

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
 Data File : VX010966.D
 Acq On : 18 Jul 2019 18:05
 Operator : JC/SP
 Sample : K3884-06
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0608

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	1.788	99	104	120	rVB	1688179	2482529	7.00%	1.520%
2	2.001	133	139	153	rVB	1272813	1788531	5.04%	1.095%
3	2.849	269	278	282	rBV	931533	2167867	6.11%	1.327%
4	2.891	282	285	289	rVB	486223	808272	2.28%	0.495%
5	3.178	321	332	347	rBV	726725	1688664	4.76%	1.034%
6	3.525	379	389	403	rBV	536818	1230934	3.47%	0.754%
7	4.312	507	518	524	rBV	252442	748629	2.11%	0.458%
8	4.409	524	534	548	rVB	2155464	6315553	17.81%	3.867%
9	5.501	702	713	717	rBV2	132336	372530	1.05%	0.228%
10	5.586	717	727	736	rVV	2341768	7058575	19.91%	4.322%
11	5.732	744	751	766	rVB	549307	1664158	4.69%	1.019%
12	5.940	770	785	797	rBV5	206781	716118	2.02%	0.438%
13	6.263	824	838	843	rBV	153646	437922	1.24%	0.268%
14	6.354	843	853	862	rVV	880105	2709451	7.64%	1.659%
15	6.458	862	870	883	rVB	199319	547260	1.54%	0.335%
16	6.860	926	936	946	rBV	339700	814026	2.30%	0.498%
17	7.464	1021	1035	1046	rBV	1955816	4342729	12.25%	2.659%
18	8.055	1121	1132	1142	rVB	776426	1562593	4.41%	0.957%
19	8.177	1142	1152	1160	rBV	1328256	2607276	7.35%	1.596%
20	8.671	1225	1233	1236	rBV3	245416	523635	1.48%	0.321%
21	8.714	1236	1240	1250	rVB	763502	1252040	3.53%	0.767%
22	10.110	1464	1469	1475	rBV	719926	982776	2.77%	0.602%
23	10.256	1486	1493	1498	rBV	12696285	16762509	47.27%	10.264%
24	10.366	1502	1511	1516	rBV	25238556	35457964	100.00%	21.711%
25	10.701	1560	1566	1576	rVB	9566716	12159454	34.29%	7.445%
26	11.018	1612	1618	1631	rVB	1059533	1331075	3.75%	0.815%
27	11.134	1631	1637	1642	rBV	687215	874181	2.47%	0.535%
28	11.359	1668	1674	1681	rBV	1405809	1676329	4.73%	1.026%
29	11.433	1681	1686	1688	rBV	4308742	5636827	15.90%	3.451%
30	11.506	1694	1698	1705	rVB	3371440	3975823	11.21%	2.434%
31	11.664	1719	1724	1734	rBV	2995526	3713665	10.47%	2.274%
32	11.804	1743	1747	1753	rVB	9612114	12187045	34.37%	7.462%
33	12.073	1786	1791	1796	rVB2	903116	1261980	3.56%	0.773%
34	12.140	1797	1802	1808	rBV	4665931	5683989	16.03%	3.480%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : SW846 8260

35	12.298	1822	1828	1835	rBV2	2679926	3632731	10.25%	2.224%
36	12.371	1835	1840	1849	rVB3	683565	1044136	2.94%	0.639%
37	12.585	1870	1875	1877	rBV	427150	557260	1.57%	0.341%
38	12.609	1877	1879	1883	rVV	450564	461493	1.30%	0.283%
39	12.664	1883	1888	1891	rVV	607041	739372	2.09%	0.453%
40	12.755	1898	1903	1911	rVB2	477530	773540	2.18%	0.474%
41	12.902	1922	1927	1932	rVB2	287844	377155	1.06%	0.231%
42	12.975	1932	1939	1942	rVV	382392	463922	1.31%	0.284%
43	13.018	1942	1946	1952	rVB	512804	615283	1.74%	0.377%
44	13.225	1975	1980	1984	rVB	543297	661002	1.86%	0.405%
45	13.347	1995	2000	2005	rVB2	1372870	1845392	5.20%	1.130%
46	13.475	2016	2021	2028	rVB	947194	1209642	3.41%	0.741%
47	13.835	2071	2080	2088	rBV	3914399	5118933	14.44%	3.134%
48	14.694	2209	2221	2232	rBV	1084507	1364418	3.85%	0.835%
49	14.834	2239	2244	2254	rBV	695816	913168	2.58%	0.559%

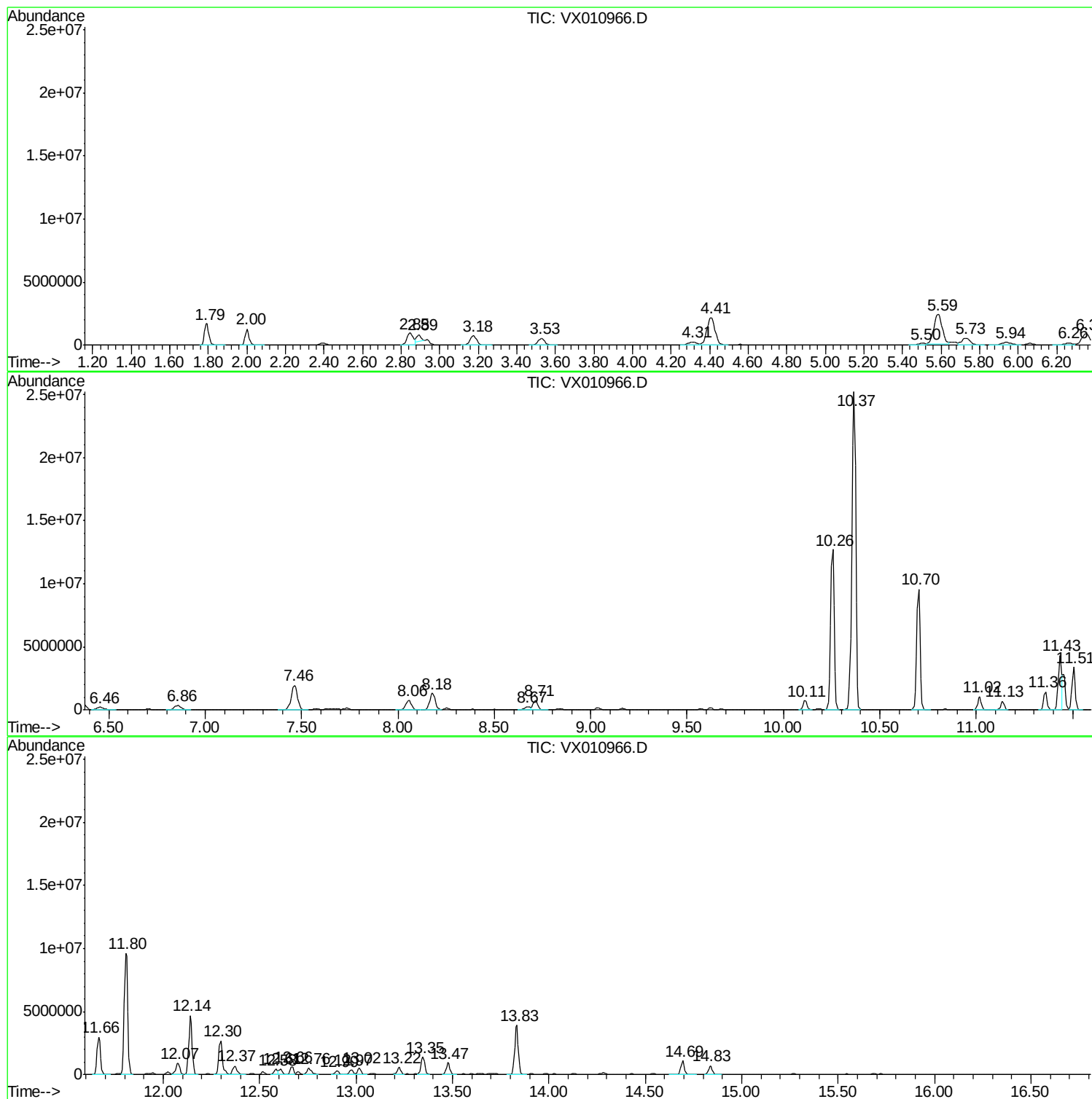
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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



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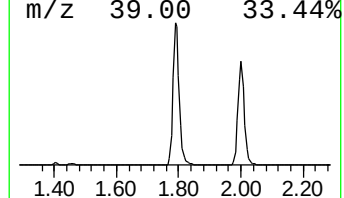
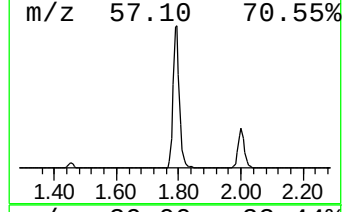
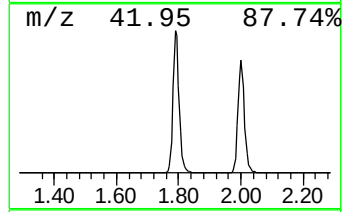
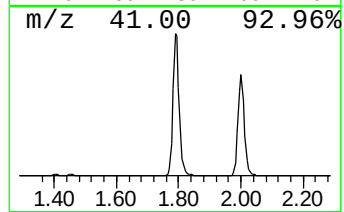
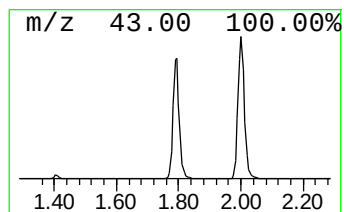
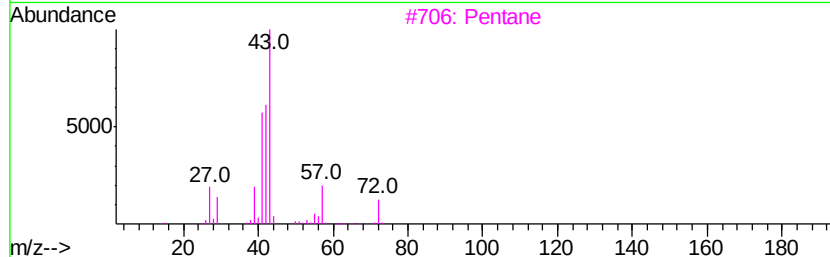
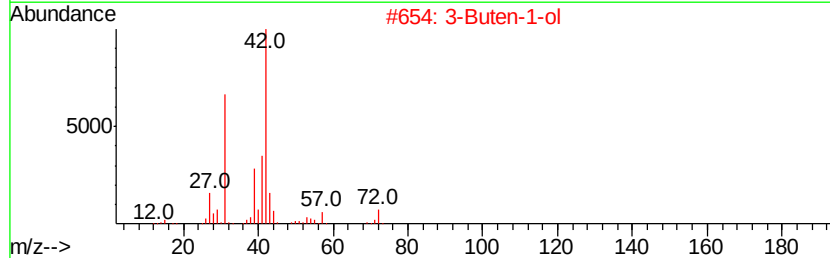
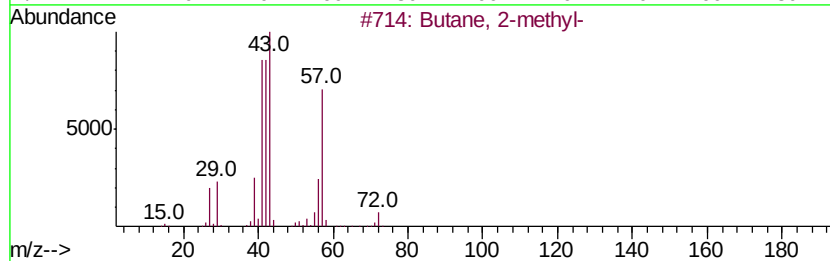
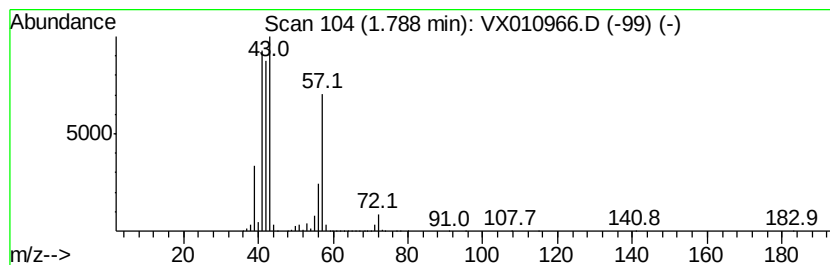
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	74.59 ug/l	2482530	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Pentane	72	C5H12	000109-66-0	36
4		1-Butene	56	C4H8	000106-98-9	10
5		Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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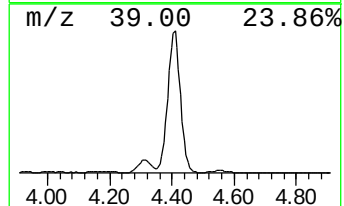
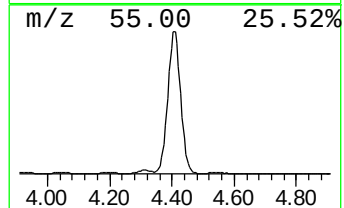
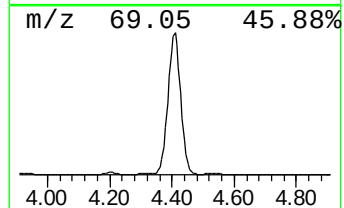
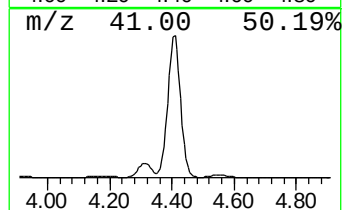
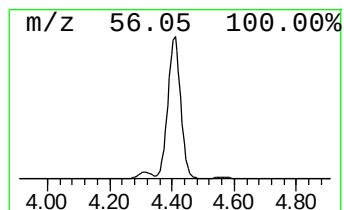
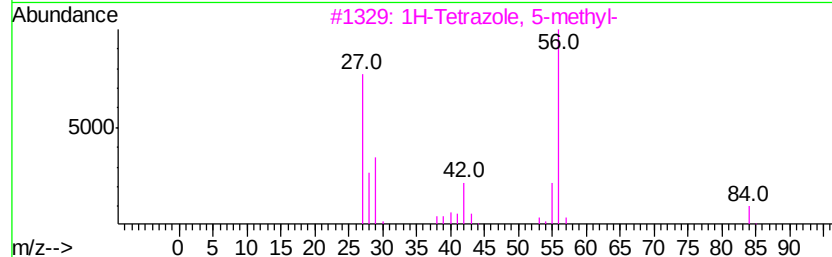
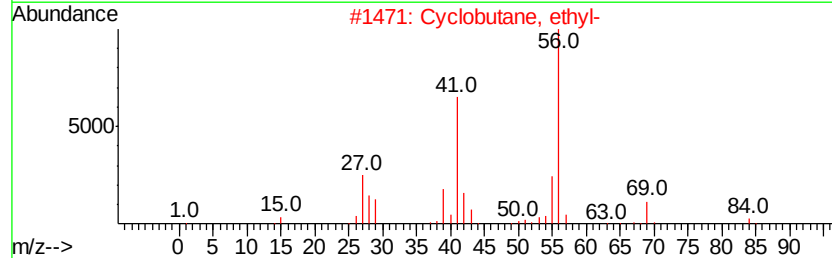
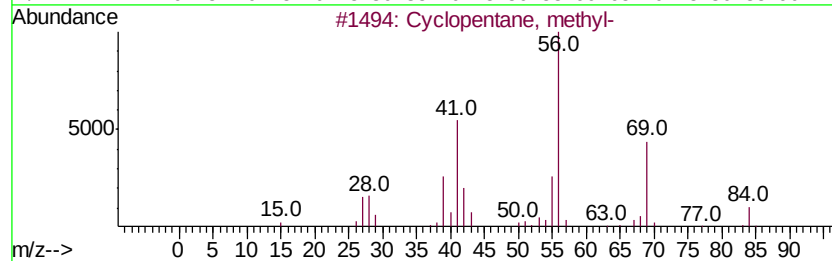
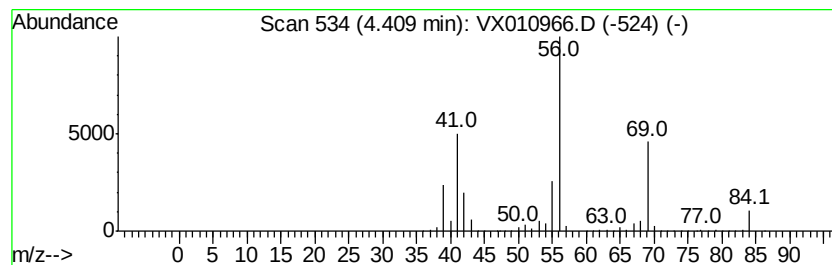
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	189.75 ug/l	6315550	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43
5		Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	35



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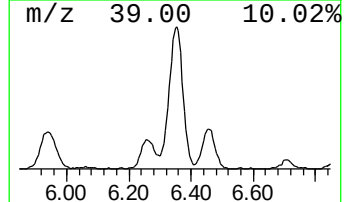
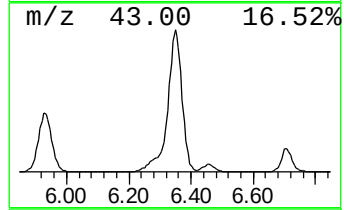
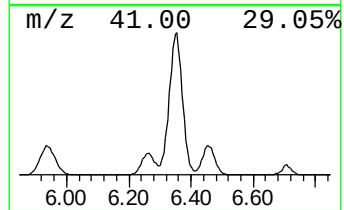
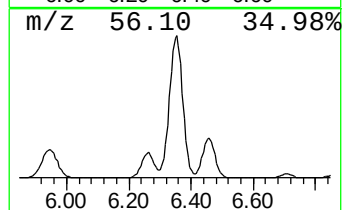
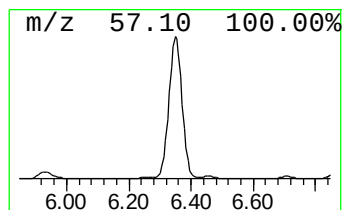
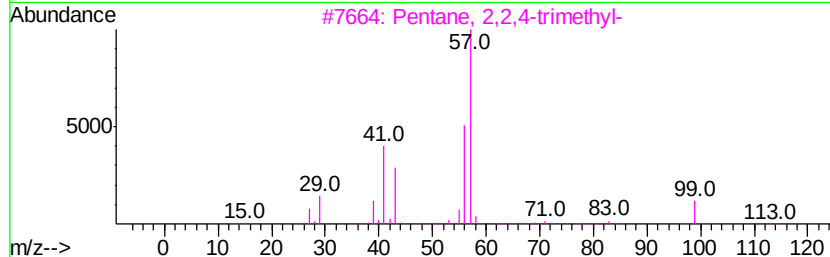
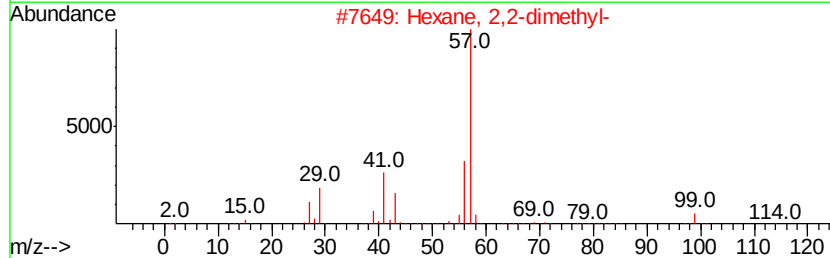
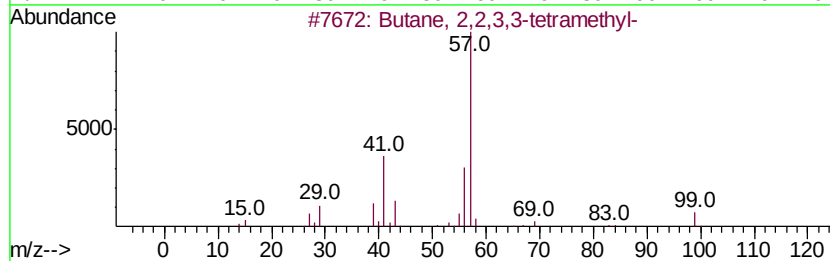
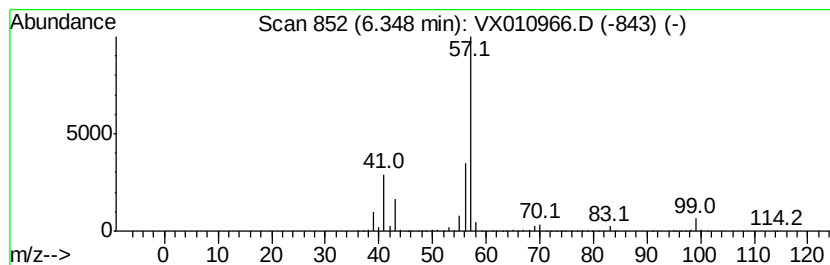
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	166.42 ug/l	2709450	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
3		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	45



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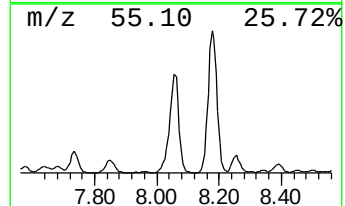
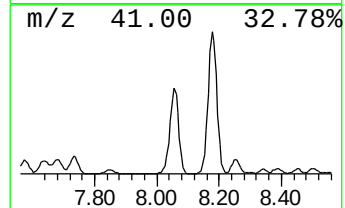
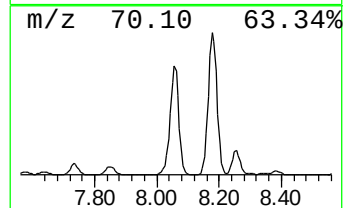
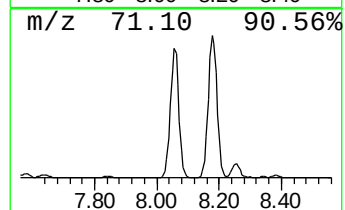
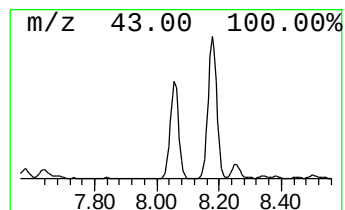
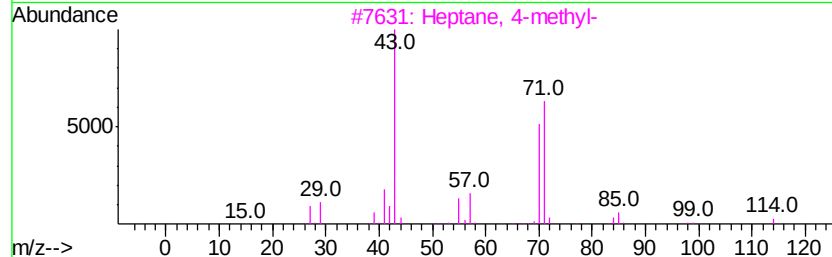
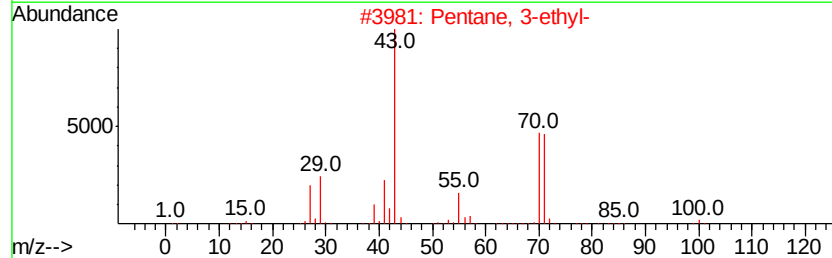
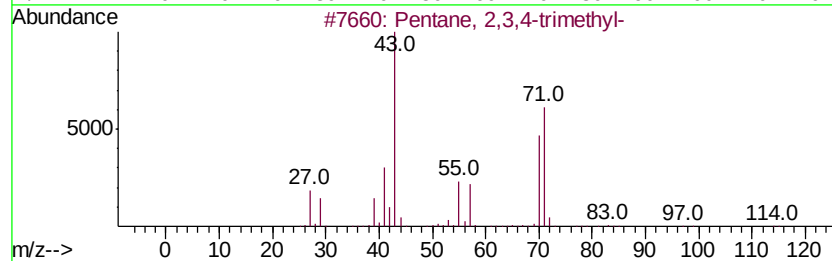
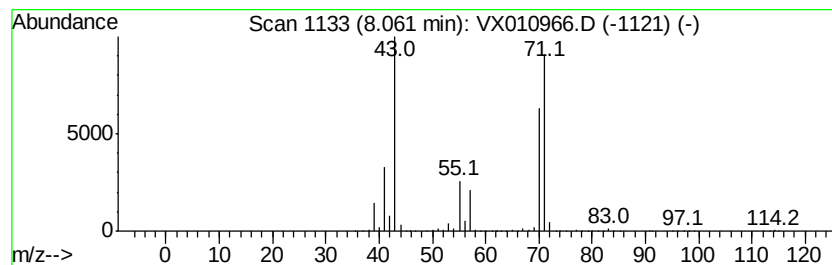
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	95.98 ug/l	1562590	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72



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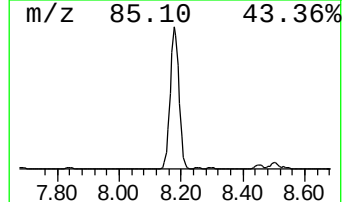
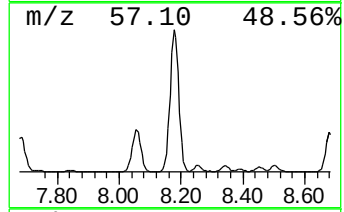
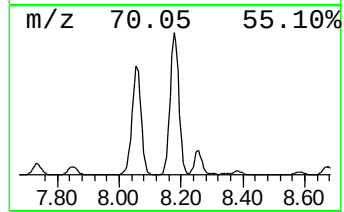
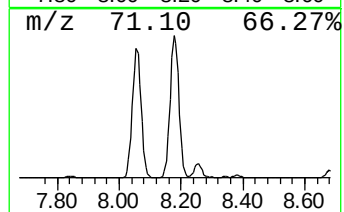
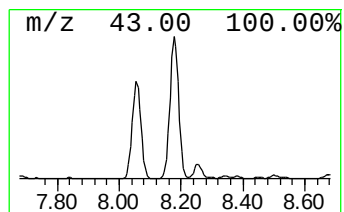
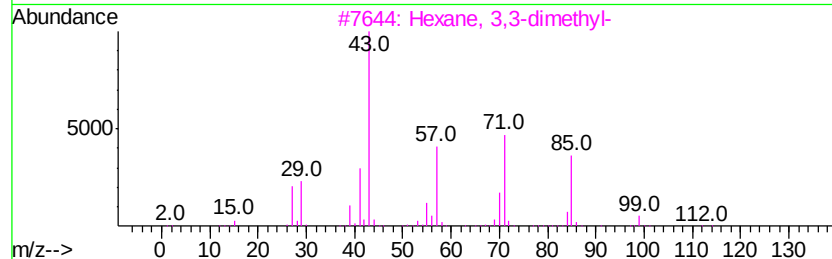
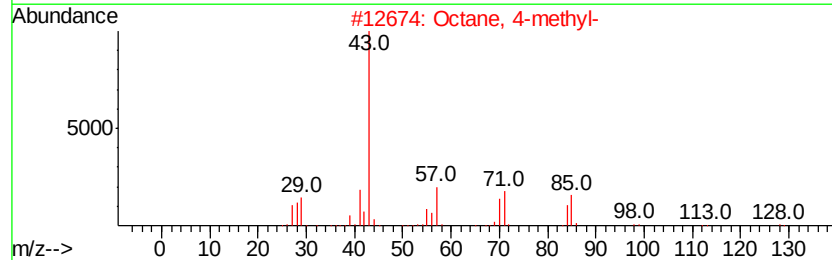
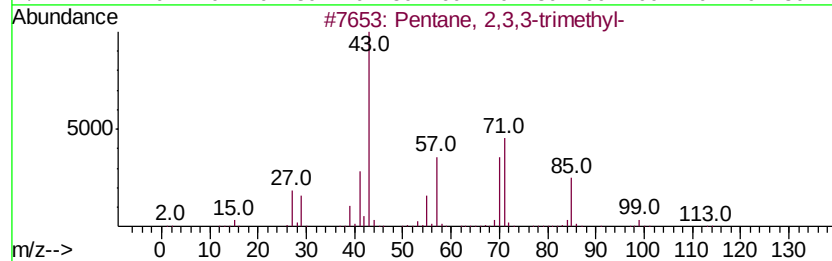
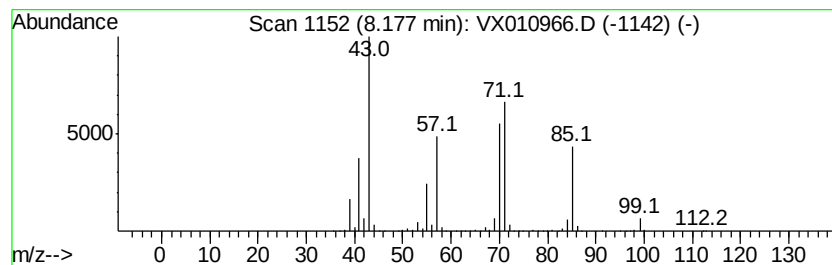
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	160.15 ug/l	2607280	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Octane, 4-methyl-	128	C9H20	002216-34-4	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010966.D
Acq On : 18 Jul 2019 18:05
Operator : JC/SP
Sample : K3884-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

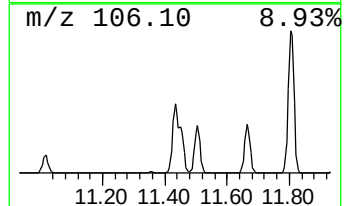
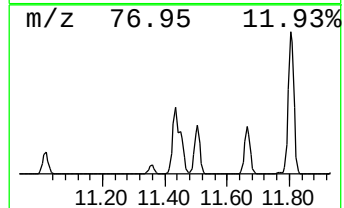
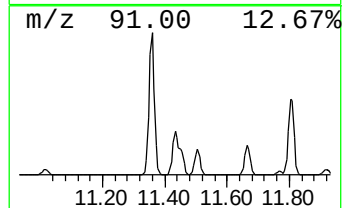
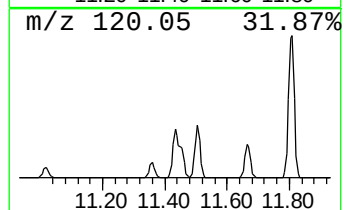
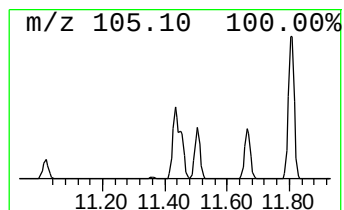
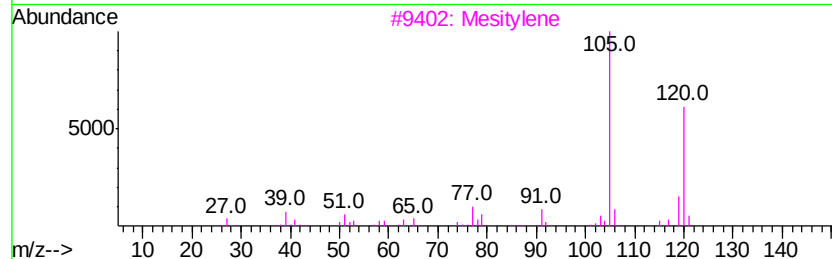
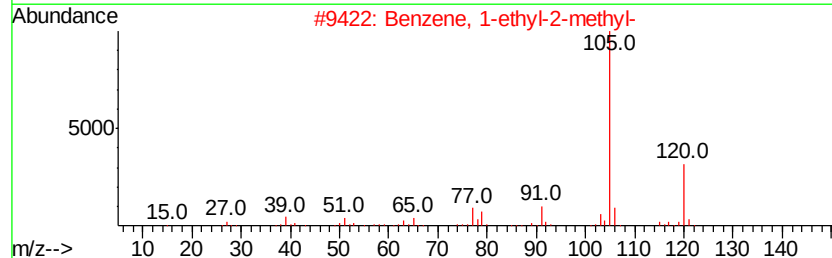
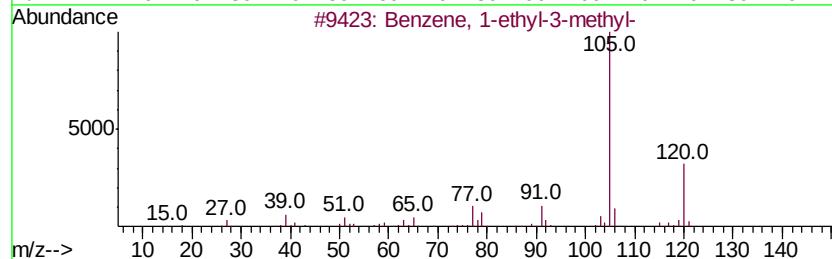
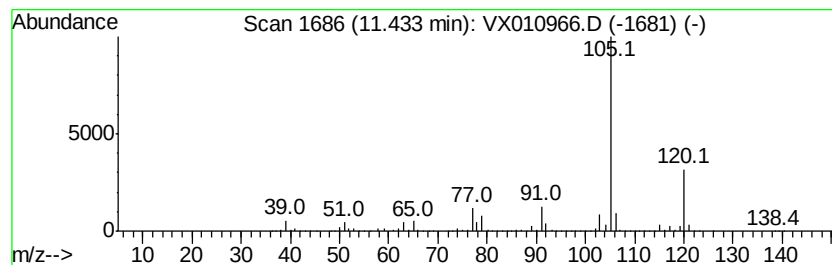
Instrument :
MSVOA_X
ClientSampleId :
FL-0608

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 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	223.33 ug/l	5636830	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 95
2		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 95
3		Mesitylene	120 C9H12	000108-67-8 91
4		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 91
5		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010966.D
Acq On : 18 Jul 2019 18:05
Operator : JC/SP
Sample : K3884-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

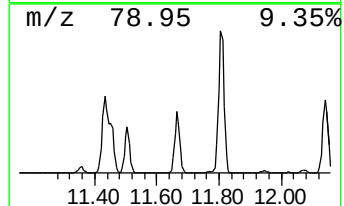
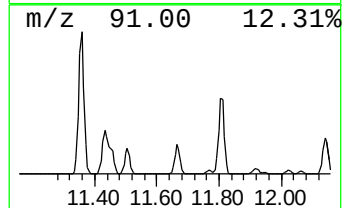
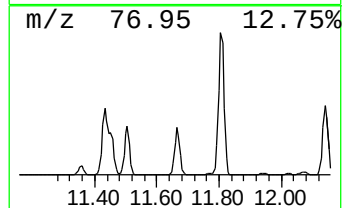
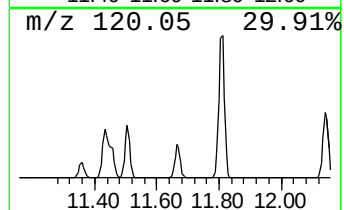
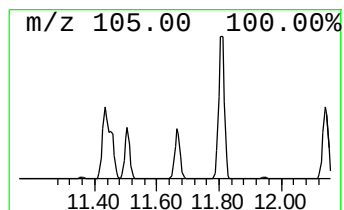
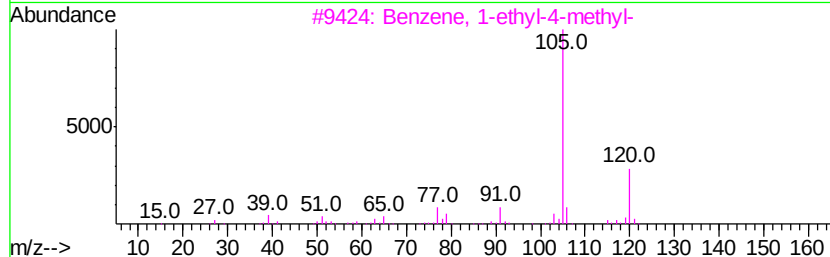
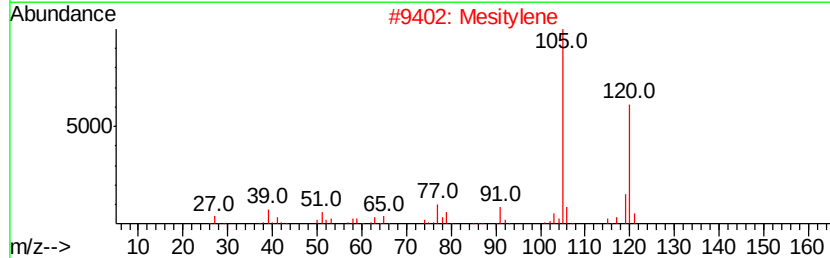
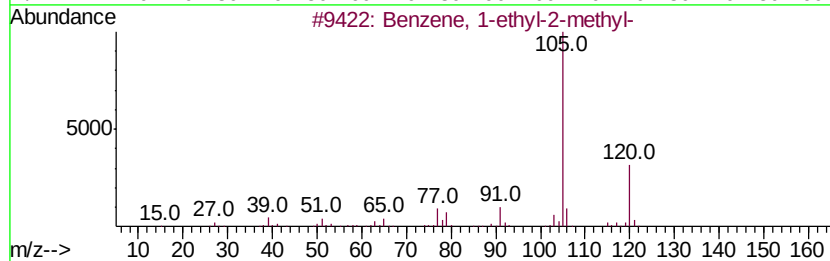
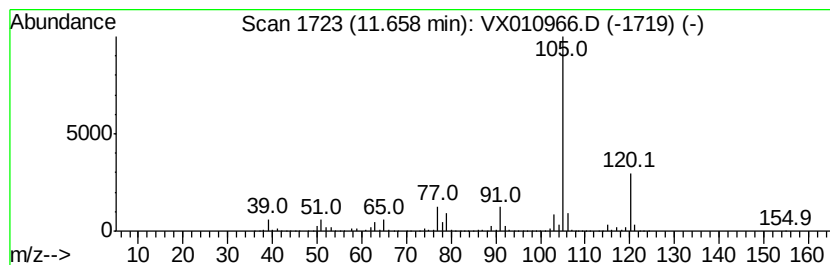
Instrument :
MSVOA_X
ClientSampleId :
FL-0608

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 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	147.14 ug/l	3713670	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 94
2		Mesitylene	120 C9H12	000108-67-8 91
3		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 91
4		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 91
5		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010966.D
Acq On : 18 Jul 2019 18:05
Operator : JC/SP
Sample : K3884-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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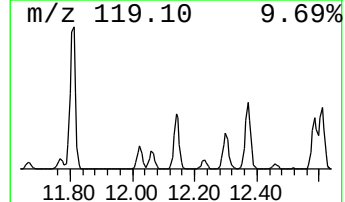
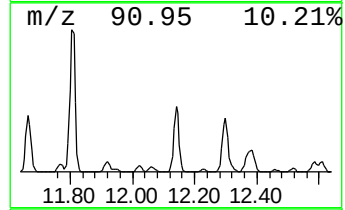
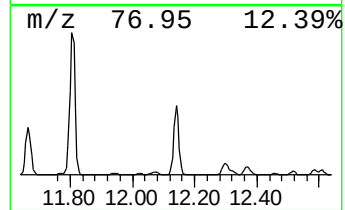
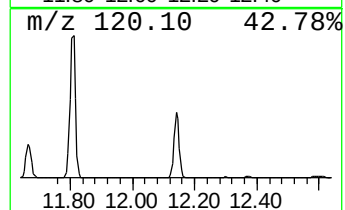
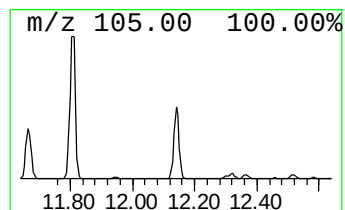
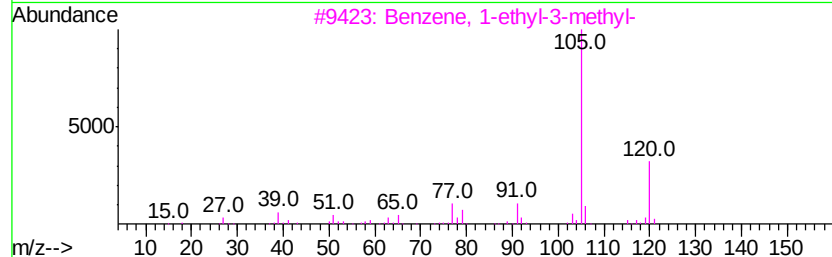
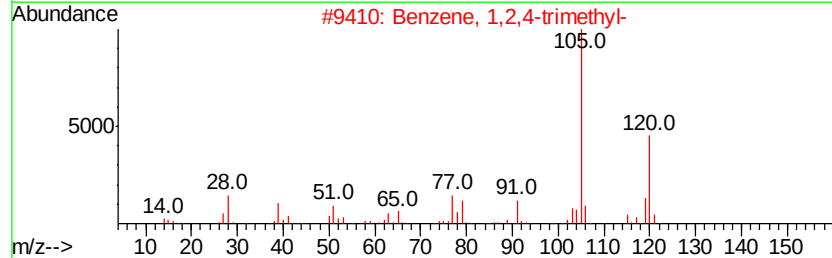
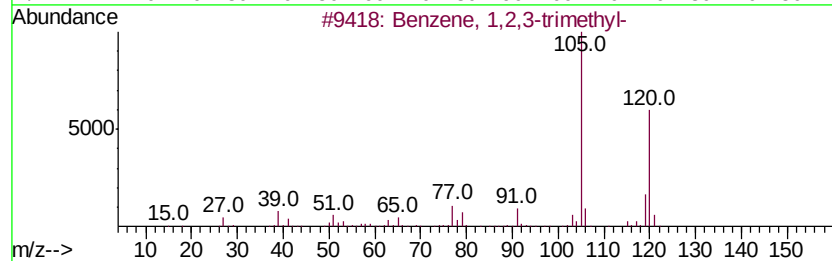
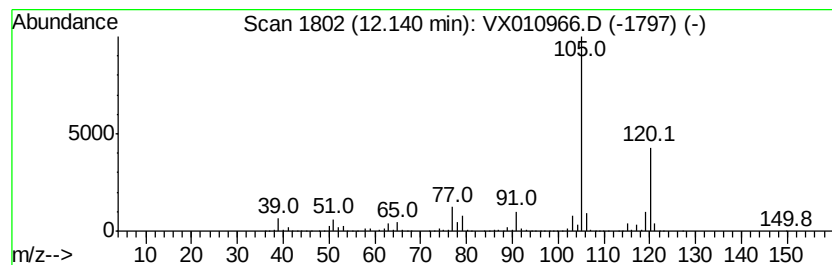
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	225.20 ug/l	5683990	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010966.D
Acq On : 18 Jul 2019 18:05
Operator : JC/SP
Sample : K3884-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

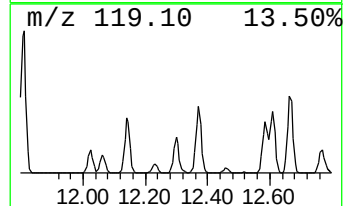
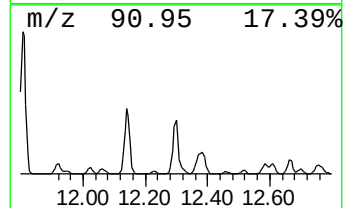
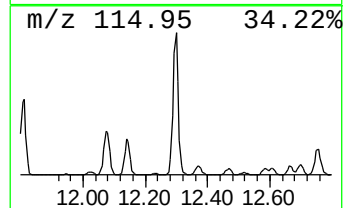
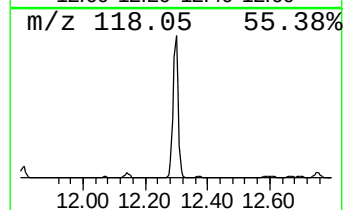
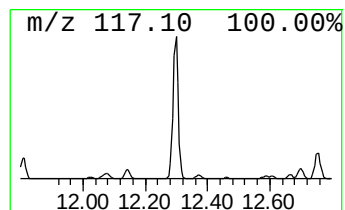
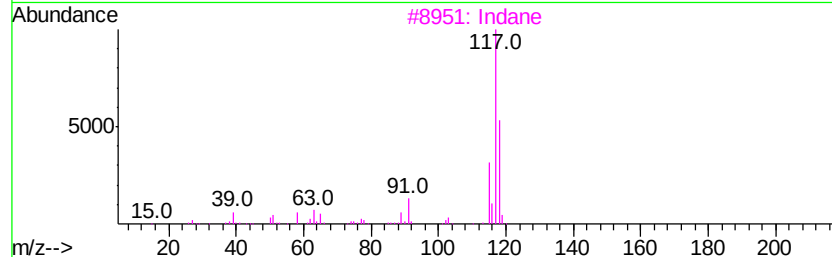
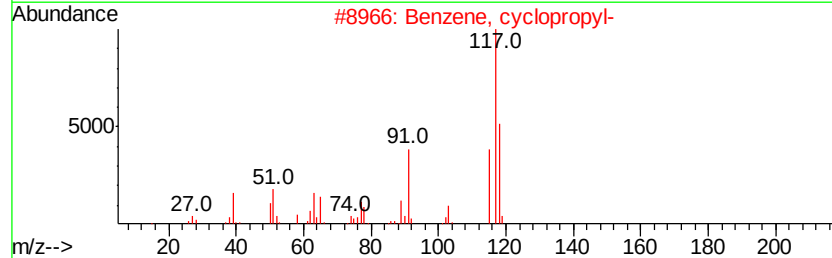
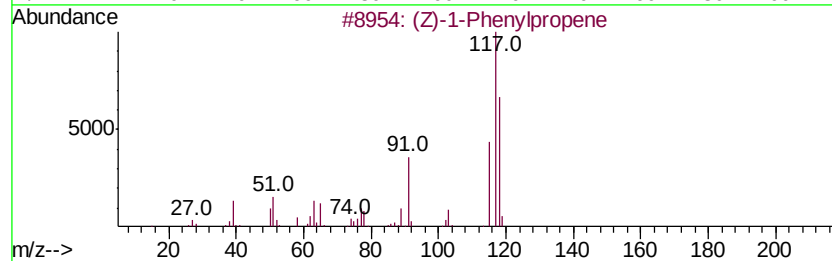
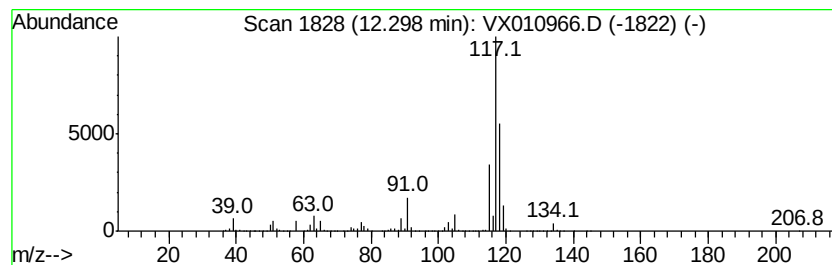
Instrument :
MSVOA_X
ClientSampleId :
FL-0608

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 9 (Z)-1-Phenylpropene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	143.93 ug/l	3632730	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		(Z)-1-Phenylpropene	118 C9H10	000766-90-5 81
2		Benzene, cyclopropyl-	118 C9H10	000873-49-4 81
3		Indane	118 C9H10	000496-11-7 81
4		Benzene, 2-propenyl-	118 C9H10	000300-57-2 74
5		Deltacyclene	118 C9H10	007785-10-6 64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010966.D
Acq On : 18 Jul 2019 18:05
Operator : JC/SP
Sample : K3884-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0608

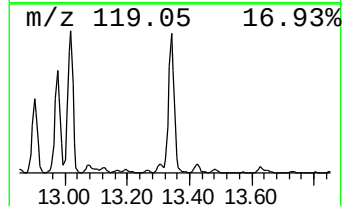
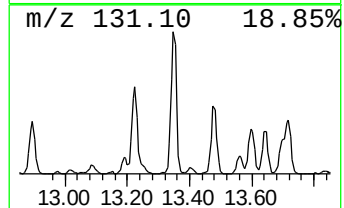
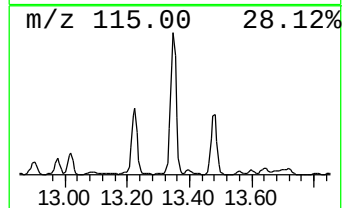
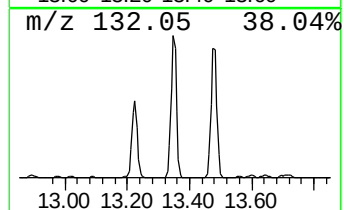
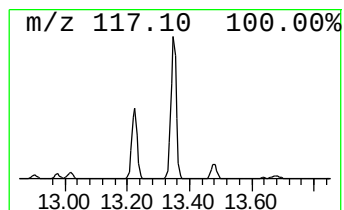
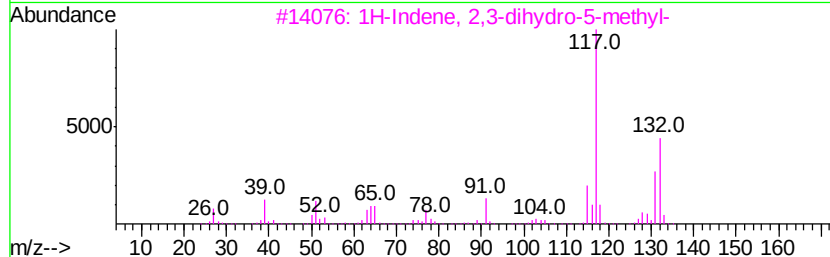
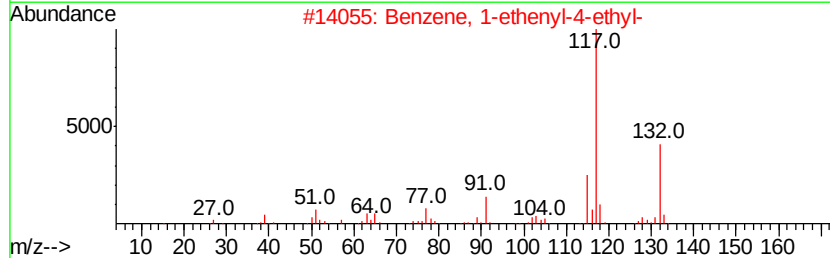
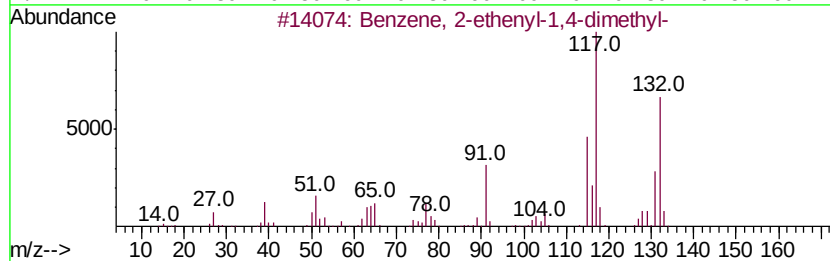
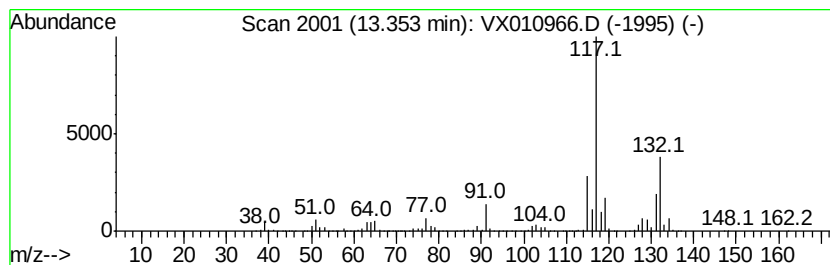
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	73.11 ug/l	1845390	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010966.D
Acq On : 18 Jul 2019 18:05
Operator : JC/SP
Sample : K3884-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0608

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, 2-methyl-	1.79	74.6	ug/l	2482530	1	5.67	1664160	50.0
Cyclopentane, met...	4.41	189.8	ug/l	6315550	1	5.67	1664160	50.0
Butane, 2,2,3,3-t...	6.35	166.4	ug/l	2709450	2	6.86	814026	50.0
Pentane, 2,3,4-tr...	8.06	96.0	ug/l	1562590	2	6.86	814026	50.0
Pentane, 2,3,3-tr...	8.18	160.2	ug/l	2607280	2	6.86	814026	50.0
Benzene, 1-ethyl-...	11.43	223.3	ug/l	5636830	4	12.08	1261980	50.0
Benzene, 1-ethyl-...	11.66	147.1	ug/l	3713670	4	12.08	1261980	50.0
Benzene, 1,2,3-tr...	12.14	225.2	ug/l	5683990	4	12.08	1261980	50.0
(Z)-1-Phenylpropene	12.30	143.9	ug/l	3632730	4	12.08	1261980	50.0
Benzene, 2-etheny...	13.35	73.1	ug/l	1845390	4	12.08	1261980	50.0