

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071219\
 Data File : VX010842.D
 Acq On : 12 Jul 2019 17:36
 Operator : JC/SP
 Sample : K3786-07
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0597

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\82X061919W.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	133	rVB	26361638	37404534	100.00%	29.131%
2	2.001	133	139	150	rVB	929116	1302378	3.48%	1.014%
3	2.849	260	278	283	rBV	2765648	6384356	17.07%	4.972%
4	3.172	321	331	347	rBV	485772	1116701	2.99%	0.870%
5	3.525	379	389	404	rVB	218065	496933	1.33%	0.387%
6	4.312	506	518	526	rBV	481942	1462551	3.91%	1.139%
7	4.403	526	533	546	rVB	479998	1386588	3.71%	1.080%
8	5.586	718	727	734	rBV3	346465	1075232	2.87%	0.837%
9	5.732	743	751	768	rVB	925496	2860386	7.65%	2.228%
10	5.934	773	784	796	rBV5	139278	451052	1.21%	0.351%
11	6.348	843	852	863	rVB	846117	2512013	6.72%	1.956%
12	6.860	926	936	946	rBV	324572	763232	2.04%	0.594%
13	7.464	1022	1035	1046	rBV	934982	2097493	5.61%	1.634%
14	8.055	1123	1132	1142	rVB	845713	1644227	4.40%	1.281%
15	8.177	1142	1152	1160	rBV	1318851	2586788	6.92%	2.015%
16	8.714	1235	1240	1250	rVB	725515	1189829	3.18%	0.927%
17	10.110	1464	1469	1475	rBV	689590	921826	2.46%	0.718%
18	10.250	1486	1492	1498	rBV	1804293	2267451	6.06%	1.766%
19	10.360	1502	1510	1517	rBV	9651996	12969494	34.67%	10.101%
20	10.695	1560	1565	1576	rVB	2782041	3656551	9.78%	2.848%
21	11.018	1612	1618	1624	rBV	662073	831068	2.22%	0.647%
22	11.134	1632	1637	1642	rBV	616517	794390	2.12%	0.619%
23	11.359	1668	1674	1681	rBV	732267	884895	2.37%	0.689%
24	11.433	1681	1686	1694	rVV	4756792	8082877	21.61%	6.295%
25	11.506	1694	1698	1705	rVB	2994434	3529333	9.44%	2.749%
26	11.664	1719	1724	1734	rBV	3431784	4266798	11.41%	3.323%
27	11.804	1742	1747	1753	rVB	8536858	10293860	27.52%	8.017%
28	12.024	1778	1783	1786	rBV	319557	382041	1.02%	0.298%
29	12.073	1786	1791	1797	rVB2	861866	1234206	3.30%	0.961%
30	12.140	1797	1802	1808	rBV	4466817	5526341	14.77%	4.304%
31	12.298	1821	1828	1831	rBV	1068642	1485744	3.97%	1.157%
32	12.371	1835	1840	1849	rVB2	553031	833788	2.23%	0.649%
33	12.518	1859	1864	1870	rBV	324855	393094	1.05%	0.306%
34	12.585	1870	1875	1877	rBV	335769	437387	1.17%	0.341%

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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 >
Peak separation: 5

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Title : SW846 8260

35	12.609	1877	1879	1883	rVB	384289	383155	1.02%	0.298%
36	12.664	1883	1888	1891	rBV	422385	496295	1.33%	0.387%
37	12.756	1898	1903	1910	rBV2	387551	640213	1.71%	0.499%
38	13.018	1942	1946	1951	rVB	462366	553573	1.48%	0.431%
39	13.341	1995	1999	2005	rVB2	708742	990117	2.65%	0.771%
40	13.481	2016	2022	2026	rBV	334899	429994	1.15%	0.335%
41	13.835	2070	2080	2086	rBV	1029849	1380162	3.69%	1.075%

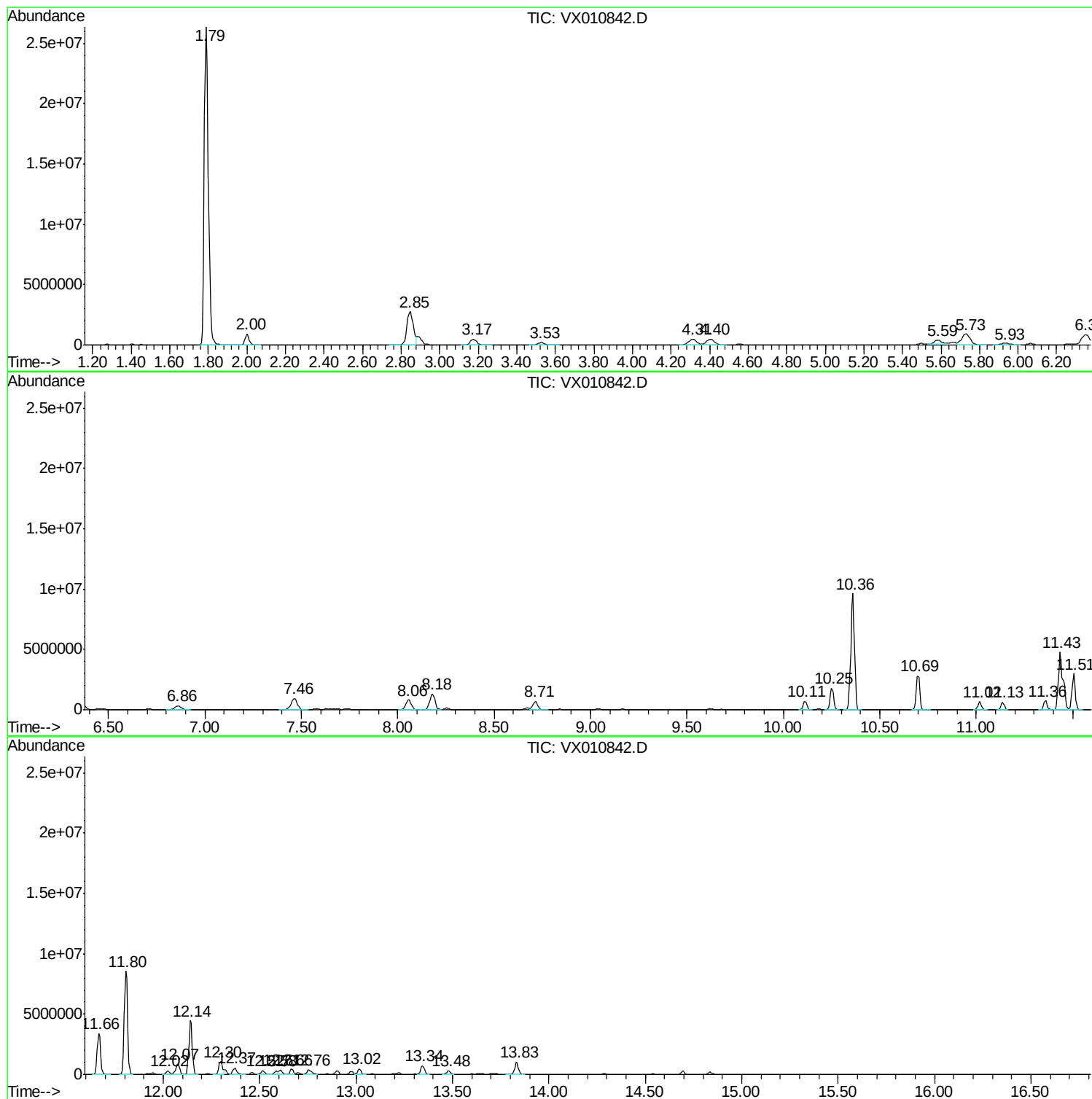
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X061919W.M
Quant Title : SW846 8260

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



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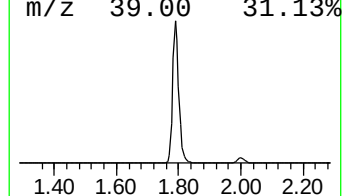
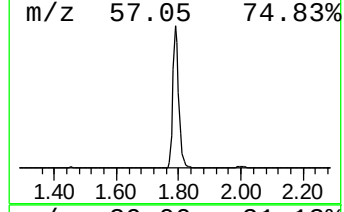
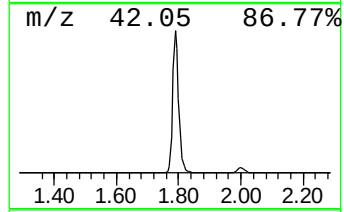
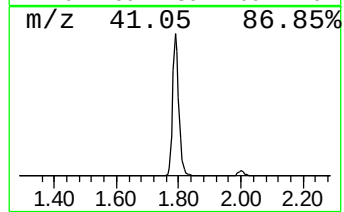
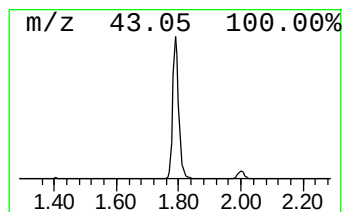
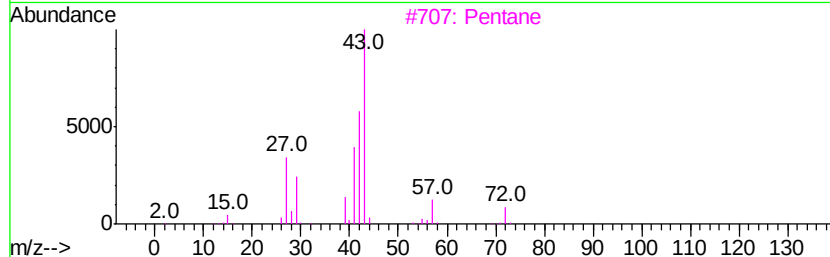
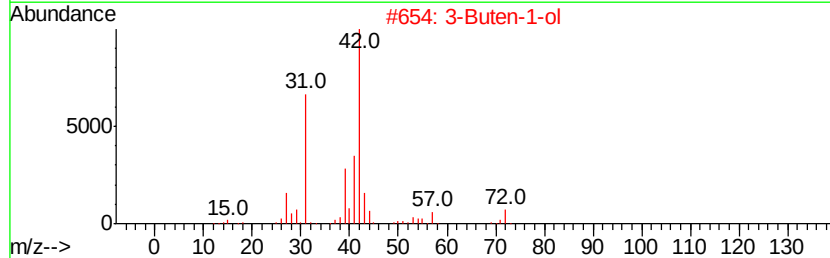
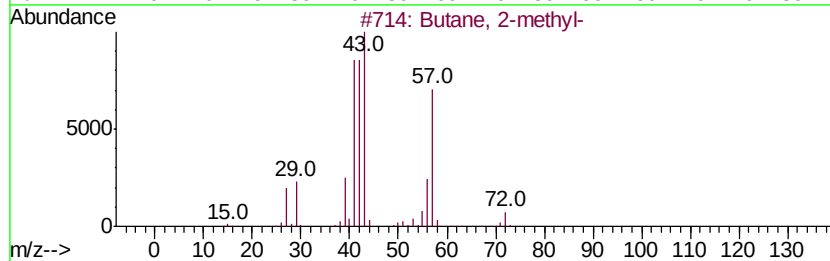
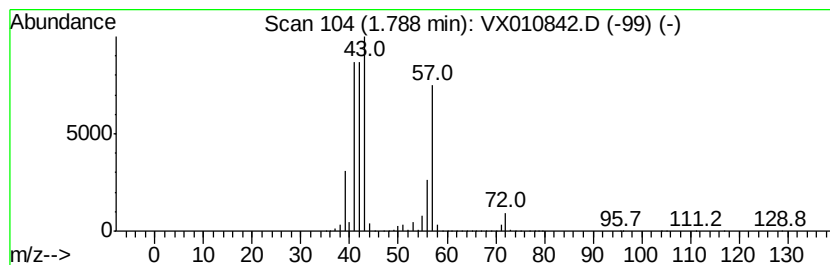
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X061919W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	653.84 ug/l	37404500	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	42
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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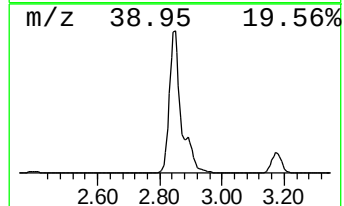
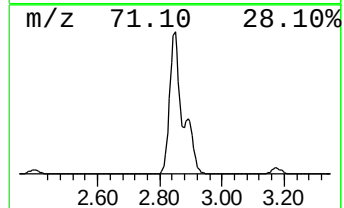
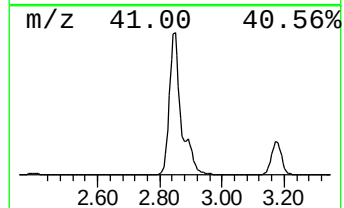
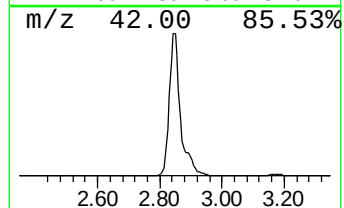
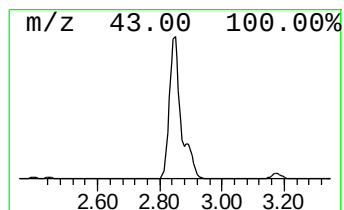
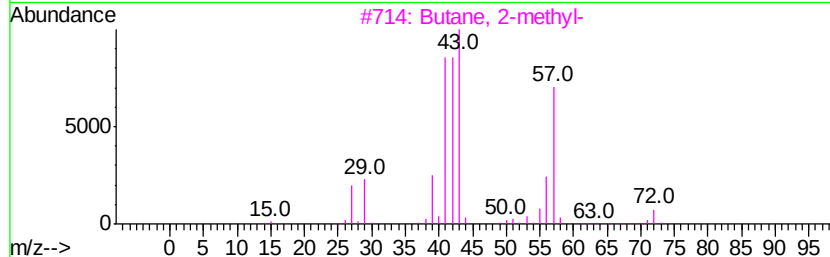
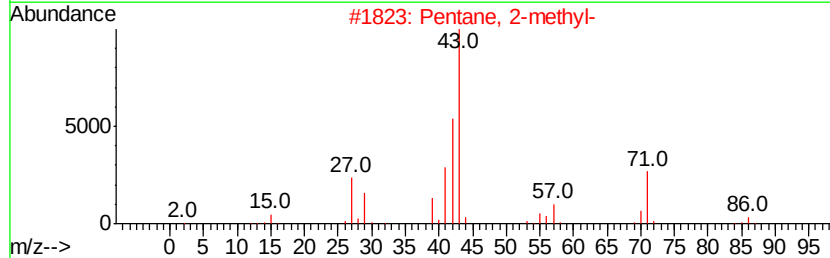
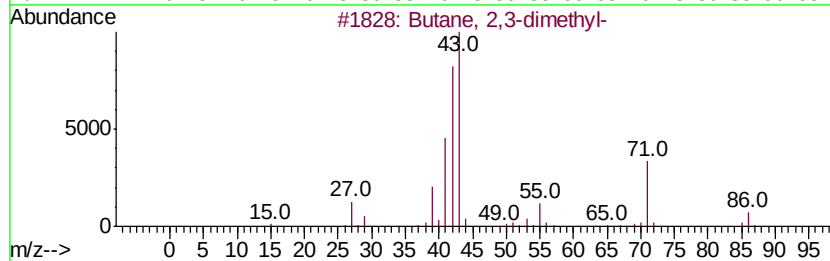
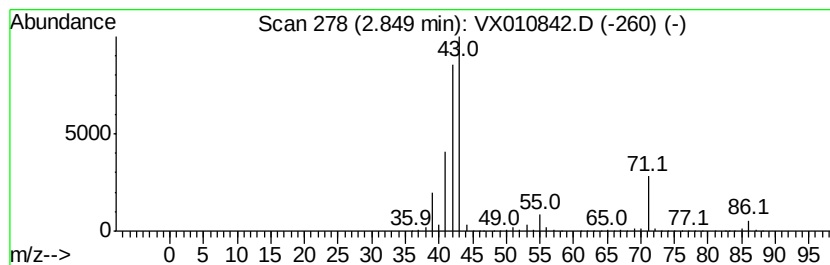
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X061919W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	111.60 ug/l	6384360	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Butane, 2-methyl-	72	C5H12	000078-78-4	36
4			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	12



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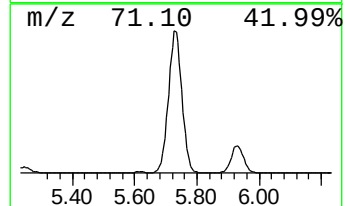
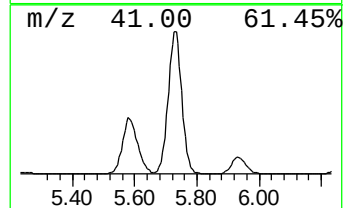
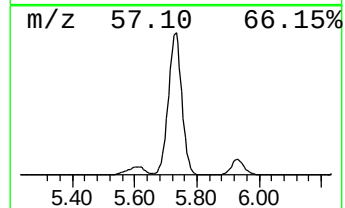
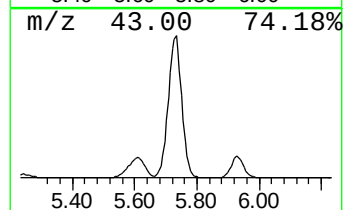
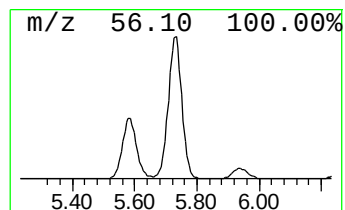
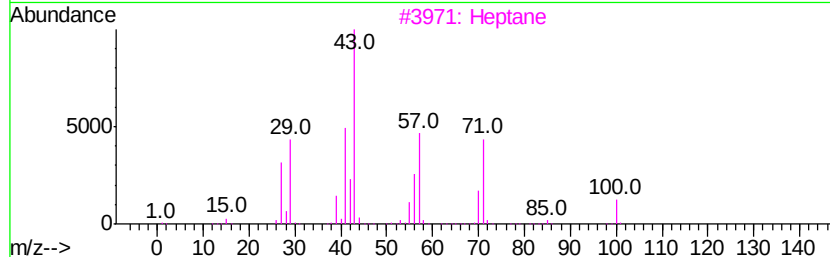
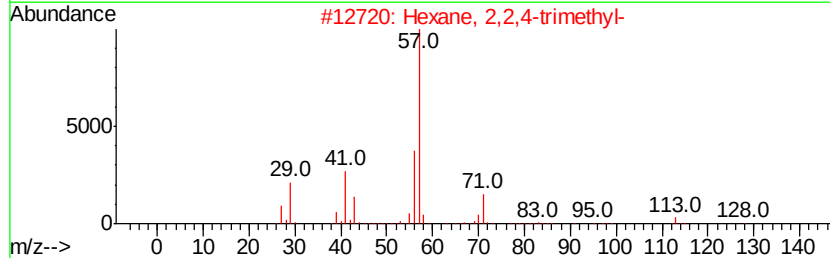
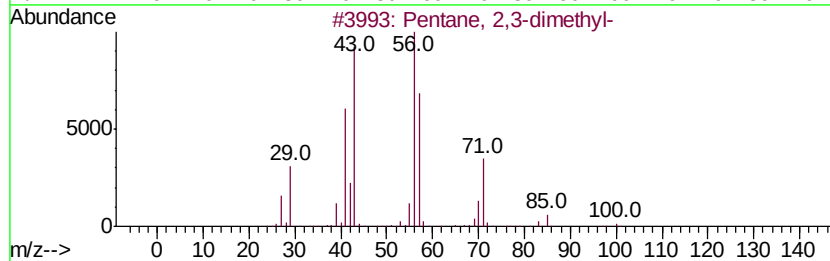
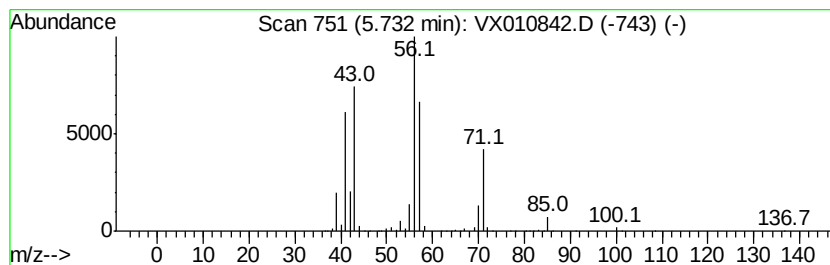
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	50.00 ug/l	2860390	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
3		Heptane	100	C7H16	000142-82-5	37
4		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	37
5		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37



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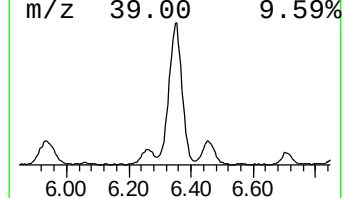
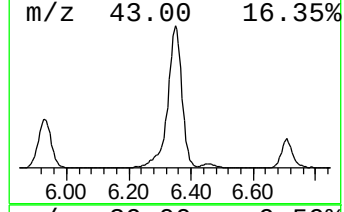
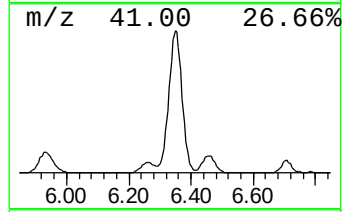
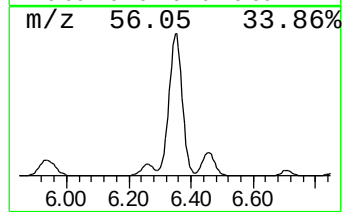
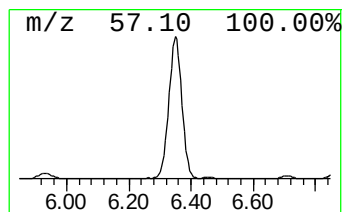
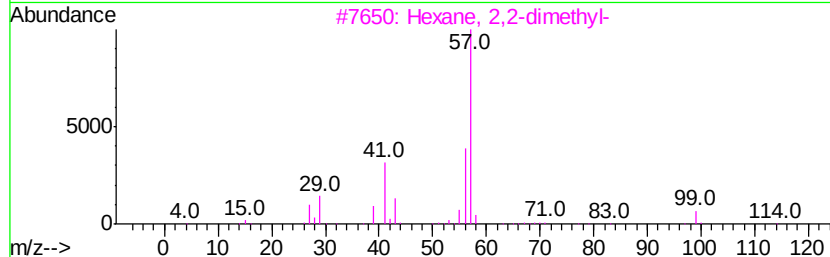
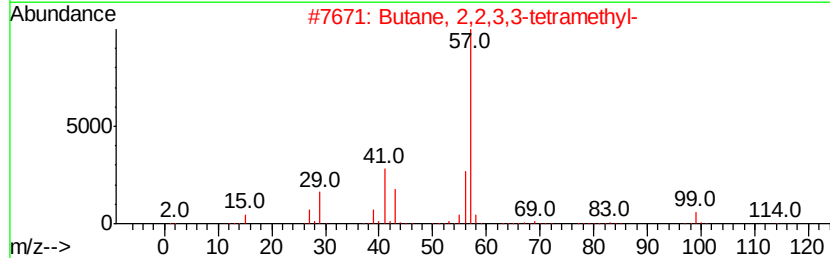
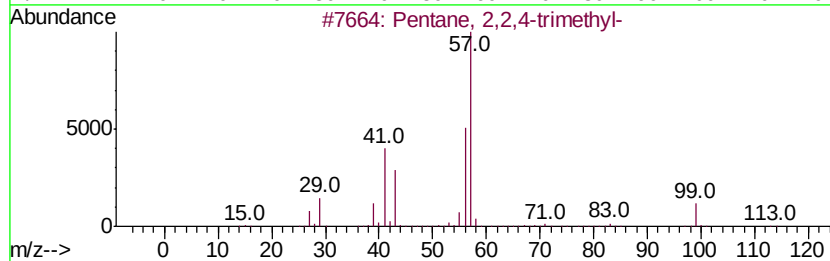
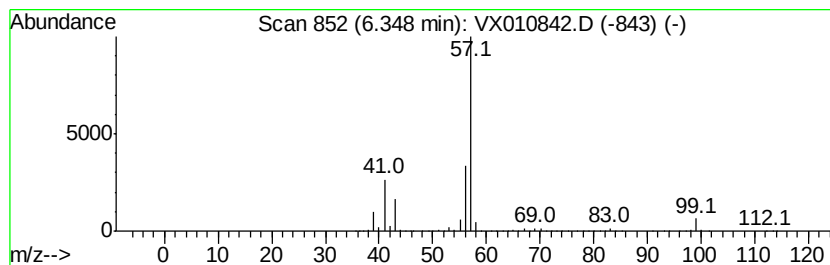
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 2,2,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	164.56 ug/l	2512010	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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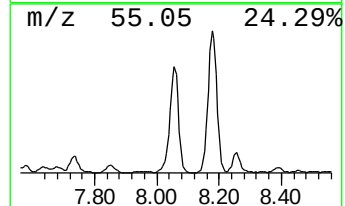
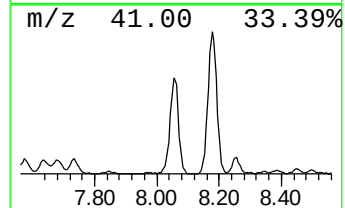
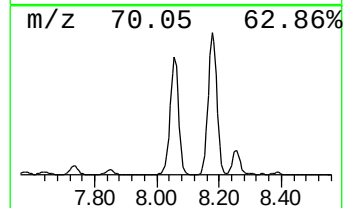
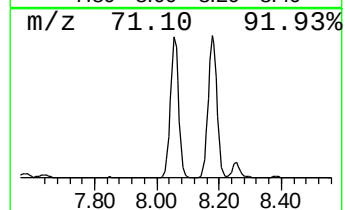
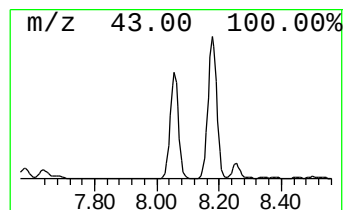
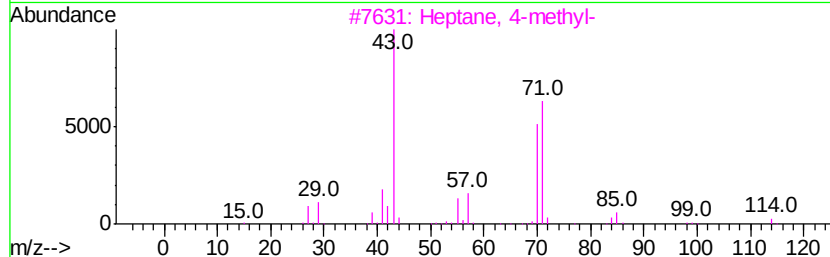
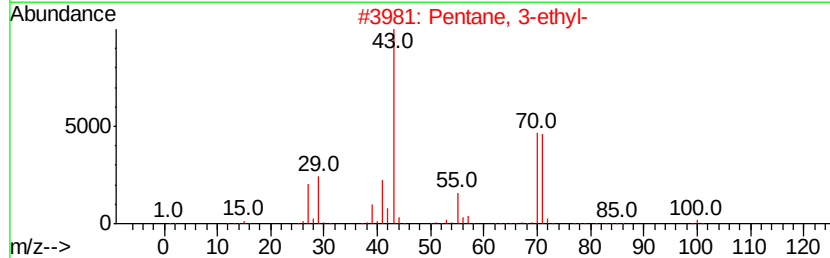
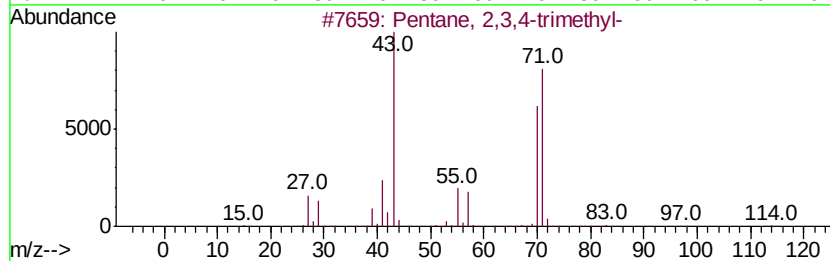
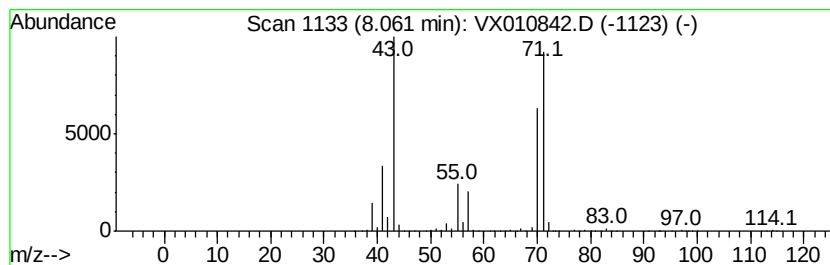
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	107.72 ug/l	1644230	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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071219\
Data File : VX010842.D
Acq On : 12 Jul 2019 17:36
Operator : JC/SP
Sample : K3786-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0597

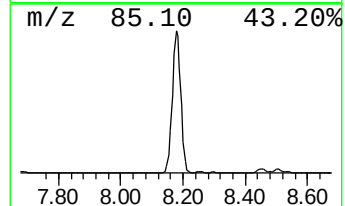
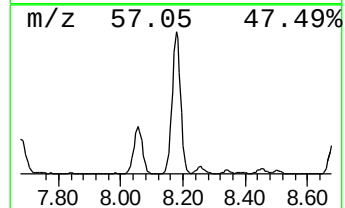
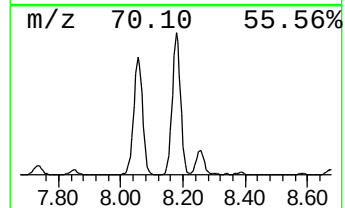
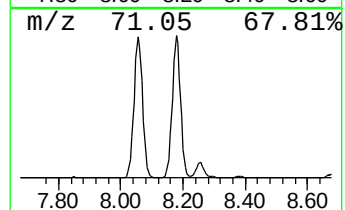
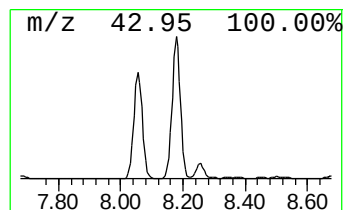
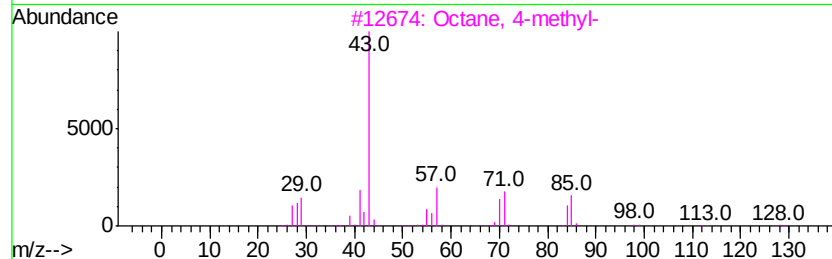
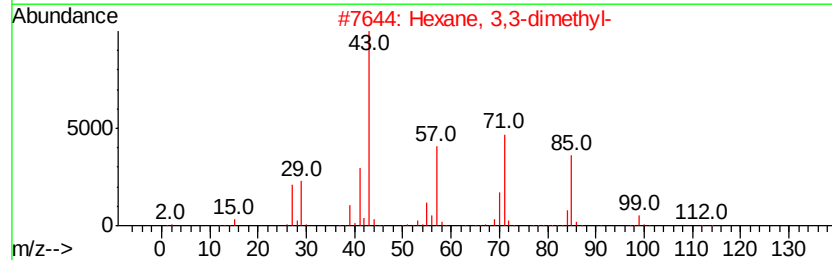
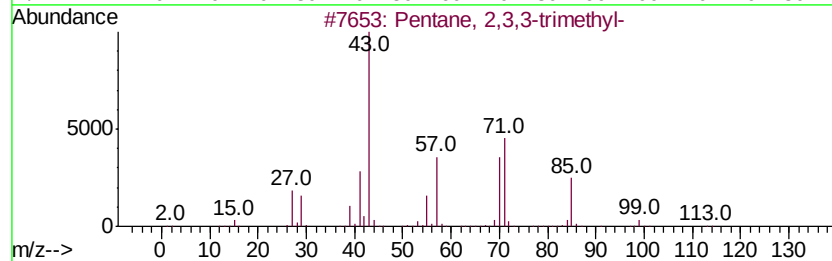
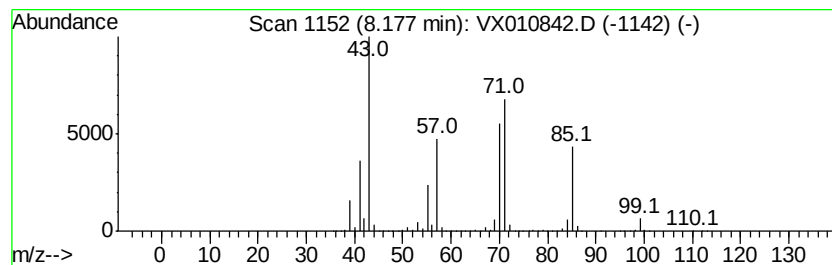
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	169.46 ug/l	2586790	1,4-Difluorobenzene	6.86

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071219\
Data File : VX010842.D
Acq On : 12 Jul 2019 17:36
Operator : JC/SP
Sample : K3786-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

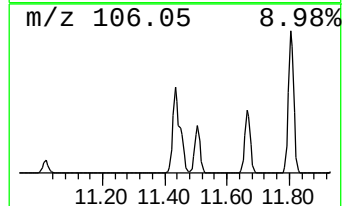
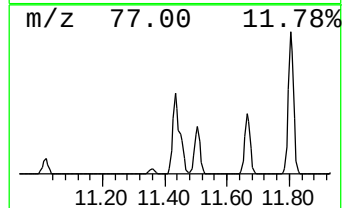
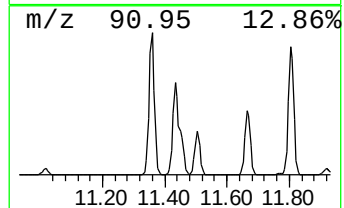
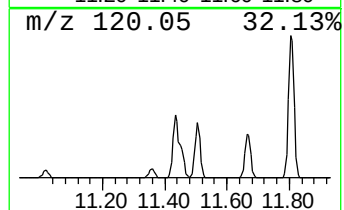
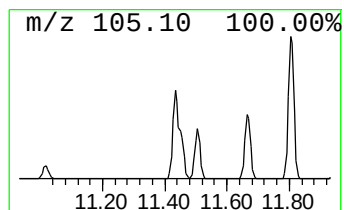
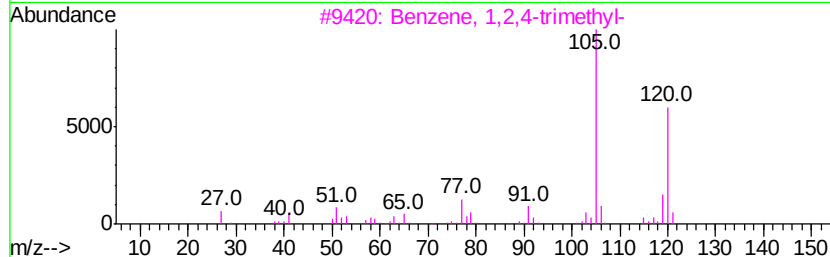
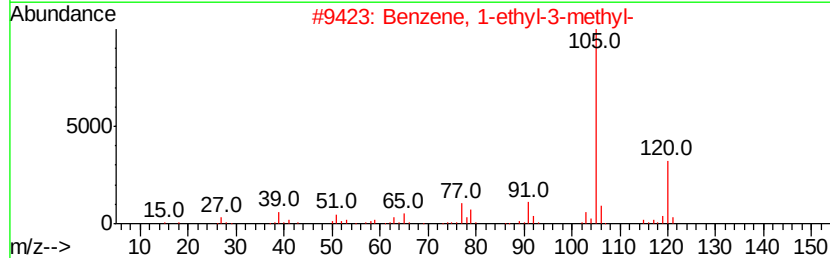
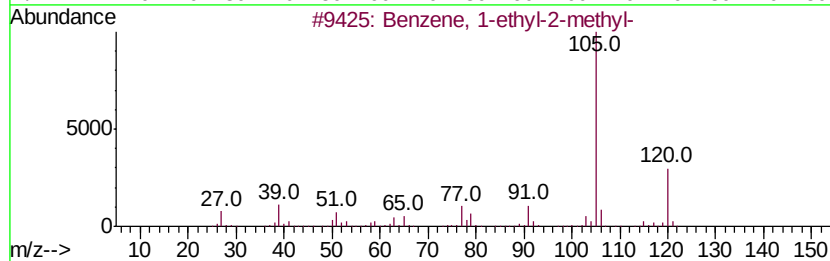
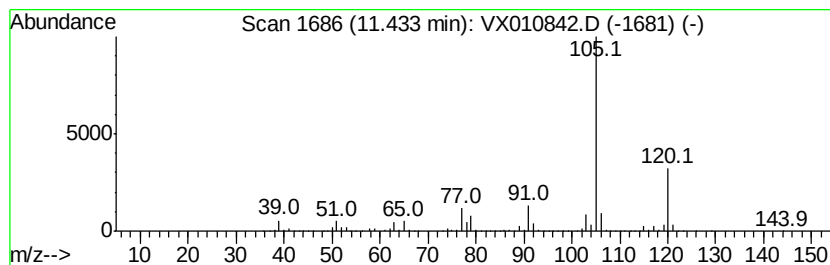
Instrument :
MSVOA_X
ClientSampled :
FL-0597

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X061919W.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	327.45 ug/l	8082880	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 95
2		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 95
3		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 91
4		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 91
5		Mesitylene	120 C9H12	000108-67-8 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071219\
Data File : VX010842.D
Acq On : 12 Jul 2019 17:36
Operator : JC/SP
Sample : K3786-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0597

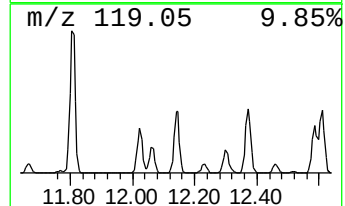
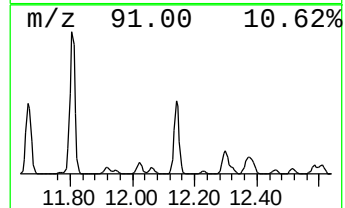
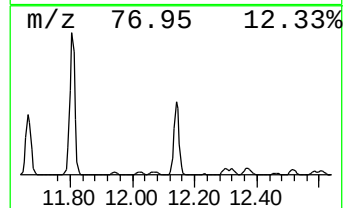
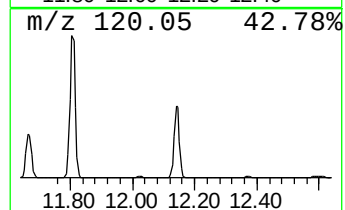
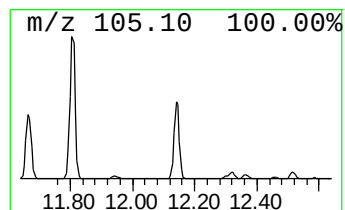
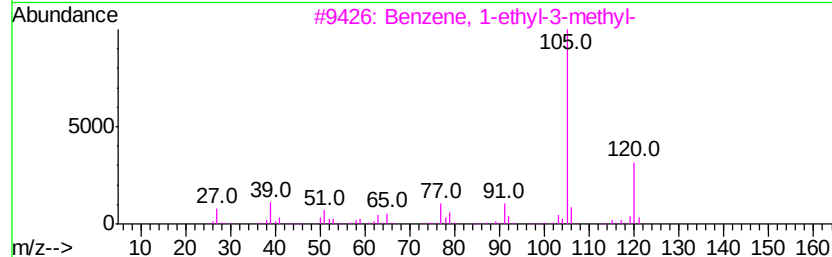
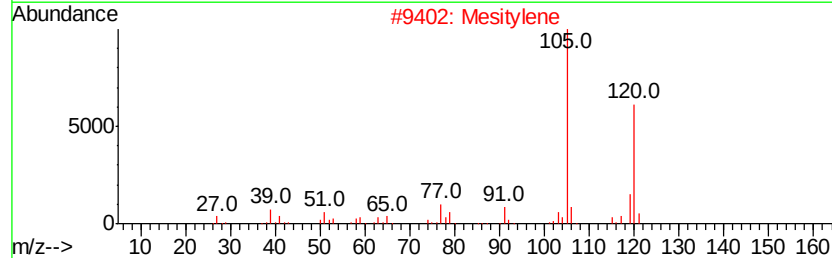
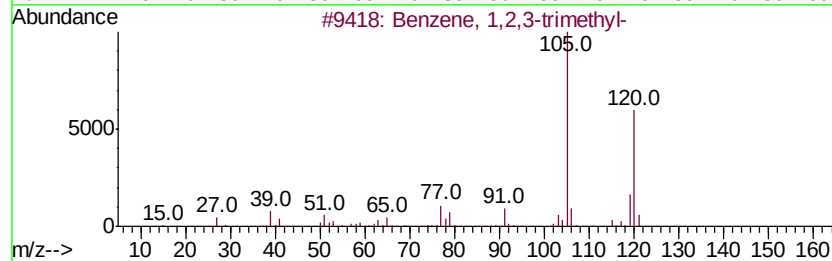
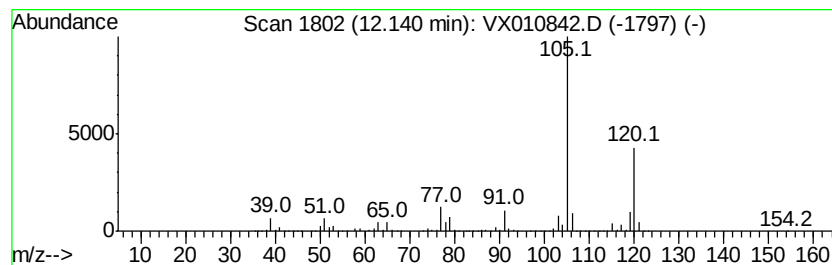
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	223.88 ug/l	5526340	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		Mesitylene	120	C9H12	000108-67-8	93
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071219\
Data File : VX010842.D
Acq On : 12 Jul 2019 17:36
Operator : JC/SP
Sample : K3786-07
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

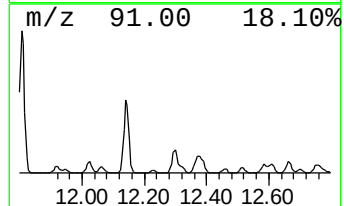
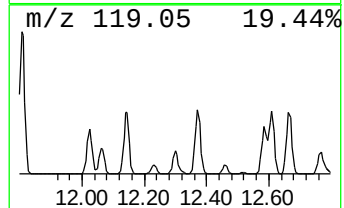
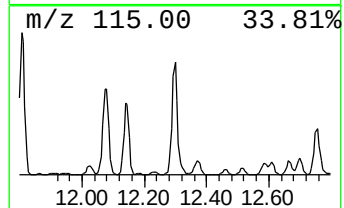
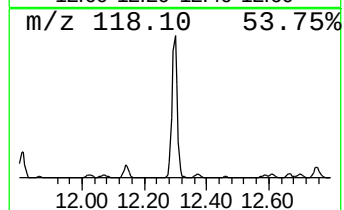
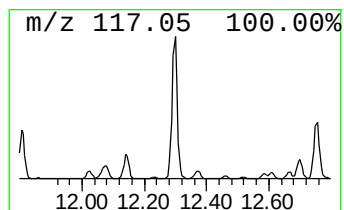
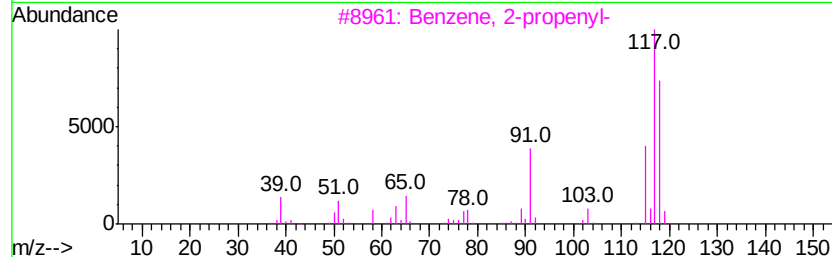
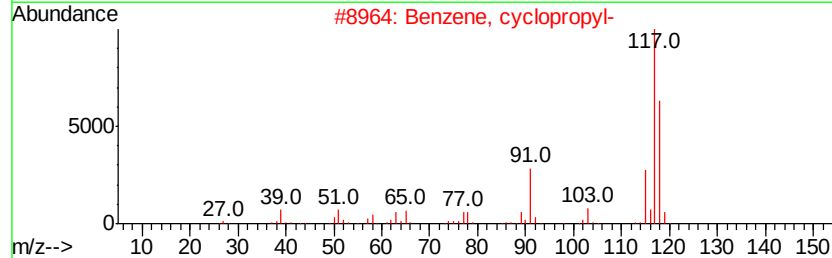
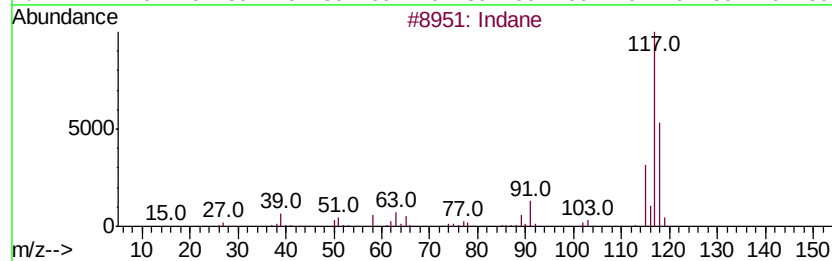
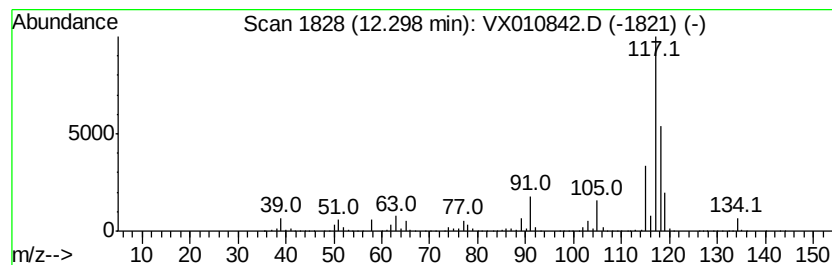
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X061919W.M
Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	60.19 ug/l	1485740	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indane		118 C9H10	000496-11-7 92
2	Benzene, cyclopropyl-		118 C9H10	000873-49-4 76
3	Benzene, 2-propenyl-		118 C9H10	000300-57-2 76
4	Deltacyclene		118 C9H10	007785-10-6 58
5	Benzene, 1-ethenyl-2-methyl-		118 C9H10	000611-15-4 55



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071219\
Data File : VX010842.D
Acq On : 12 Jul 2019 17:36
Operator : JC/SP
Sample : K3786-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0597

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061919W.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...	2.85	111.6	ug/l	6384360	1	5.67	2860390	50.0
Pentane, 2,3-dime...	5.73	50.0	ug/l	2860390	1	5.67	2860390	50.0
Pentane, 2,2,4-tr...	6.35	164.6	ug/l	2512010	2	6.86	763232	50.0
Pentane, 2,3,4-tr...	8.06	107.7	ug/l	1644230	2	6.86	763232	50.0
Pentane, 2,3,3-tr...	8.18	169.5	ug/l	2586790	2	6.86	763232	50.0
Benzene, 1-ethyl-...	11.43	327.4	ug/l	8082880	4	12.08	1234210	50.0
Benzene, 1,2,3-tr...	12.14	223.9	ug/l	5526340	4	12.08	1234210	50.0
Indane	12.30	60.2	ug/l	1485740	4	12.08	1234210	50.0