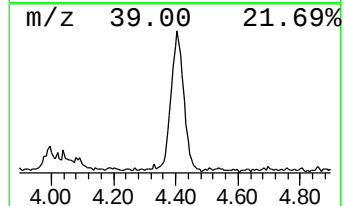
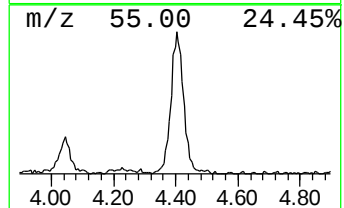
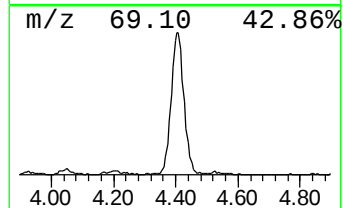
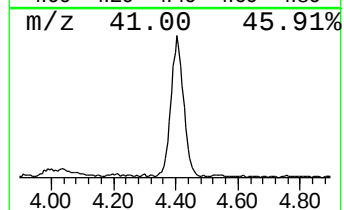
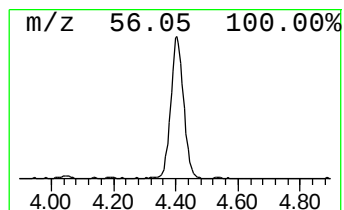
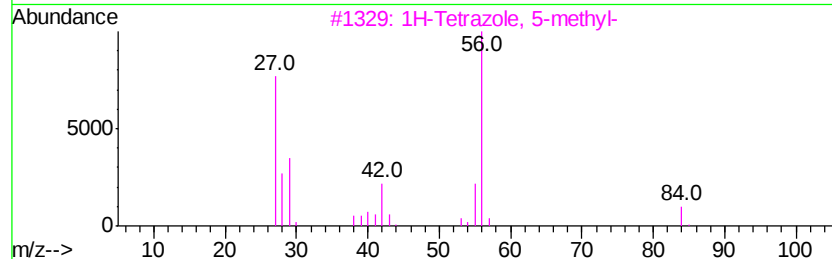
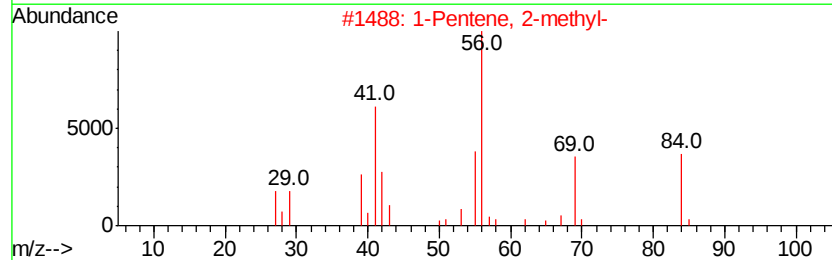
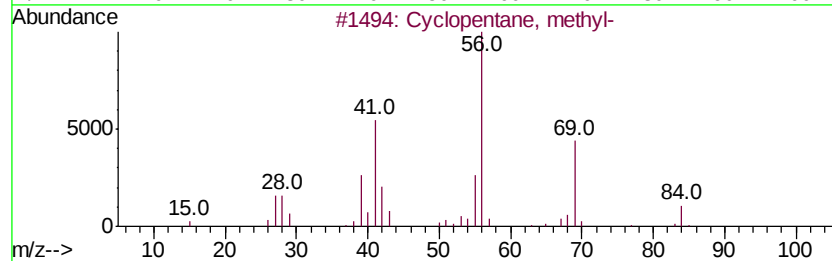
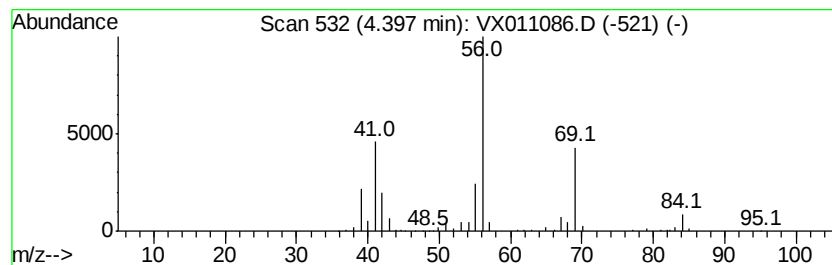
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	18.73 ug/l	215781	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	83
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
4		Cyclohexane	84	C6H12	000110-82-7	78
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX072619\
Data File : VX011086.D
Acq On : 26 Jul 2019 13:28
Operator : JC/SP
Sample : K4014-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-3

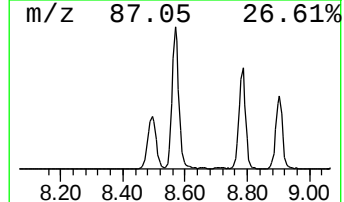
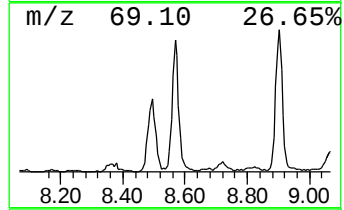
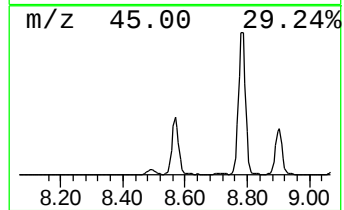
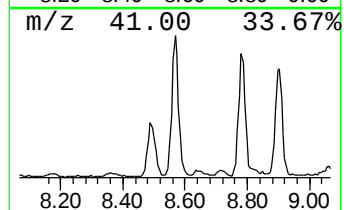
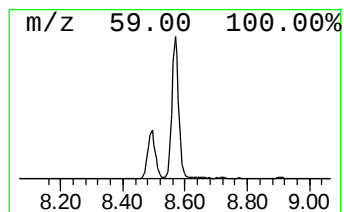
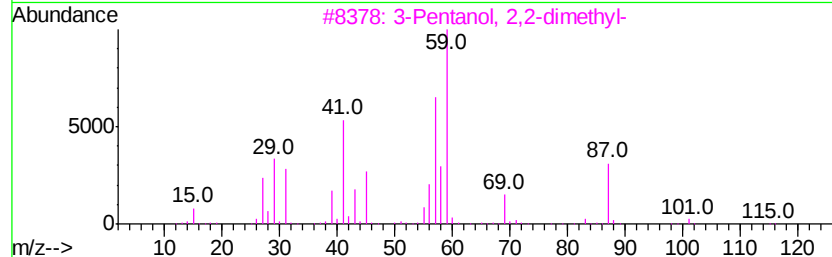
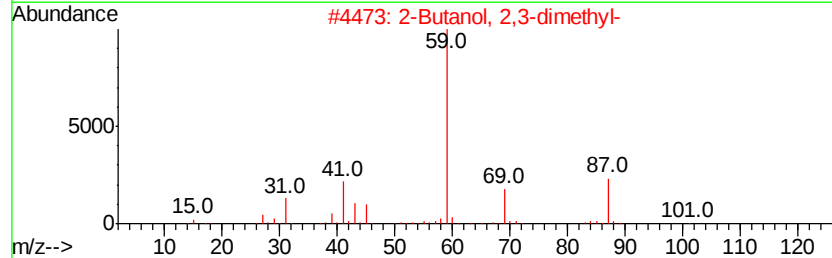
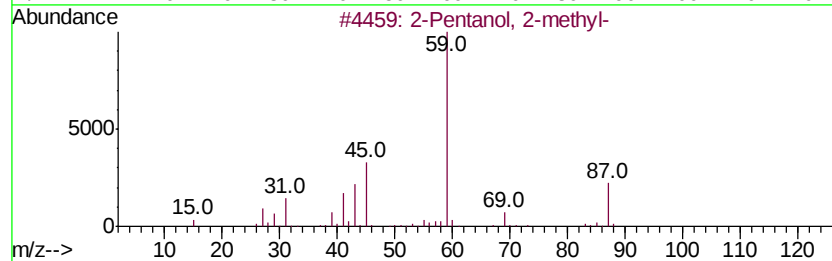
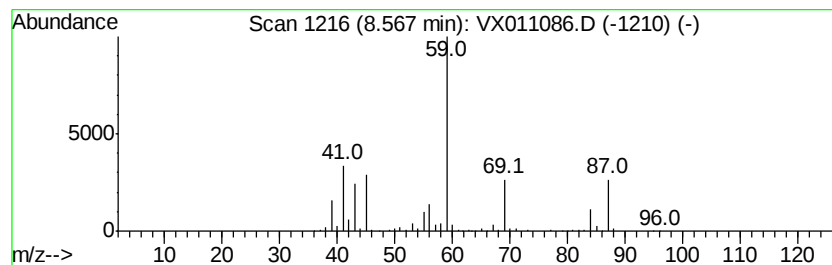
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Quant Title : SW846 8260

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

Peak Number 8 2-Pentanol, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	13.45 ug/l	240250	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
2		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72
3		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	72
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	56
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX072619\
Data File : VX011086.D
Acq On : 26 Jul 2019 13:28
Operator : JC/SP
Sample : K4014-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-3

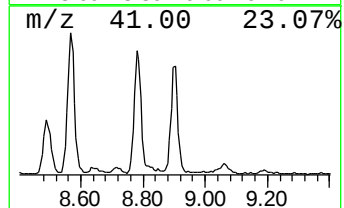
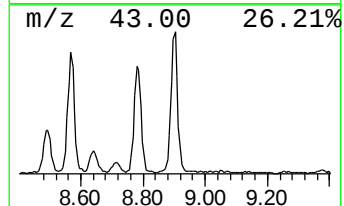
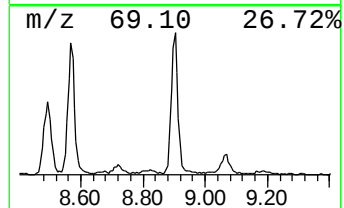
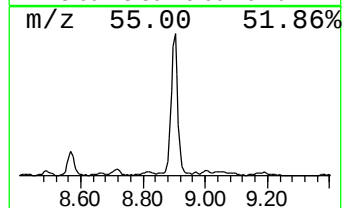
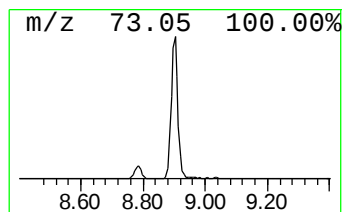
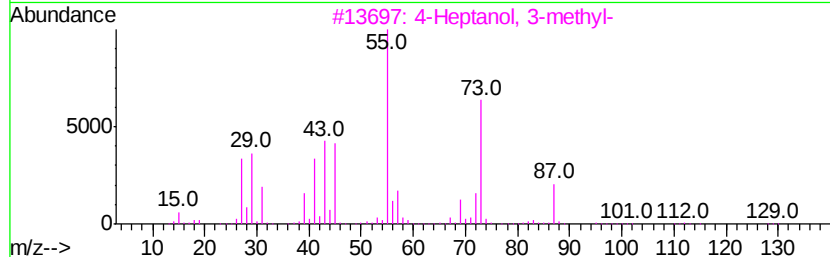
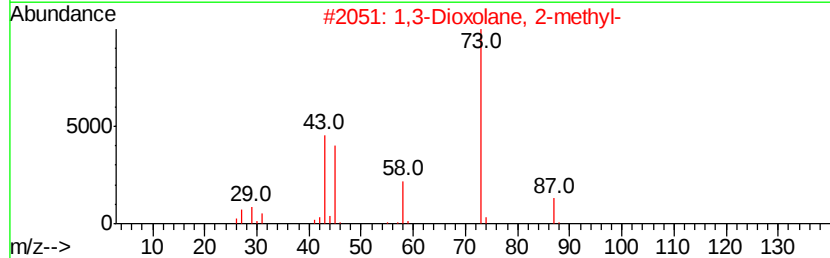
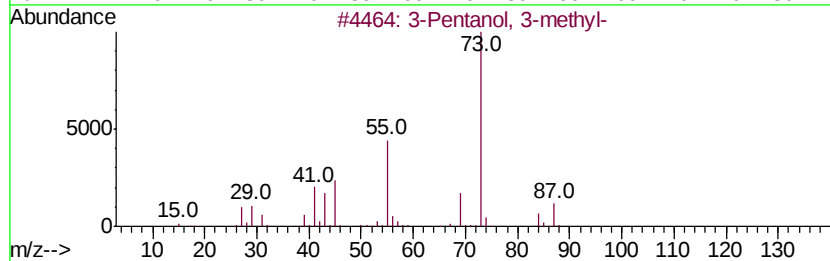
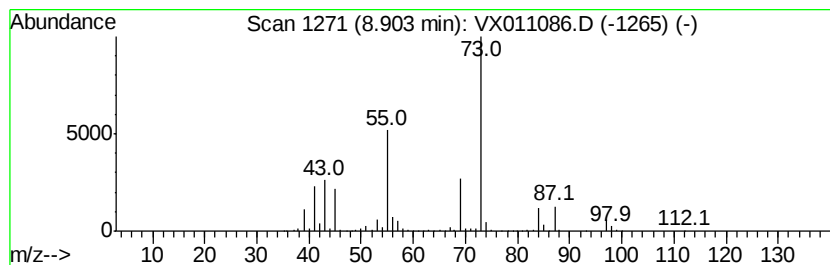
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Quant Title : SW846 8260

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

Peak Number 9 3-Pentanol, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	15.39 ug/l	275035	Chlorobenzene-d5	10.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-			102	C6H14O	000077-74-7	72
2	1,3-Dioxolane, 2-methyl-			88	C4H8O2	000497-26-7	47
3	4-Heptanol, 3-methyl-			130	C8H18O	001838-73-9	33
4	1,3-Dioxolane, 2-(1-methylethyl)-			116	C6H12O2	000822-83-3	25
5	3-Pentanol, 2,4-dimethyl-			116	C7H16O	000600-36-2	23



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX072619\
Data File : VX011086.D
Acq On : 26 Jul 2019 13:28
Operator : JC/SP
Sample : K4014-03 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-3

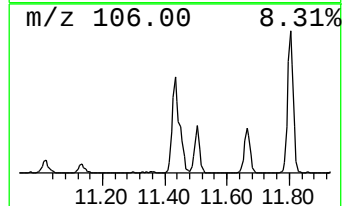
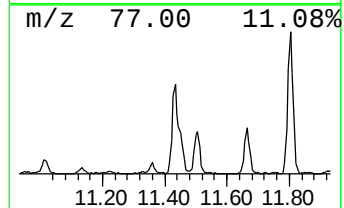
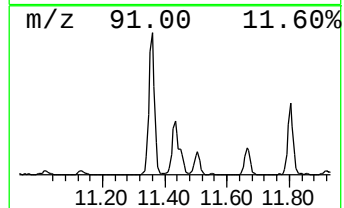
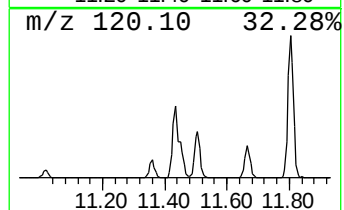
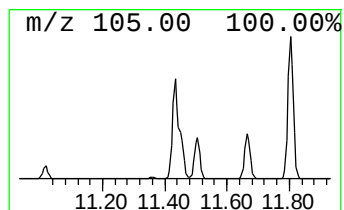
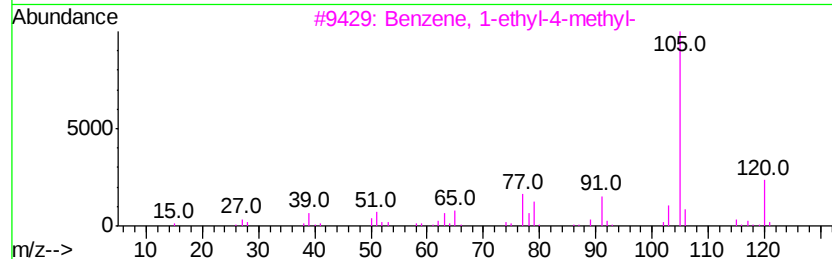
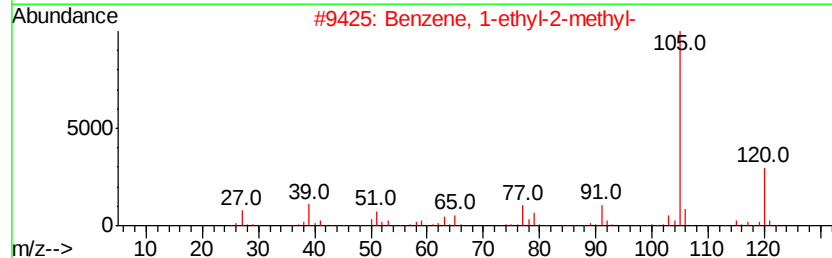
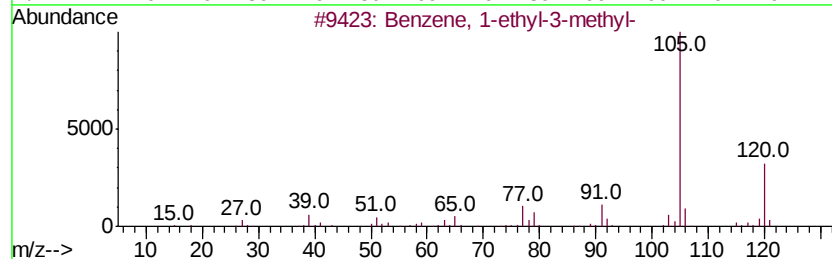
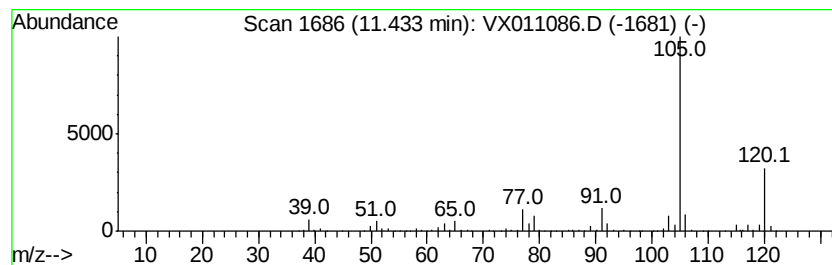
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	19.81 ug/l	366831	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX072619\
Data File : VX011086.D
Acq On : 26 Jul 2019 13:28
Operator : JC/SP
Sample : K4014-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.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	1.40	35.6	ug/l	410092	1	5.67	576023	50.0
Butane, 2-methyl-	1.79	36.3	ug/l	418678	1	5.67	576023	50.0
Pentane	2.00	21.6	ug/l	249422	1	5.67	576023	50.0
2-Pentene, (E)-	2.12	21.8	ug/l	250736	1	5.67	576023	50.0
Cyclopentene	2.81	14.2	ug/l	163393	1	5.67	576023	50.0
Cyclopentane	2.93	16.2	ug/l	187092	1	5.67	576023	50.0
Cyclopentane, met...	4.40	18.7	ug/l	215781	1	5.67	576023	50.0
2-Pentanol, 2-met...	8.57	13.4	ug/l	240250	3	10.11	893334	50.0
3-Pentanol, 3-met...	8.90	15.4	ug/l	275035	3	10.11	893334	50.0
Benzene, 1-ethyl-...	11.43	19.8	ug/l	366831	4	12.08	925684	50.0