

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101419\
 Data File : VX013044.D
 Acq On : 14 Oct 2019 12:13
 Operator : JC/SP
 Sample : K5313-12
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FA19-JBW7338A

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\82X100819W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	43	rBV	892259	1081916	100.00%	10.456%
2	1.399	80	84	89	rBV	58171	59383	5.49%	0.574%
3	1.783	141	147	160	rBV	689840	940898	86.97%	9.093%
4	1.991	177	181	189	rVB2	22164	34758	3.21%	0.336%
5	2.259	220	225	233	rVB2	7151	12314	1.14%	0.119%
6	2.387	238	246	250	rBV6	6511	15465	1.43%	0.149%
7	2.436	250	254	263	rVB	10161	17010	1.57%	0.164%
8	2.594	272	280	293	rBV	57391	109517	10.12%	1.058%
9	2.838	308	320	331	rBV	186085	419104	38.74%	4.050%
10	2.923	331	334	343	rVB3	10877	20784	1.92%	0.201%
11	3.167	363	374	384	rBV2	25641	59169	5.47%	0.572%
12	4.301	549	560	569	rBV2	37024	112913	10.44%	1.091%
13	4.393	569	575	588	rVB2	14637	42063	3.89%	0.406%
14	4.551	588	601	602	rBV2	8451	18563	1.72%	0.179%
15	4.582	603	606	618	rVB3	10577	25063	2.32%	0.242%
16	5.490	742	755	764	rBV2	102952	297909	27.54%	2.879%
17	5.569	764	768	772	rBV3	7892	13438	1.24%	0.130%
18	5.654	773	782	789	rBV	189416	523348	48.37%	5.058%
19	5.947	821	830	838	rBV5	5718	17195	1.59%	0.166%
20	6.051	838	847	855	rBV	118027	309610	28.62%	2.992%
21	6.136	855	861	871	rVB2	42587	111741	10.33%	1.080%
22	6.337	883	894	907	rVB	348248	1037409	95.89%	10.025%
23	6.849	969	978	994	rBV	300623	701780	64.86%	6.782%
24	7.209	1029	1037	1050	rVB4	8819	20170	1.86%	0.195%
25	7.447	1069	1076	1084	rBV5	6796	16886	1.56%	0.163%
26	7.569	1088	1096	1101	rBV2	16446	32758	3.03%	0.317%
27	7.636	1101	1107	1110	rVV2	17746	39270	3.63%	0.380%
28	7.672	1110	1113	1121	rVB	23006	43832	4.05%	0.424%
29	8.050	1164	1175	1185	rVB	202299	395038	36.51%	3.818%
30	8.172	1185	1195	1205	rBV	292461	563675	52.10%	5.447%
31	8.709	1270	1283	1298	rBV	592871	1001713	92.59%	9.680%
32	8.837	1298	1304	1314	rVB3	9670	18660	1.72%	0.180%
33	9.038	1331	1337	1343	rVB2	15235	25123	2.32%	0.243%
34	9.160	1348	1357	1363	rBV5	5635	11498	1.06%	0.111%

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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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35	10.111	1507	1513	1521	rBV	555402	778475	71.95%	7.523%
36	11.013	1656	1661	1669	rVB	23320	30349	2.81%	0.293%
37	11.135	1675	1681	1692	rBV	432446	566133	52.33%	5.471%
38	12.074	1829	1835	1843	rBV	539395	668176	61.76%	6.457%
39	12.294	1864	1871	1876	rBV	42661	53696	4.96%	0.519%
40	12.696	1932	1937	1942	rBV	10729	14130	1.31%	0.137%
41	12.751	1942	1946	1953	rVB	29384	37582	3.47%	0.363%
42	13.714	2101	2104	2111	rVB	14308	19645	1.82%	0.190%
43	13.976	2142	2147	2152	rBV3	11124	15207	1.41%	0.147%
44	14.653	2252	2258	2267	rBV4	5816	14404	1.33%	0.139%

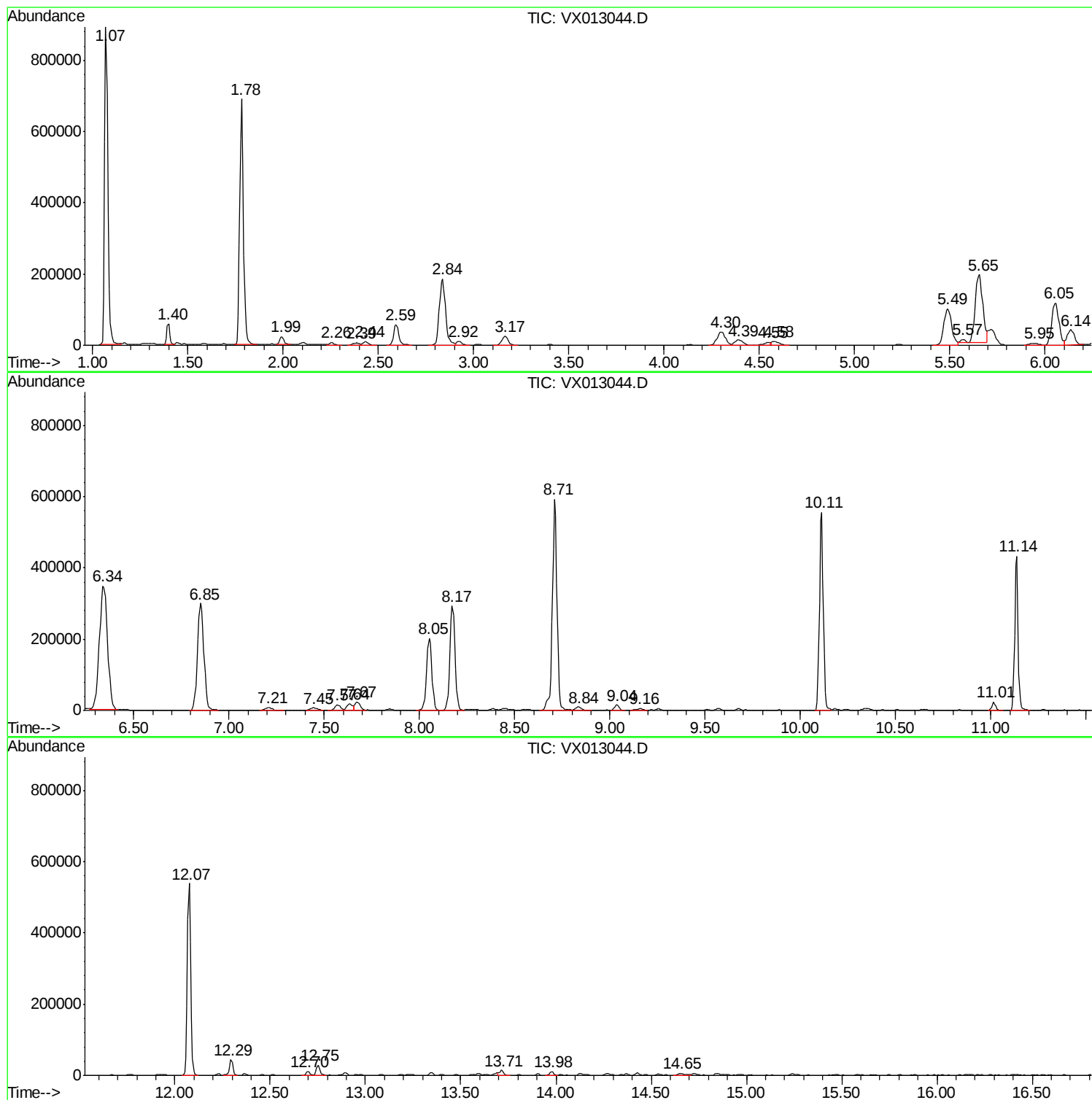
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Quant Title : SW846 8260

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



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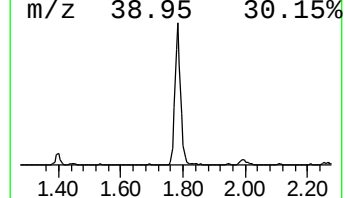
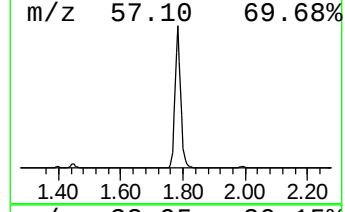
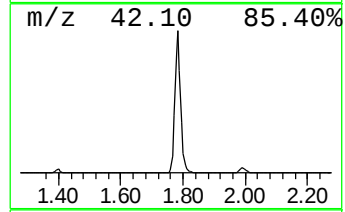
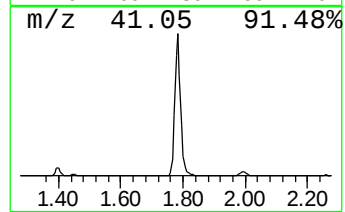
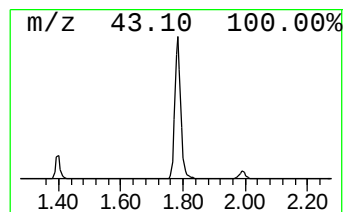
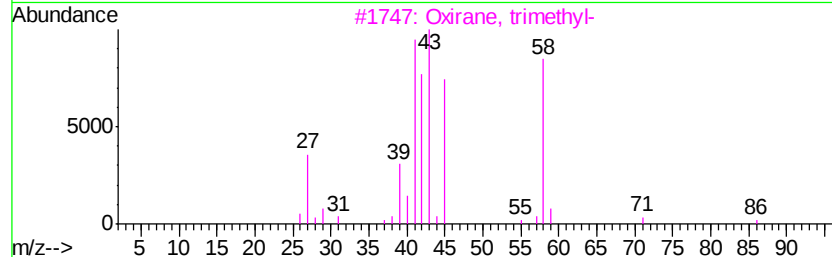
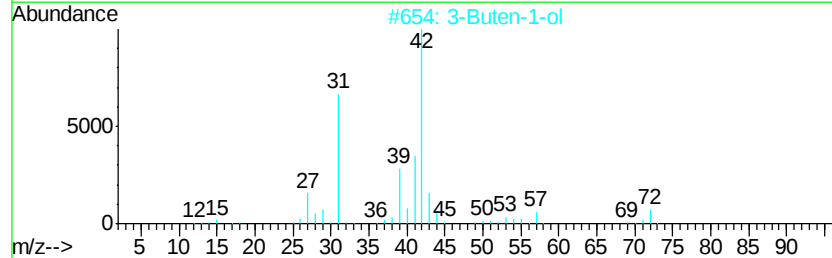
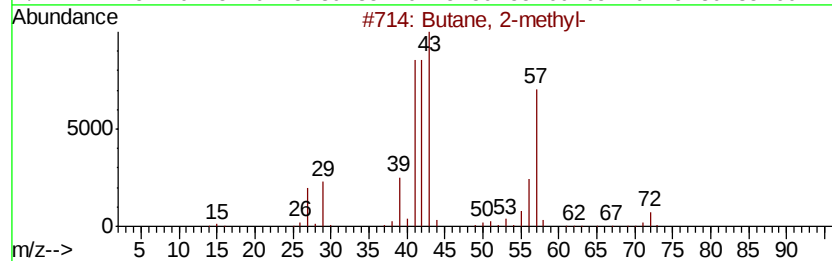
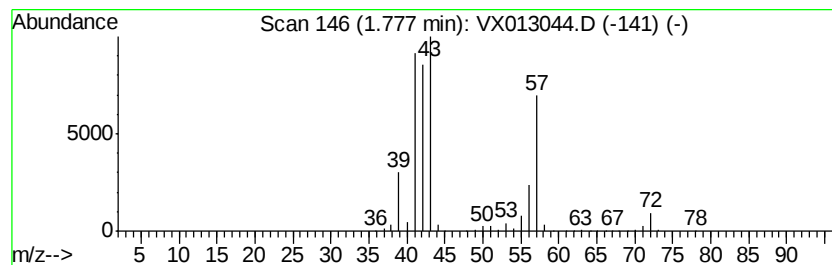
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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	89.89 ug/l	940898	Pentafluorobenzene	5.65

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		Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
4		Pentane	72	C5H12	000109-66-0	32
5		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12



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Instrument :
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ClientSampleId :
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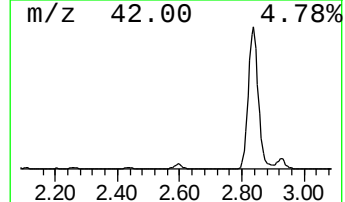
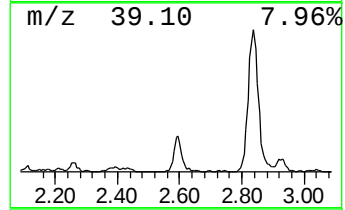
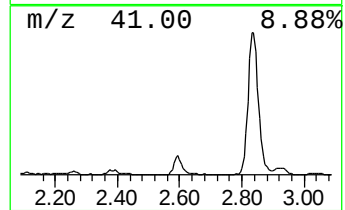
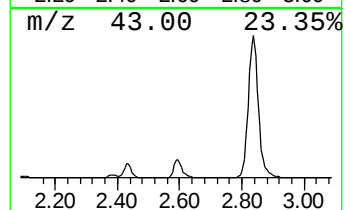
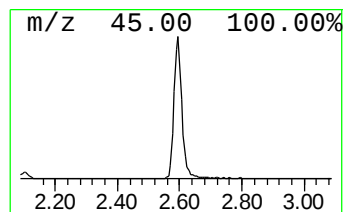
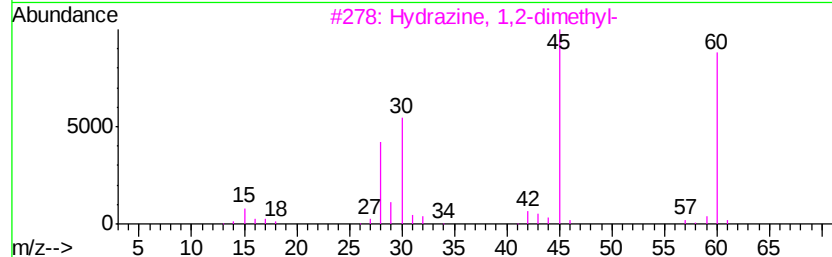
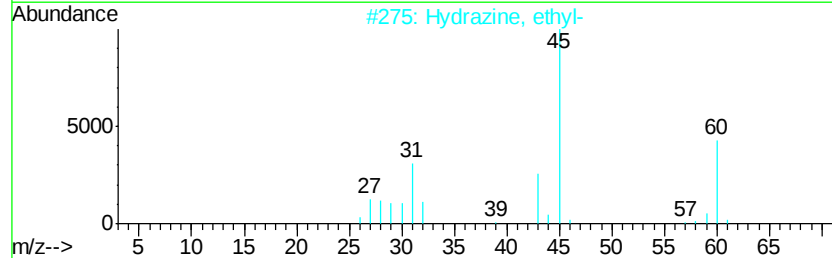
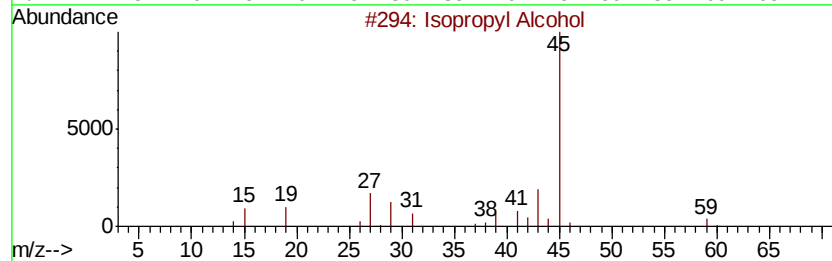
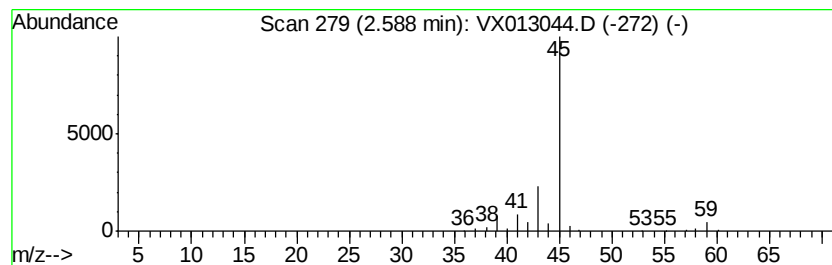
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.59	10.46 ug/l	109517	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hvdrazine, ethyl-	60	C2H8N2	000624-80-6	40
3		Hvdrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4		4-Penten-2-ol	86	C5H10O	000625-31-0	9
5		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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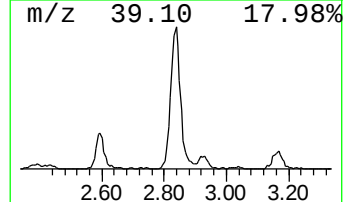
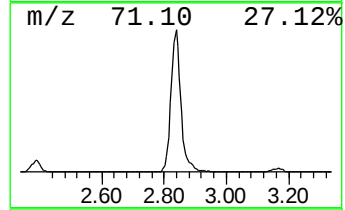
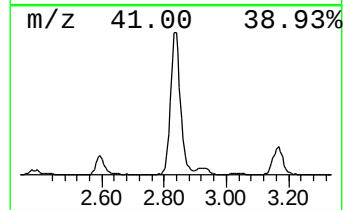
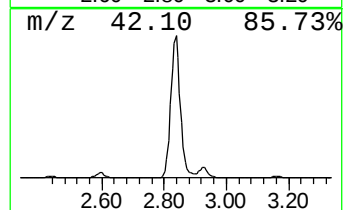
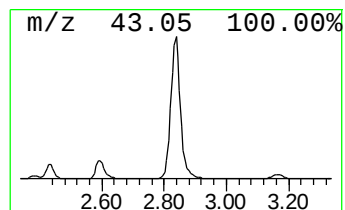
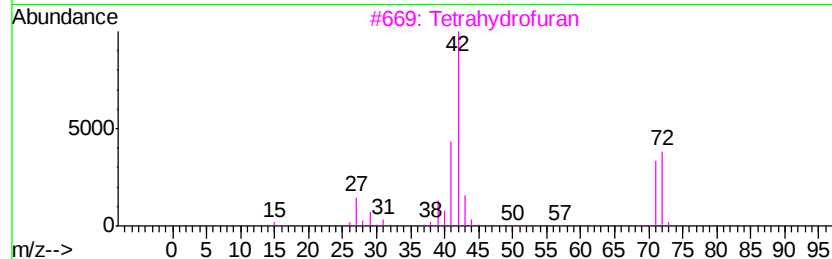
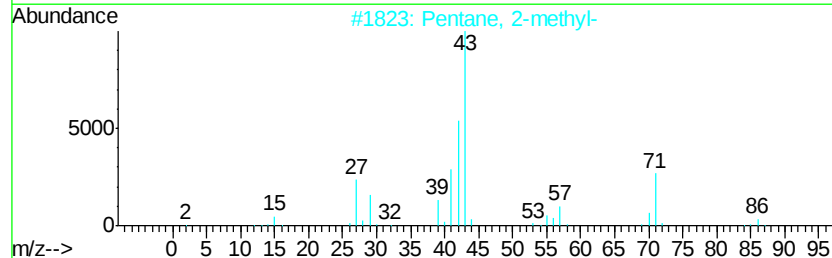
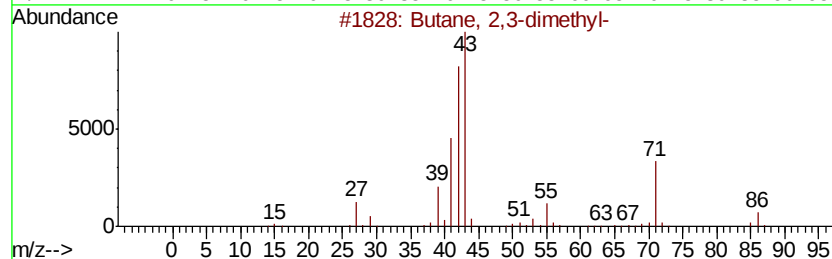
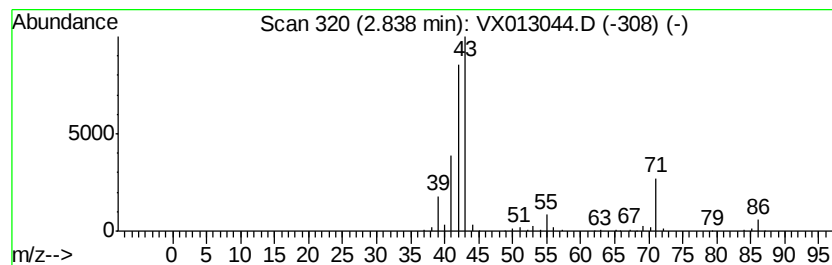
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	40.04 ug/l	419104	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Tetrahydrofuran	72	C4H8O	000109-99-9	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	36
5		1-Pentene	70	C5H10	000109-67-1	28



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ClientSampleId :
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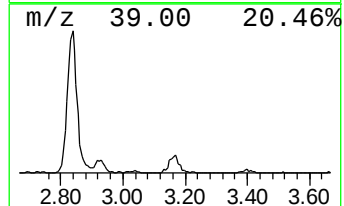
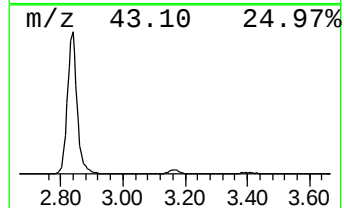
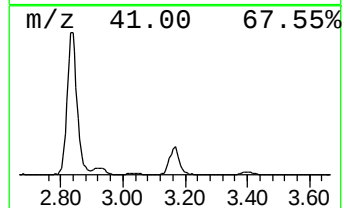
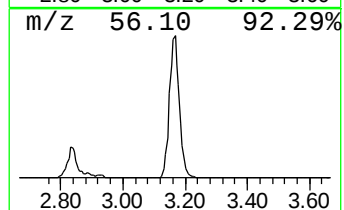
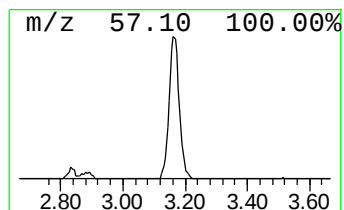
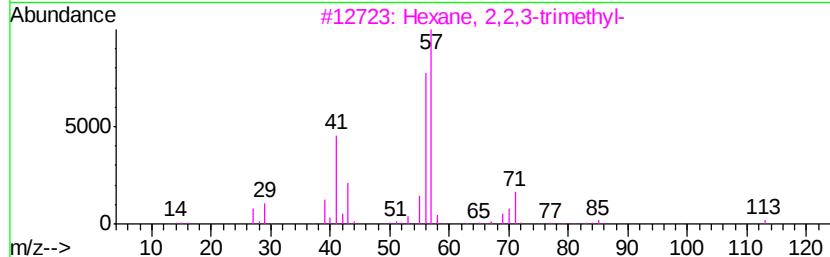
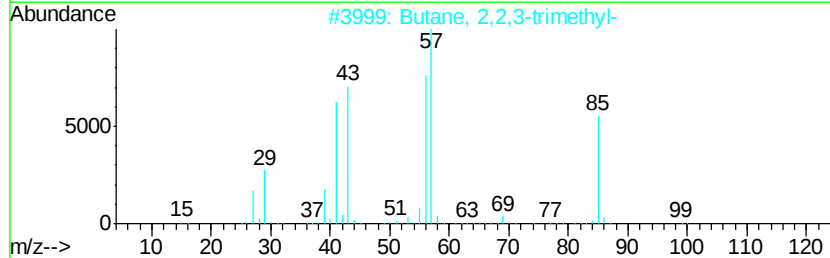
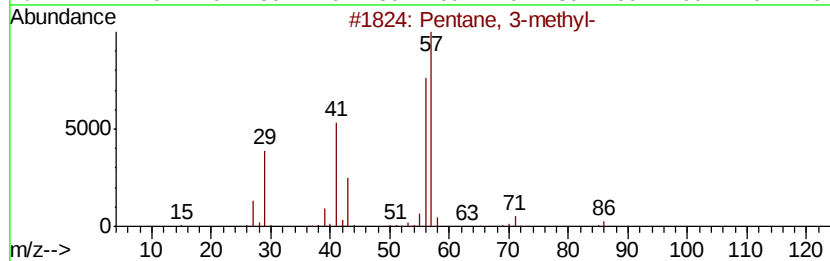
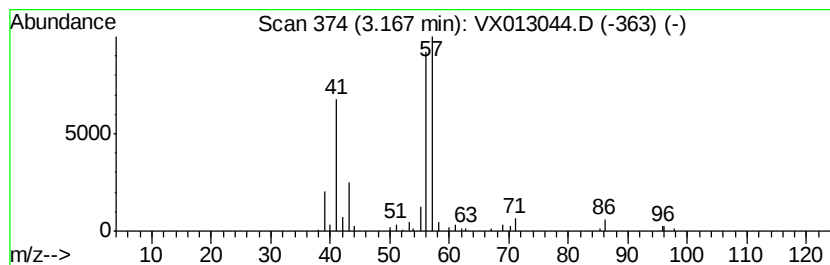
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	5.65 ug/l	59169	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	83
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	59
4		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	50
5		Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	45



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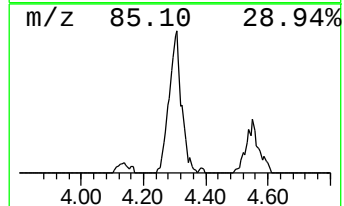
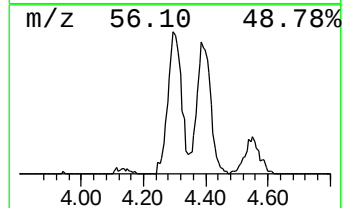
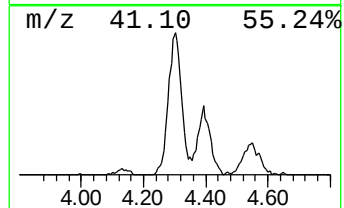
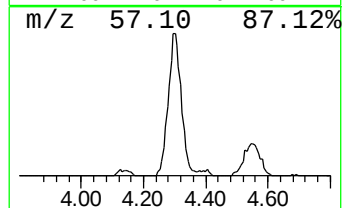
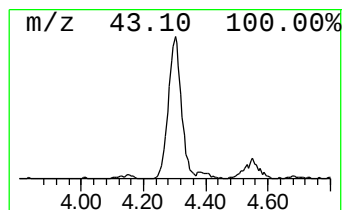
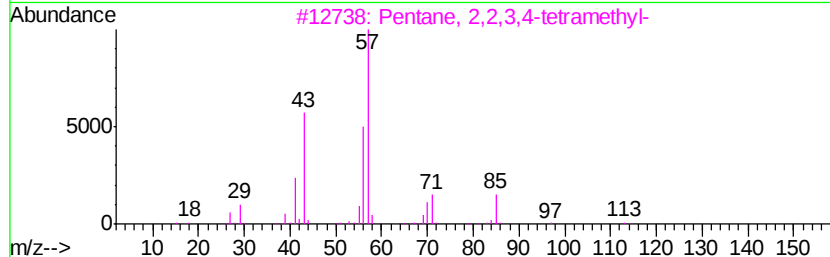
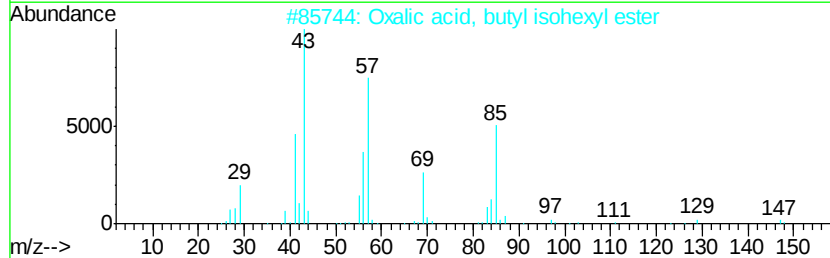
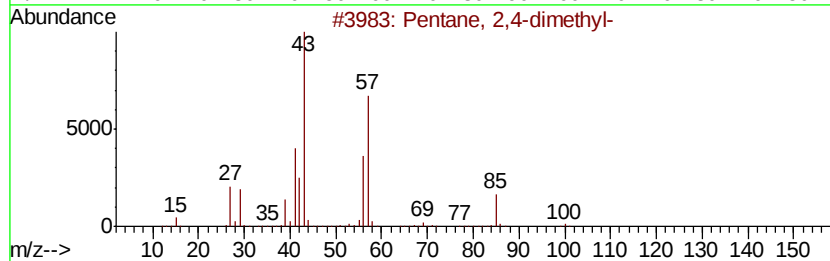
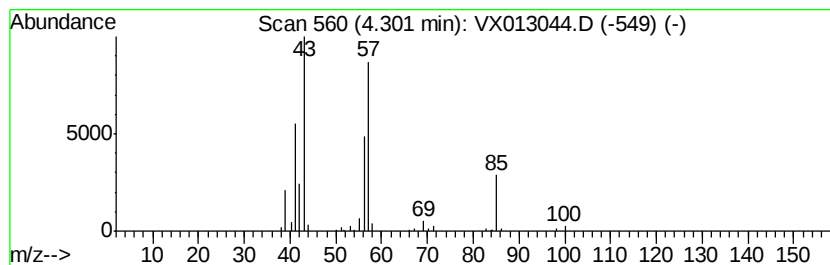
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentane, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	10.79 ug/l	112913	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2		Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	64
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013044.D
Acq On : 14 Oct 2019 12:13
Operator : JC/SP
Sample : K5313-12
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7338A

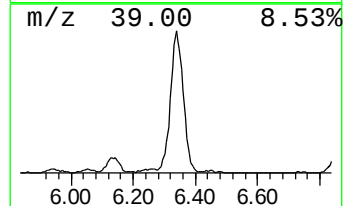
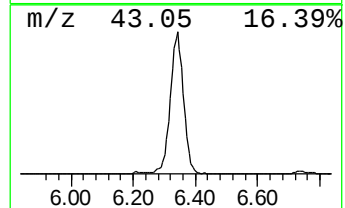
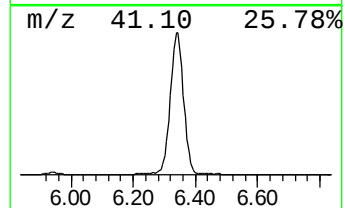
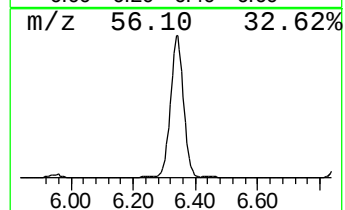
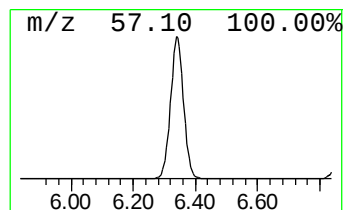
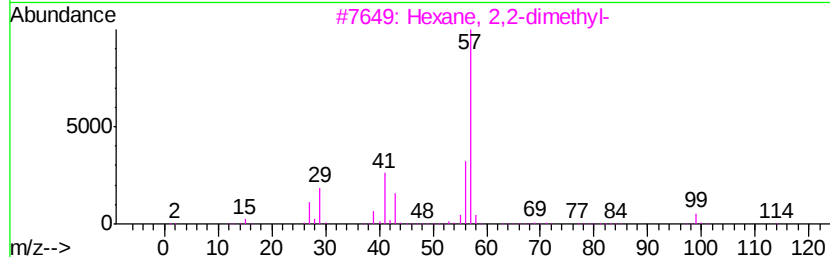
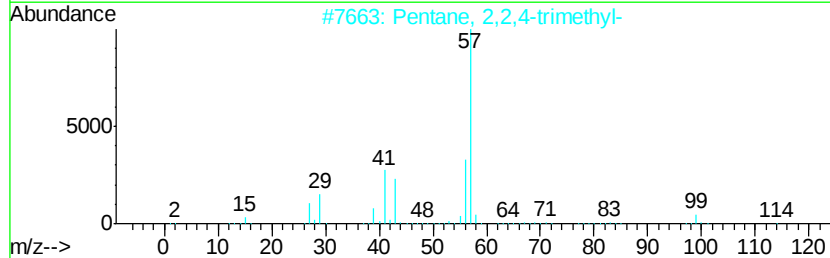
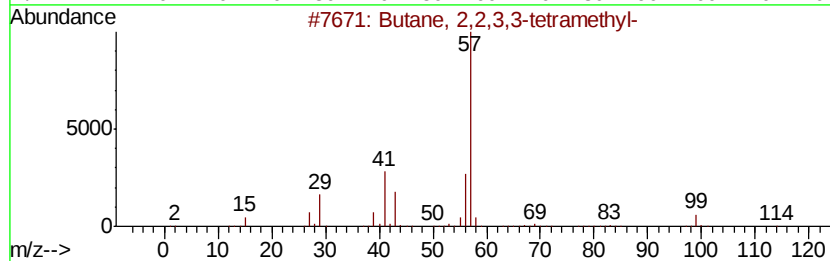
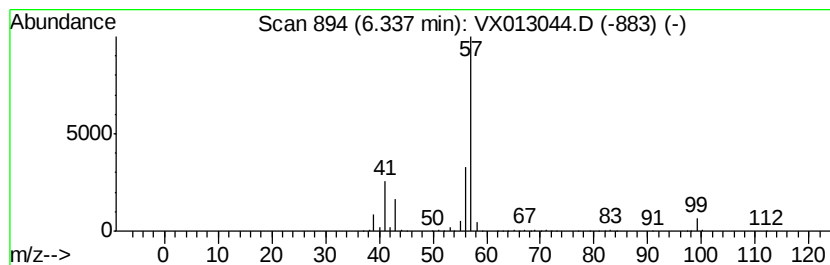
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	73.91 ug/l	1037410	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013044.D
Acq On : 14 Oct 2019 12:13
Operator : JC/SP
Sample : K5313-12
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7338A

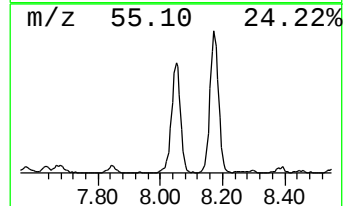
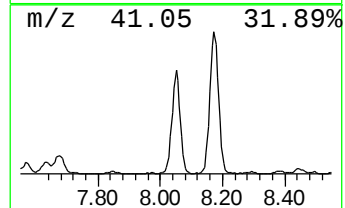
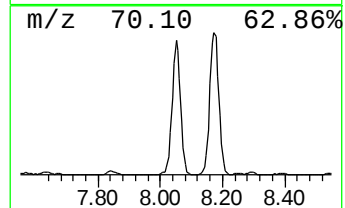
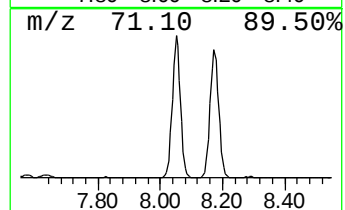
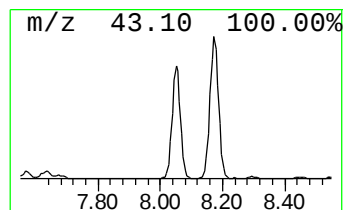
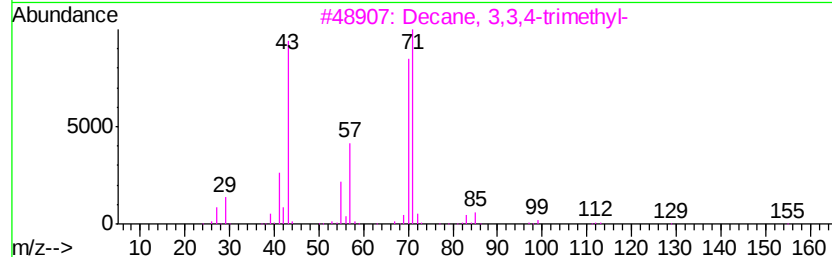
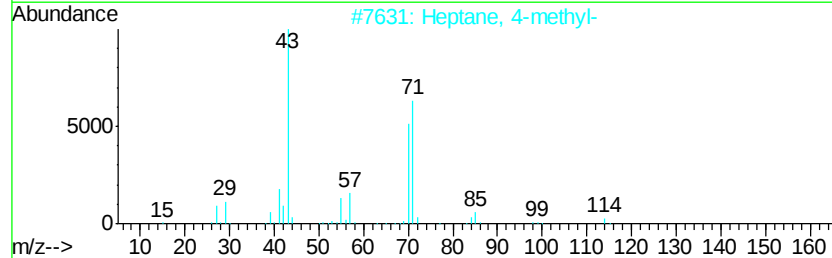
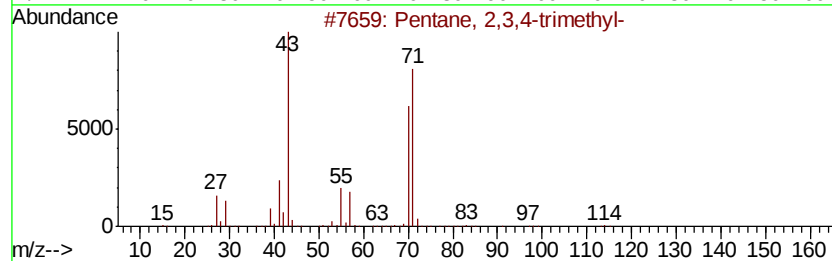
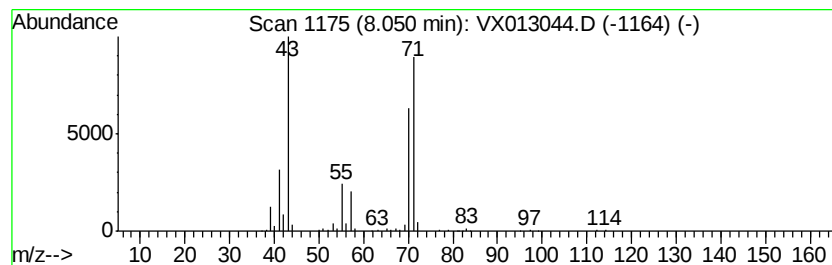
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.05	28.15 ug/l	395038	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013044.D
Acq On : 14 Oct 2019 12:13
Operator : JC/SP
Sample : K5313-12
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7338A

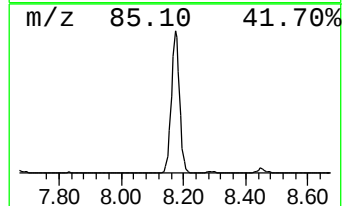
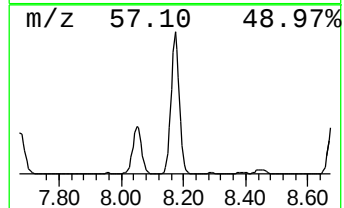
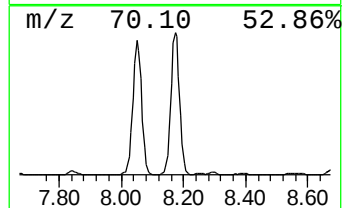
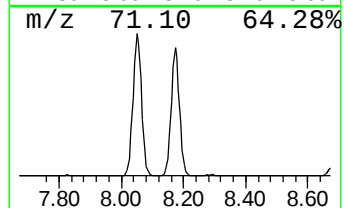
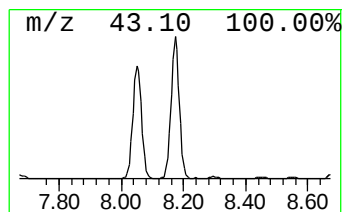
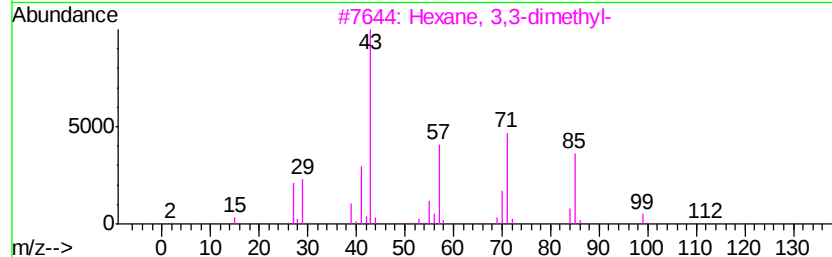
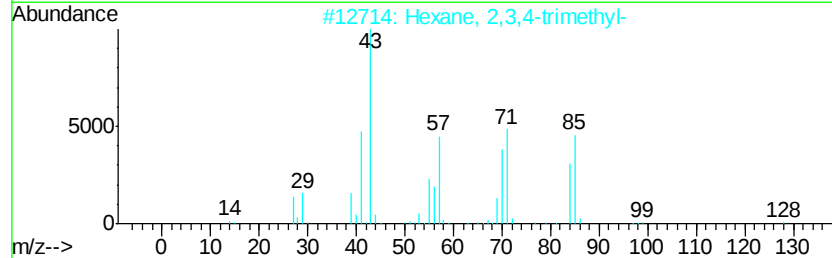
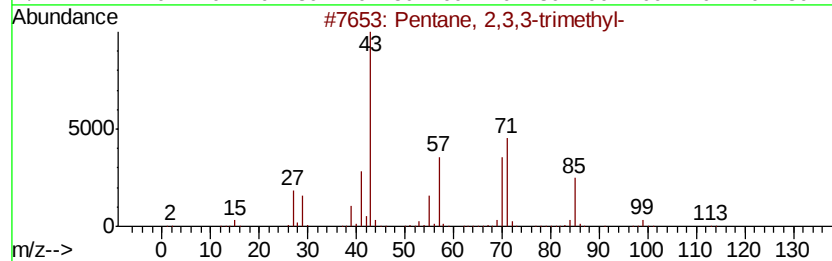
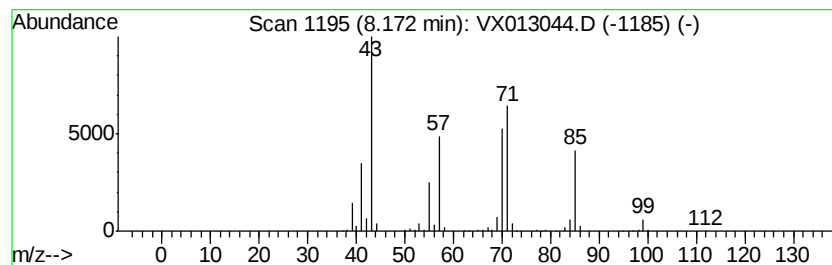
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	40.16 ug/l	563675	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX101419\
Data File : VX013044.D
Acq On : 14 Oct 2019 12:13
Operator : JC/SP
Sample : K5313-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7338A

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.78	89.9	ug/l	940898	1	5.65	523348	50.0
Isopropyl Alcohol	2.59	10.5	ug/l	109517	1	5.65	523348	50.0
Butane, 2,3-dimet...	2.84	40.0	ug/l	419104	1	5.65	523348	50.0
Pentane, 3-methyl-	3.17	5.7	ug/l	59169	1	5.65	523348	50.0
Pentane, 2,4-dime...	4.30	10.8	ug/l	112913	1	5.65	523348	50.0
Butane, 2,2,3,3-t...	6.34	73.9	ug/l	1037410	2	6.85	701780	50.0
Pentane, 2,3,4-tr...	8.05	28.1	ug/l	395038	2	6.85	701780	50.0
Pentane, 2,3,3-tr...	8.17	40.2	ug/l	563675	2	6.85	701780	50.0