

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
 Data File : VU027267.D
 Acq On : 28 Sep 2018 13:32
 Operator : MD/SY
 Sample : J5104-04
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 FA18-JEB5-2

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_U\METHOD\82U092218W.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	1.402	61	71	80	rBV	36451	42172	1.41%	0.191%
2	1.759	172	182	195	rVB	130547	170502	5.70%	0.771%
3	1.948	231	241	253	rVB	226087	305649	10.21%	1.381%
4	2.051	265	273	283	rVB	24612	32929	1.10%	0.149%
5	2.321	344	357	368	rBV	359574	566044	18.92%	2.558%
6	2.379	368	375	384	rVV	89583	141526	4.73%	0.640%
7	2.444	384	395	419	rVB	322964	547734	18.31%	2.475%
8	2.707	466	477	485	rBV2	36823	77319	2.58%	0.349%
9	2.997	554	567	584	rVB3	14061	30351	1.01%	0.137%
10	3.305	650	663	680	rVB2	23674	49295	1.65%	0.223%
11	3.997	860	878	895	rBV4	21259	60248	2.01%	0.272%
12	4.103	895	911	928	rVB5	20199	56922	1.90%	0.257%
13	4.228	928	950	982	rBV2	65128	196978	6.58%	0.890%
14	4.884	1137	1154	1171	rBV	99051	222555	7.44%	1.006%
15	4.987	1171	1186	1203	rVV3	171169	397044	13.27%	1.794%
16	5.083	1203	1216	1234	rVB2	35511	85258	2.85%	0.385%
17	5.222	1246	1259	1274	rBV5	15985	43558	1.46%	0.197%
18	5.312	1275	1287	1304	rVB	122573	258516	8.64%	1.168%
19	5.540	1326	1358	1374	rBV	248476	623456	20.84%	2.818%
20	5.627	1375	1385	1413	rVB5	21330	57452	1.92%	0.260%
21	5.787	1423	1435	1445	rBV3	18742	37263	1.25%	0.168%
22	5.887	1454	1466	1483	rBV	213037	408270	13.64%	1.845%
23	6.189	1546	1560	1578	rBV2	61879	124953	4.18%	0.565%
24	6.418	1608	1631	1644	rBV	448295	868864	29.04%	3.927%
25	6.479	1644	1650	1658	rVV2	42900	84739	2.83%	0.383%
26	6.533	1659	1667	1675	rVV3	62046	125872	4.21%	0.569%
27	6.582	1675	1682	1694	rVV2	44130	94507	3.16%	0.427%
28	6.778	1719	1743	1773	rBV2	148003	319460	10.68%	1.444%
29	6.929	1774	1790	1806	rVB	154499	312824	10.45%	1.414%
30	7.051	1814	1828	1838	rBV	187336	375904	12.56%	1.699%
31	7.106	1839	1845	1856	rVB2	41751	71291	2.38%	0.322%
32	7.524	1961	1975	1980	rBV3	86309	156735	5.24%	0.708%
33	7.566	1980	1988	2002	rVV	433808	765473	25.58%	3.459%
34	7.639	2004	2011	2022	rVB	33310	58584	1.96%	0.265%

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35	7.919	2087	2098	2109	rBV2	26428	49403	1.65%	0.223%
36	8.366	2212	2237	2257	rBV2	111266	238618	7.97%	1.078%
37	8.466	2257	2268	2285	rBV	137101	254265	8.50%	1.149%
38	8.546	2285	2293	2296	rBV2	26077	35323	1.18%	0.160%
39	8.578	2297	2303	2308	rBV	38131	48976	1.64%	0.221%
40	9.090	2451	2462	2485	rVB	309984	522098	17.45%	2.359%
41	9.250	2502	2512	2529	rVB	39575	64579	2.16%	0.292%
42	9.376	2531	2551	2565	rVV	146162	276512	9.24%	1.250%
43	9.446	2565	2573	2596	rVB4	23645	49241	1.65%	0.223%
44	9.684	2634	2647	2657	rBV	33629	67537	2.26%	0.305%
45	9.781	2668	2677	2683	rBV	30388	47036	1.57%	0.213%
46	9.816	2683	2688	2708	rVB2	22895	49235	1.65%	0.223%
47	9.919	2708	2720	2746	rBV	795112	1265086	42.28%	5.717%
48	10.048	2746	2760	2787	rVV	606165	997313	33.33%	4.507%
49	10.167	2789	2797	2805	rVV2	21239	32398	1.08%	0.146%
50	10.308	2830	2841	2853	rBV	303561	492742	16.47%	2.227%
51	10.591	2920	2929	2931	rBV	24918	31527	1.05%	0.142%
52	10.620	2932	2938	2948	rVB	70545	107051	3.58%	0.484%
53	10.681	2948	2957	2972	rBV2	70622	161269	5.39%	0.729%
54	10.771	2973	2985	2994	rVV	74344	118961	3.98%	0.538%
55	10.948	3031	3040	3043	rBV	60594	82853	2.77%	0.374%
56	11.022	3056	3063	3070	rVB2	27877	38439	1.28%	0.174%
57	11.154	3093	3104	3116	rBV2	529912	788192	26.34%	3.562%
58	11.257	3124	3136	3150	rBV2	1739658	2908750	97.21%	13.145%
59	11.337	3150	3161	3182	rVB	2021504	2992171	100.00%	13.522%
60	11.485	3196	3207	3224	rVB	380613	602683	20.14%	2.724%
61	11.572	3225	3234	3243	rVV	64898	95980	3.21%	0.434%
62	11.636	3246	3254	3268	rVB4	22658	40267	1.35%	0.182%
63	11.810	3304	3308	3316	rVB	28127	34649	1.16%	0.157%
64	11.874	3317	3328	3341	rBV4	39034	79882	2.67%	0.361%
65	12.054	3378	3384	3397	rVB	29594	50535	1.69%	0.228%
66	12.183	3417	3424	3428	rBV3	24488	33260	1.11%	0.150%
67	12.218	3428	3435	3441	rBV	104108	142348	4.76%	0.643%
68	12.360	3469	3479	3497	rBV4	62230	122651	4.10%	0.554%
69	12.453	3497	3508	3515	rBV2	297808	466618	15.59%	2.109%
70	12.498	3515	3522	3534	rVB	404443	580912	19.41%	2.625%
71	12.704	3579	3586	3598	rVB	26222	42648	1.43%	0.193%

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72	12.967	3660	3668	3677	rVB3	22094	33380	1.12%	0.151%
73	13.125	3708	3717	3729	rVB6	37798	69298	2.32%	0.313%
74	13.318	3771	3777	3797	rVB3	41137	76851	2.57%	0.347%
75	13.549	3841	3849	3864	rVB3	40820	100918	3.37%	0.456%
76	14.877	4252	4262	4272	rBV	20485	33327	1.11%	0.151%
77	15.064	4310	4320	4333	rBV2	18203	31568	1.06%	0.143%

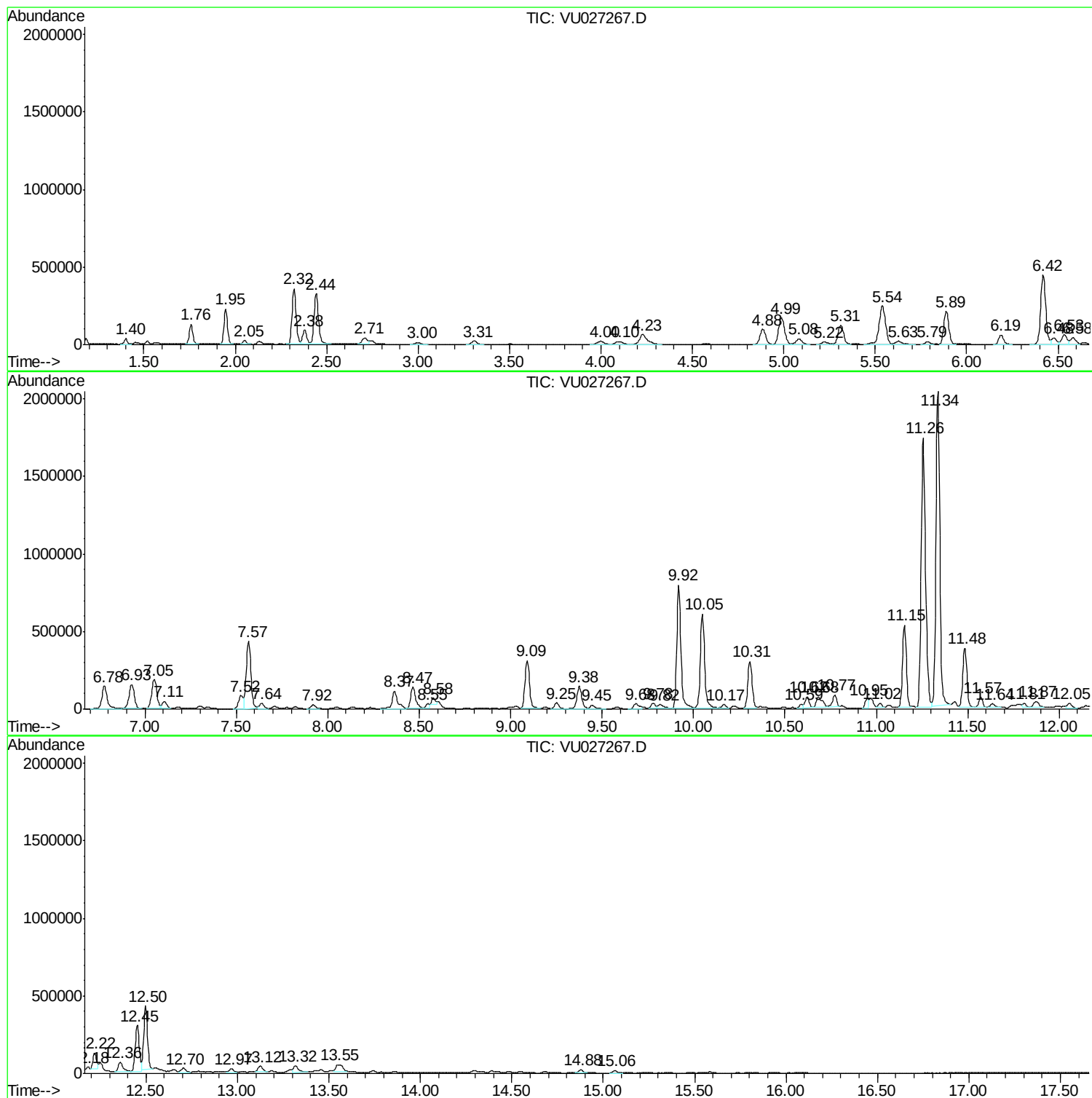
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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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



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Instrument :
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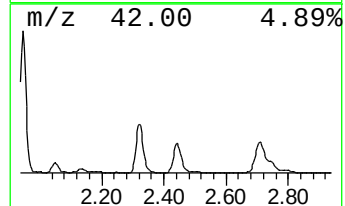
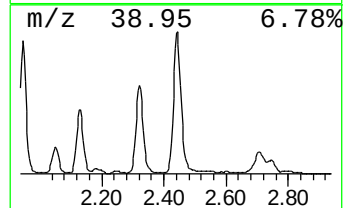
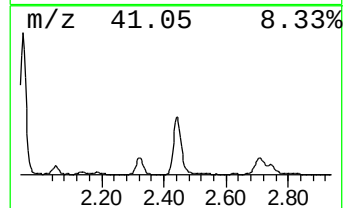
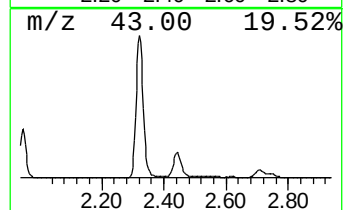
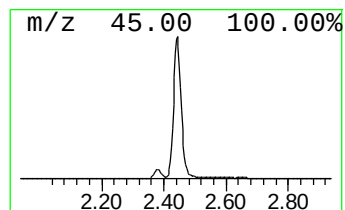
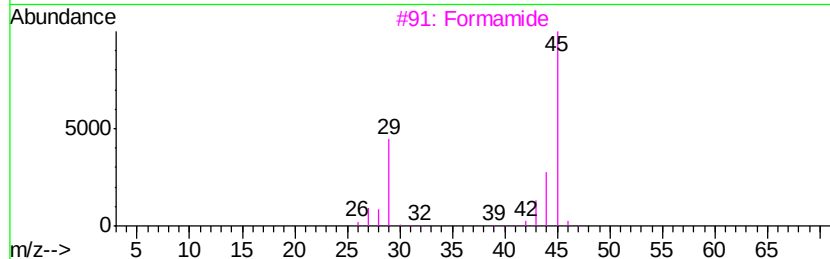
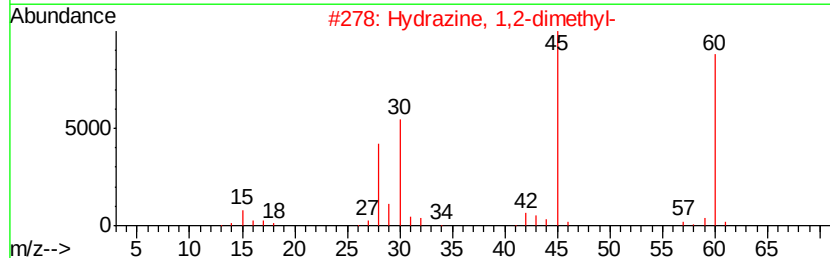
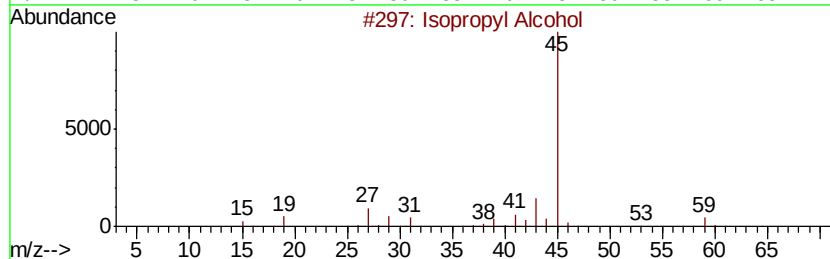
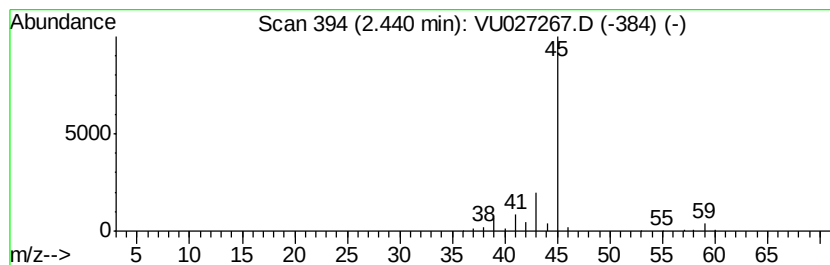
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	68.98 ug/l	547734	Pentafluorobenzene	4.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Formamide	45	CH3NO	000075-12-7	4
4			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4
5			4-Penten-2-ol	86	C5H10O	000625-31-0	4



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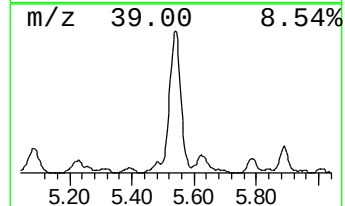
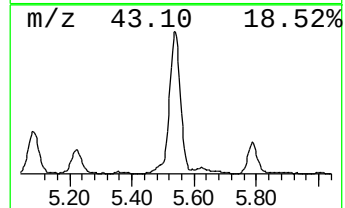
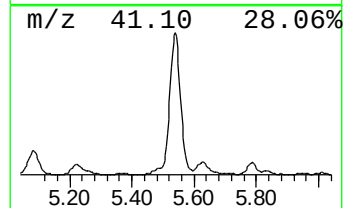
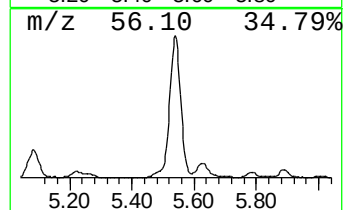
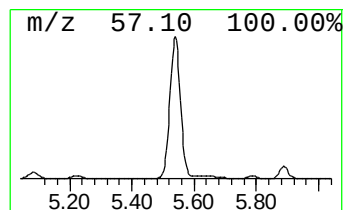
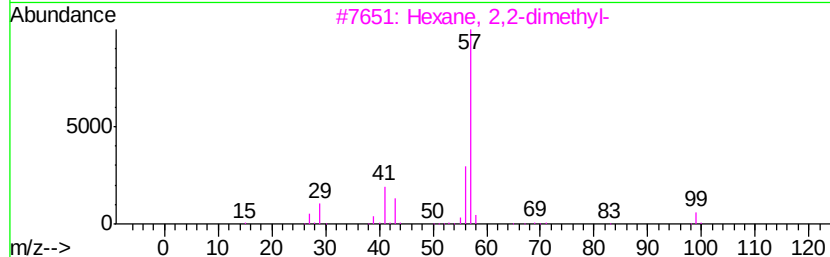
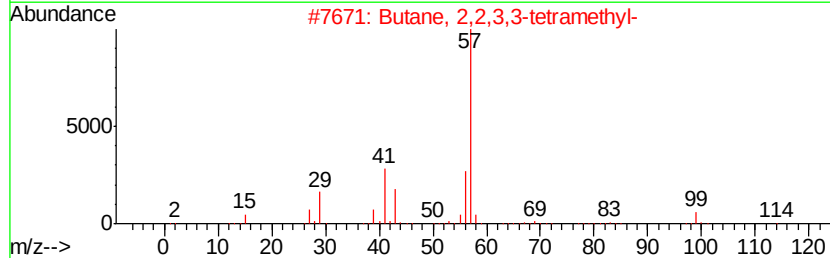
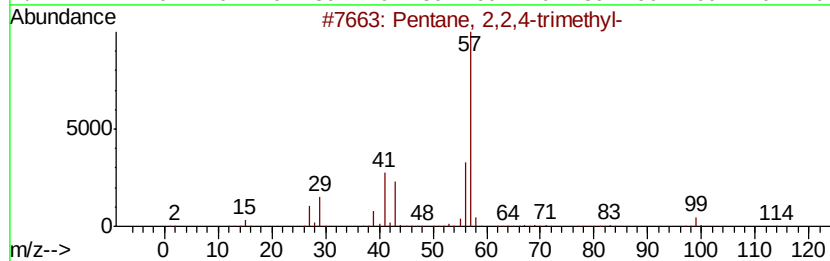
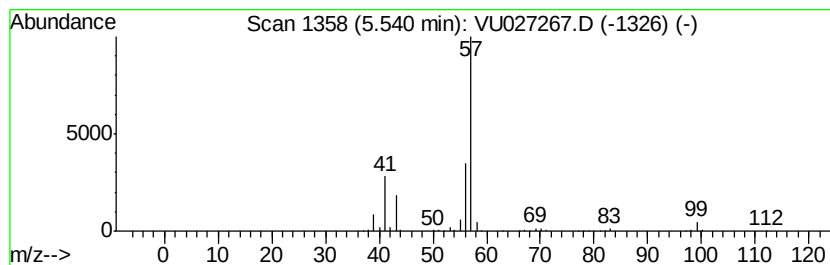
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	76.35 ug/l	623456	1,4-Difluorobenzene	5.89

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	64
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	59



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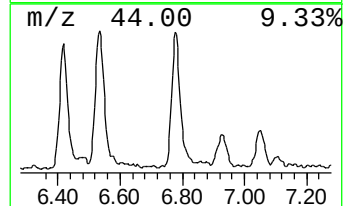
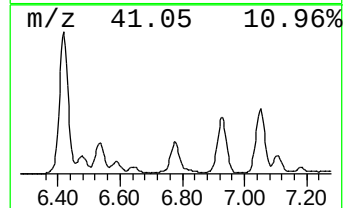
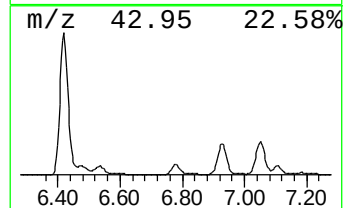
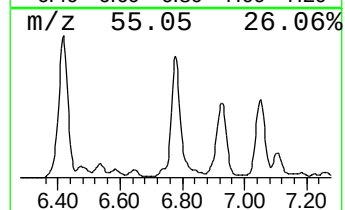
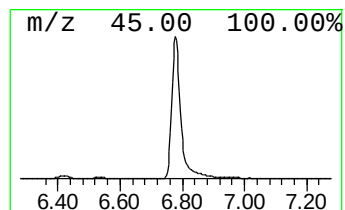
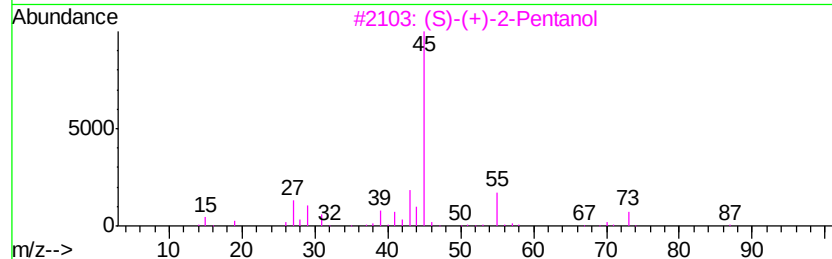
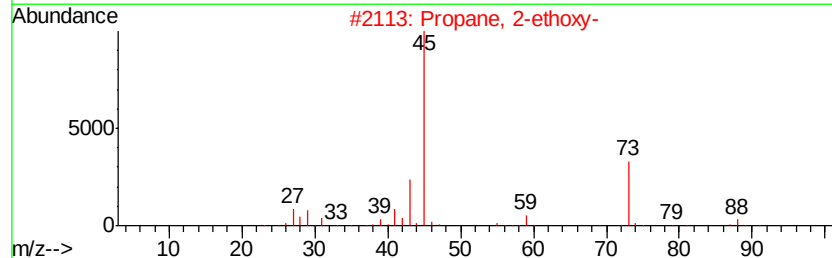
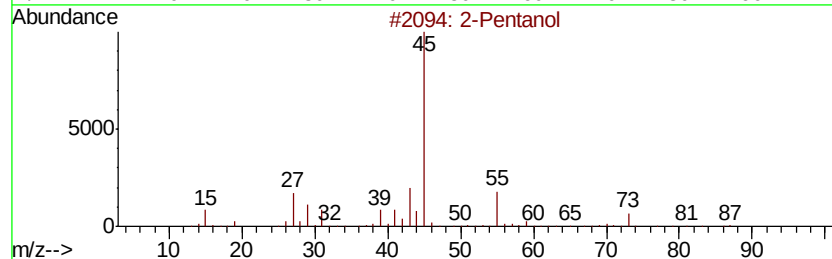
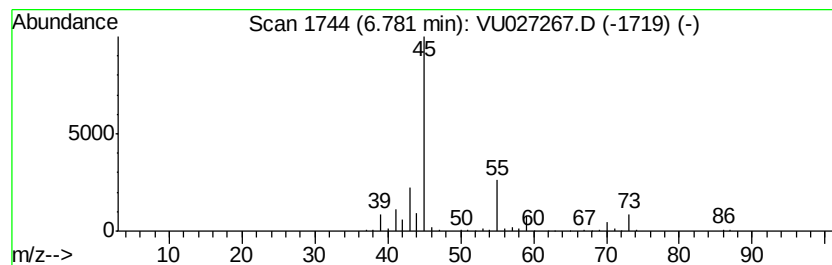
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	39.12 ug/l	319460	1,4-Difluorobenzene	5.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Pentanol		88 C5H12O	006032-29-7 72
2	Propane, 2-ethoxy-		88 C5H12O	000625-54-7 72
3	(S)-(+)-2-Pentanol		88 C5H12O	026184-62-3 72
4	2-Butanol, 3-methyl-, (S)-		88 C5H12O	001517-66-4 72
5	(R)-(-)-3-Methyl-2-butanol		88 C5H12O	001572-93-6 64



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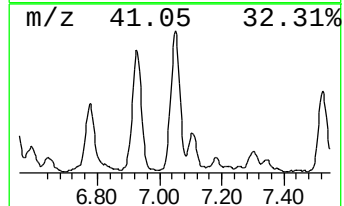
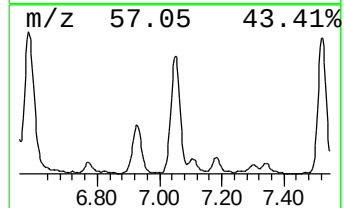
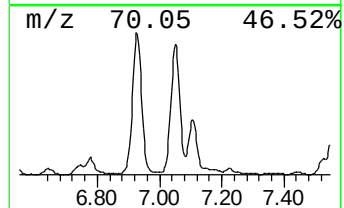
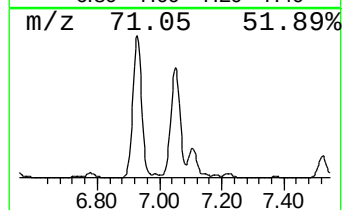
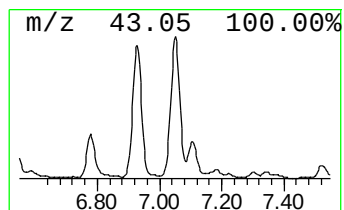
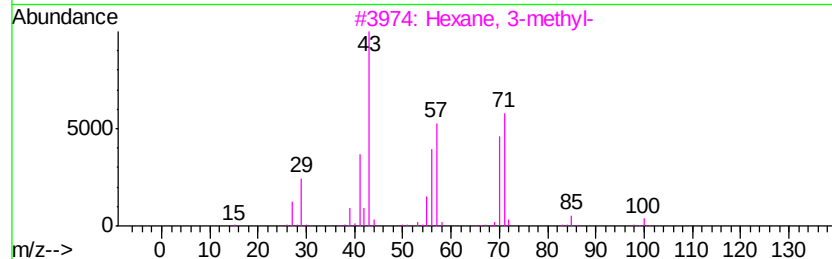
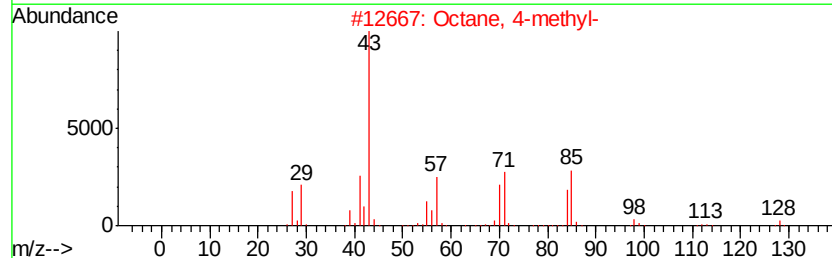
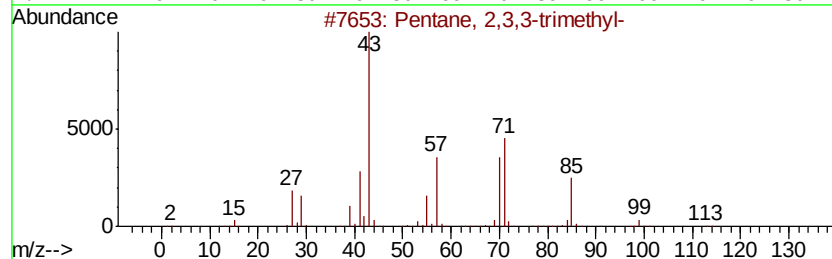
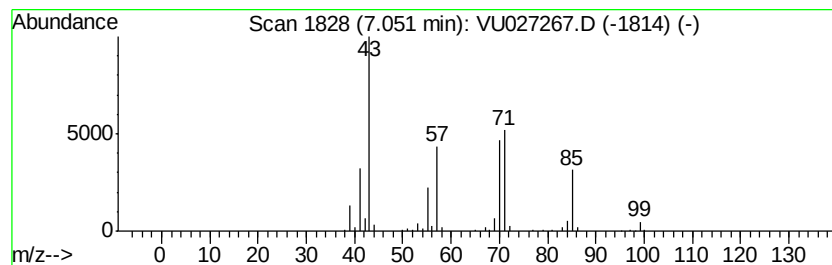
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	46.04 ug/l	375904	1,4-Difluorobenzene	5.89

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	78
3		Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FA18-JEB5-2

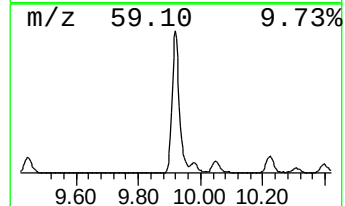
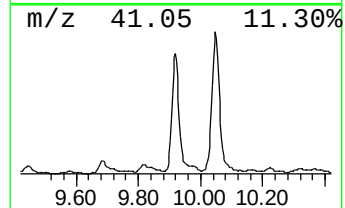
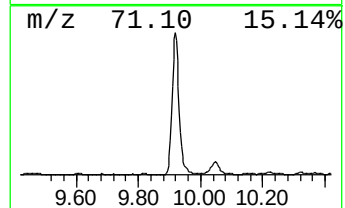
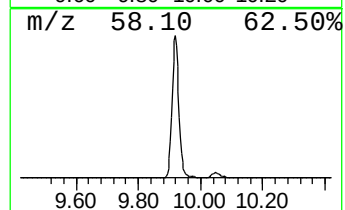
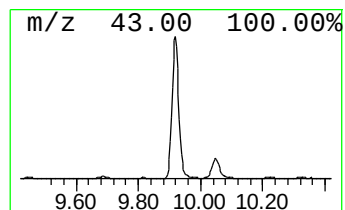
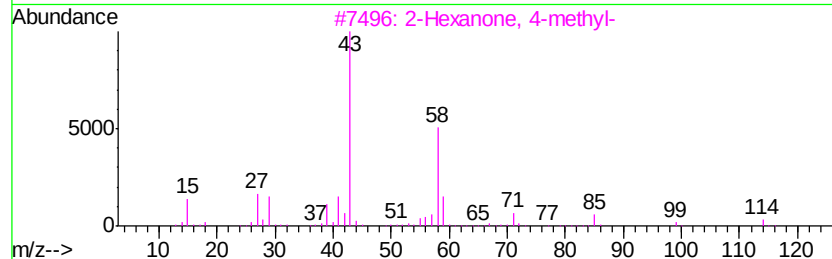
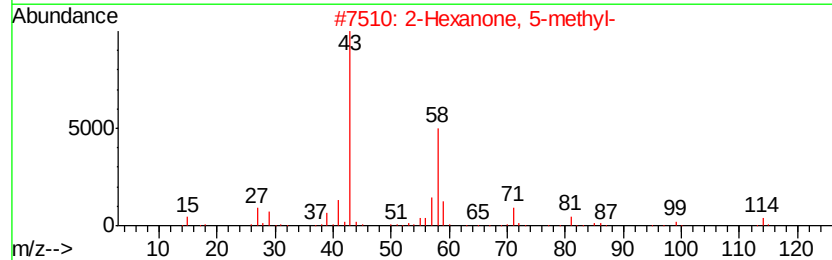
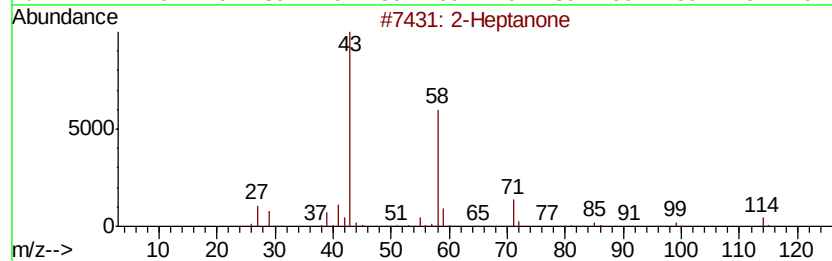
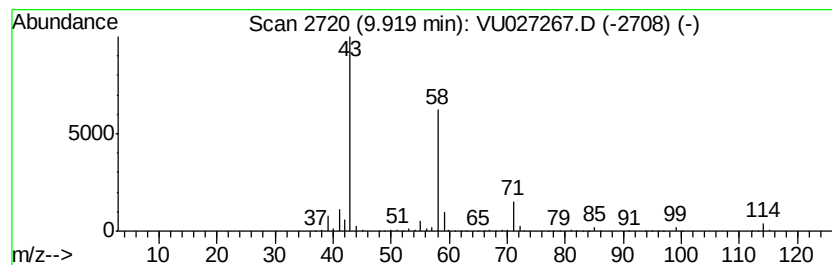
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Quant Title : SW846 8260

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

Peak Number 5 2-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	121.15 ug/l	1265090	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone		114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-		114	C7H14O	000110-12-3	72
3	2-Hexanone, 4-methyl-		114	C7H14O	000105-42-0	64
4	2-Heptanone, 6-methyl-		128	C8H16O	000928-68-7	56
5	2-Pentanone, 4,4-dimethyl-		114	C7H14O	000590-50-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FA18-JEB5-2

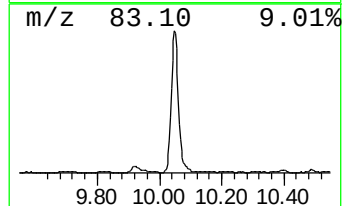
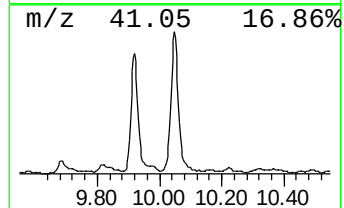
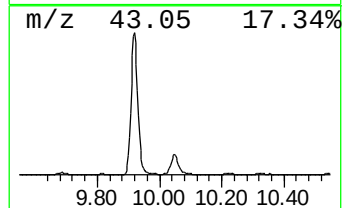
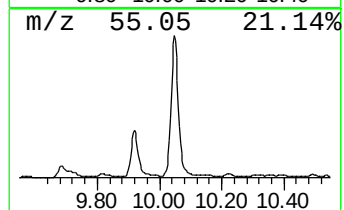
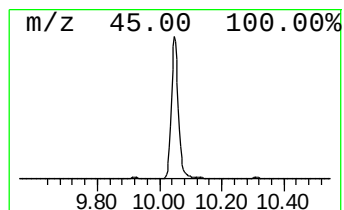
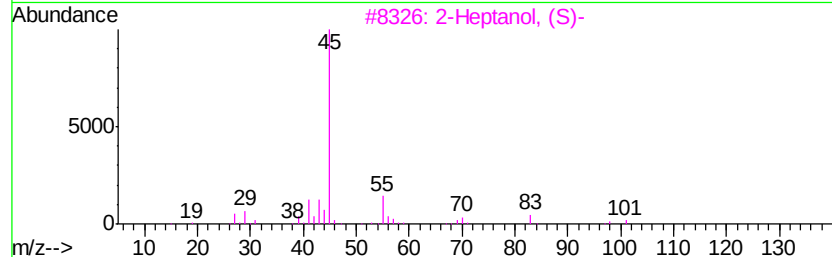
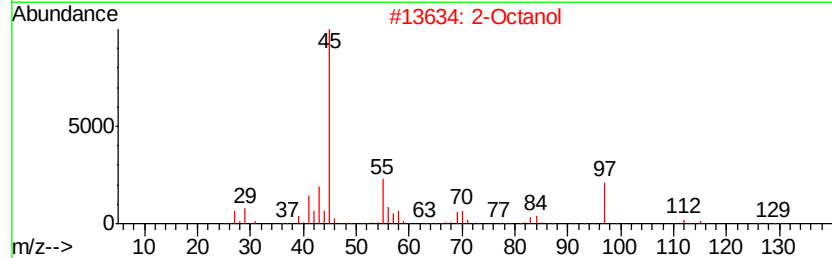
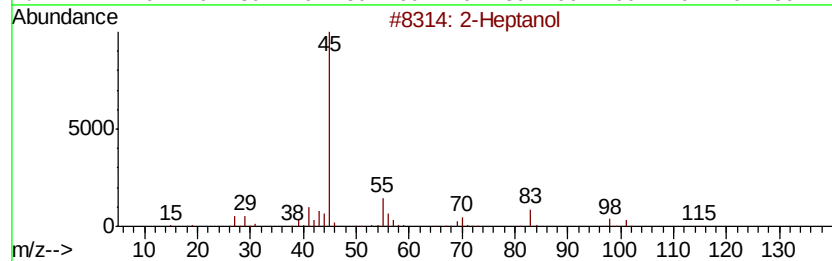
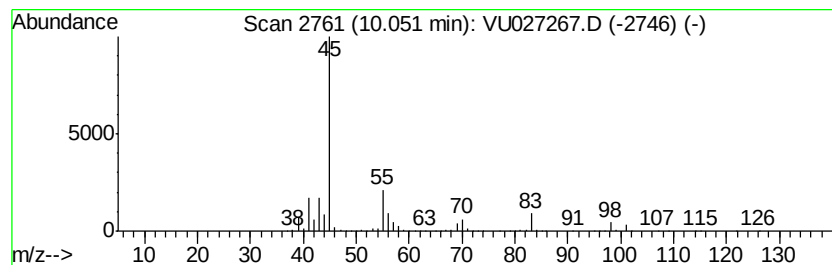
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Quant Title : SW846 8260

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

Peak Number 6 2-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	95.51 ug/l	997313	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanol	116	C7H16O	000543-49-7	83
2		2-Octanol	130	C8H18O	000123-96-6	78
3		2-Heptanol, (S)-	116	C7H16O	006033-23-4	74
4		2-Octanol, (S)-	130	C8H18O	006169-06-8	72
5		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FA18-JEB5-2

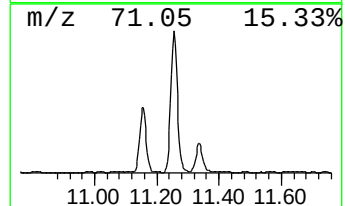
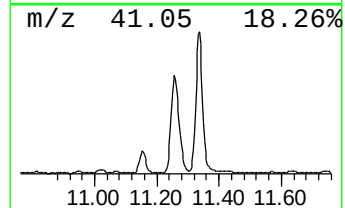
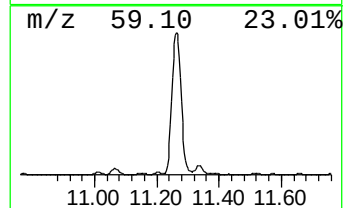
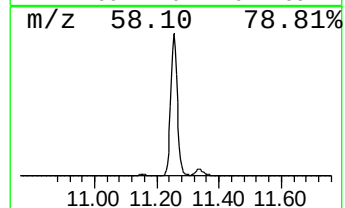
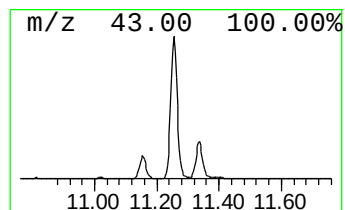
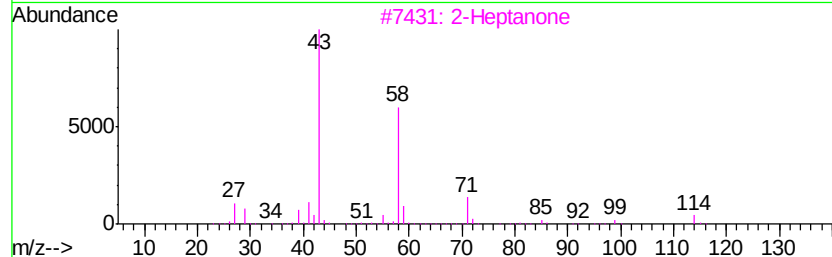
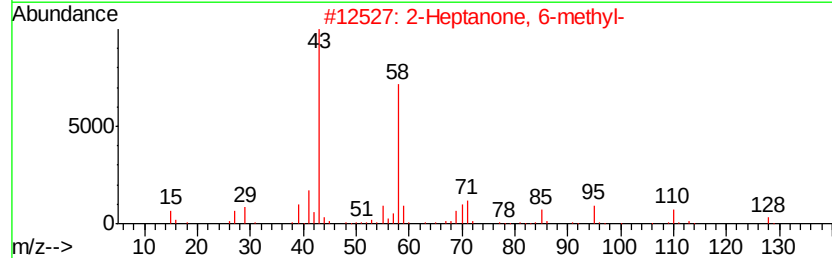
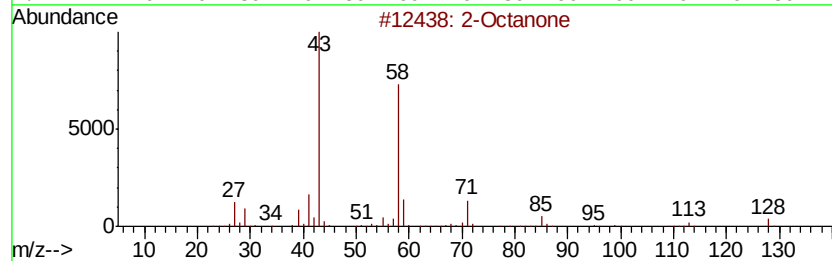
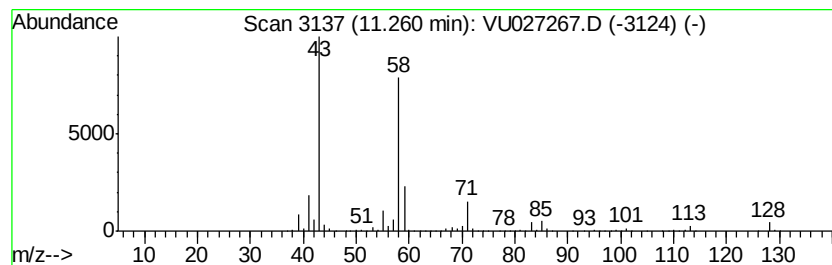
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Quant Title : SW846 8260

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

Peak Number 7 2-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	241.32 ug/l	2908750	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanone	128	C8H16O	000111-13-7	94
2		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	90
3		2-Heptanone	114	C7H14O	000110-43-0	50
4		1-Propene, 2-(1-methylethoxy)	100	C6H12O	004188-63-0	45
5		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

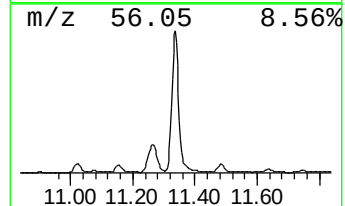
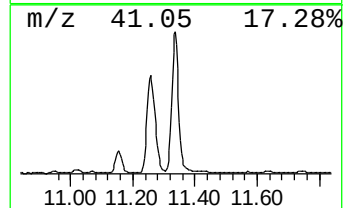
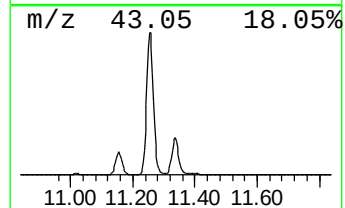
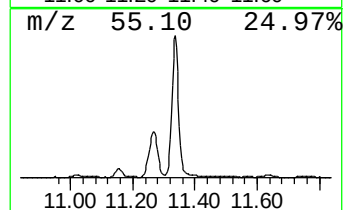
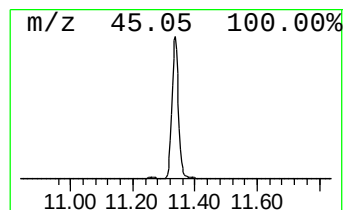
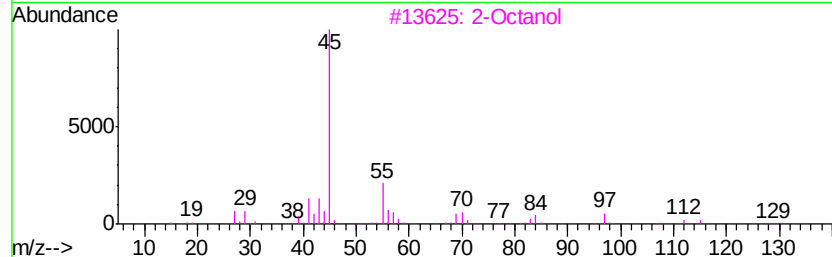
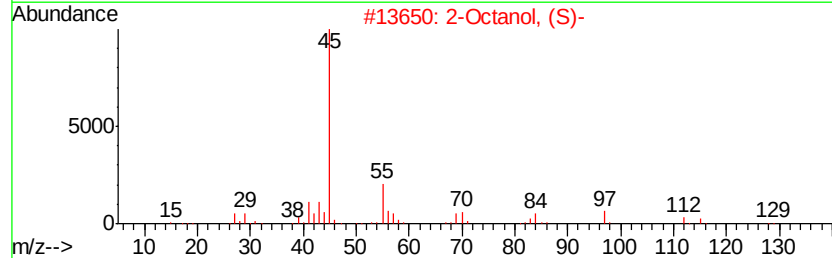
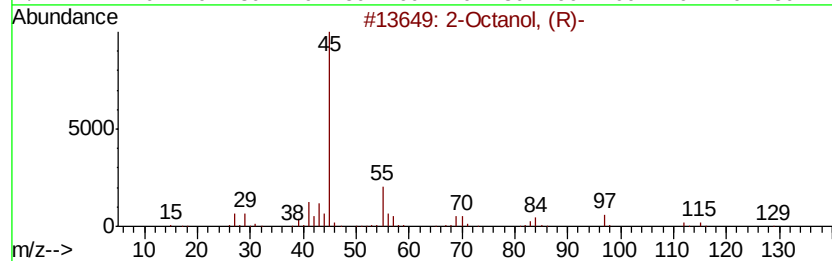
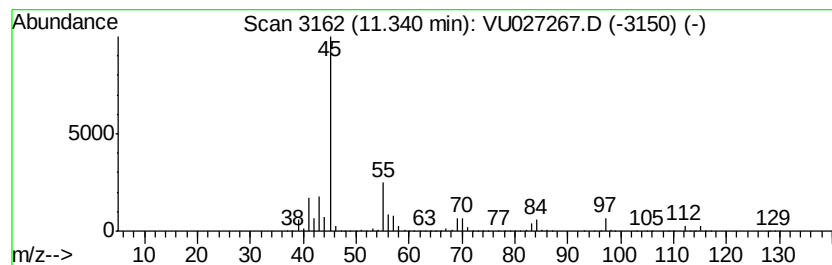
Instrument :
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ClientSampleId :
FA18-JEB5-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 8 2-Octanol, (R)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.34	248.24 ug/l	2992170	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Octanol, (R)-	130 C8H18O	005978-70-1	90
2	2-Octanol, (S)-	130 C8H18O	006169-06-8	90
3	2-Octanol	130 C8H18O	000123-96-6	90
4	2-Heptanol, 6-methyl-	130 C8H18O	004730-22-7	78
5	2-Nonanol	144 C9H20O	000628-99-9	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

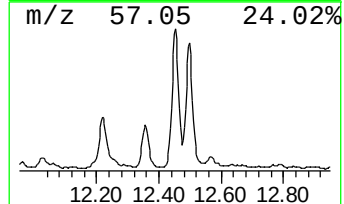
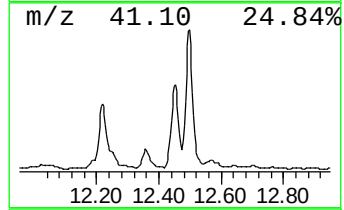
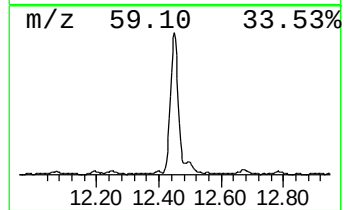
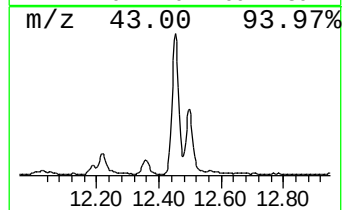
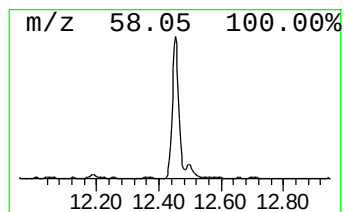
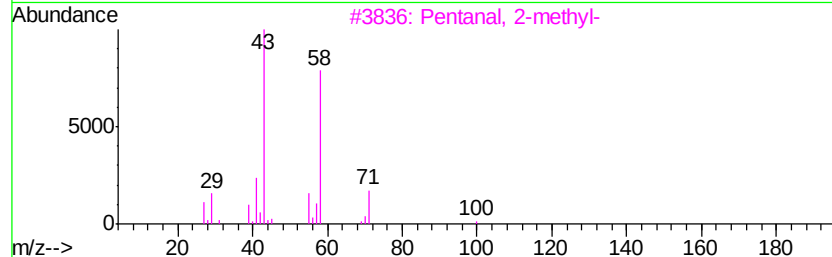
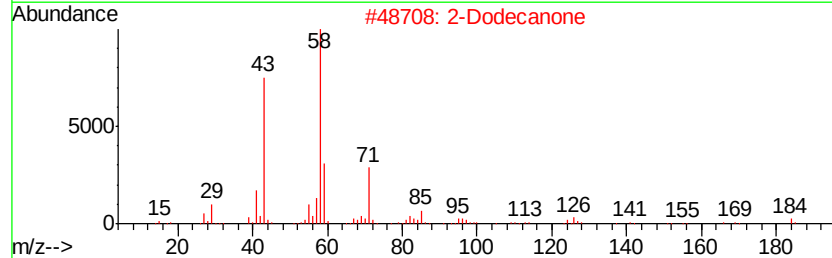
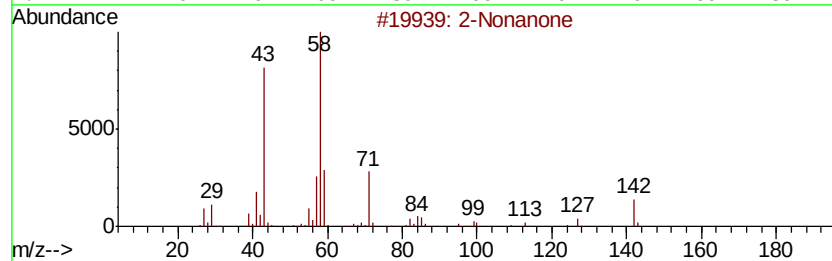
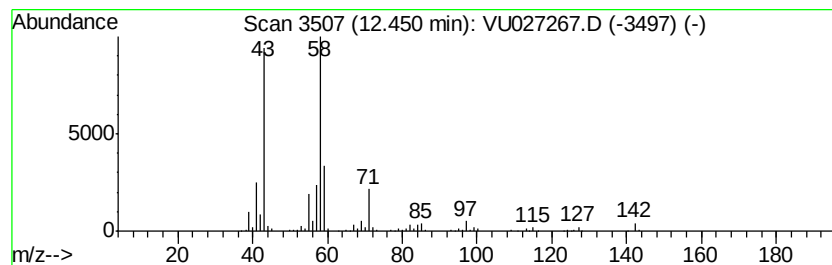
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FA18-JEB5-2

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Quant Title : SW846 8260

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

Peak Number 9 2-Nonanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	38.71 ug/l	466618	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Nonanone	142 C9H18O	000821-55-6	91
2	2-Dodecanone	184 C12H24O	006175-49-1	78
3	Pentanal, 2-methyl-	100 C6H12O	000123-15-9	53
4	2-Propenoic acid, 2-(dimethylami...	143 C7H13NO2	002439-35-2	43
5	Undecanal, 2-methyl-	184 C12H24O	000110-41-8	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FA18-JEB5-2

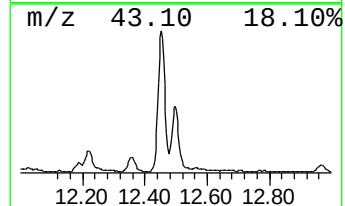
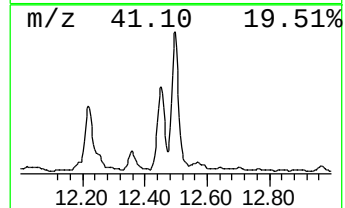
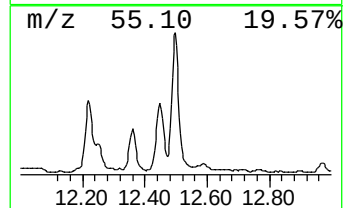
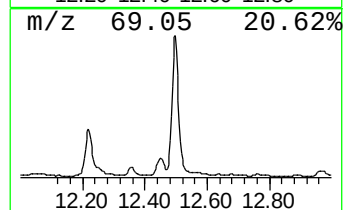
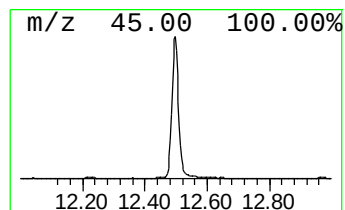
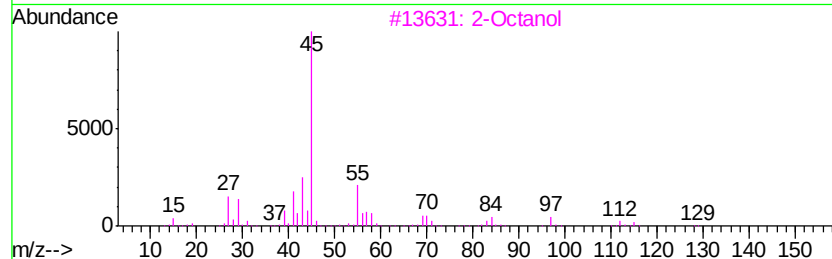
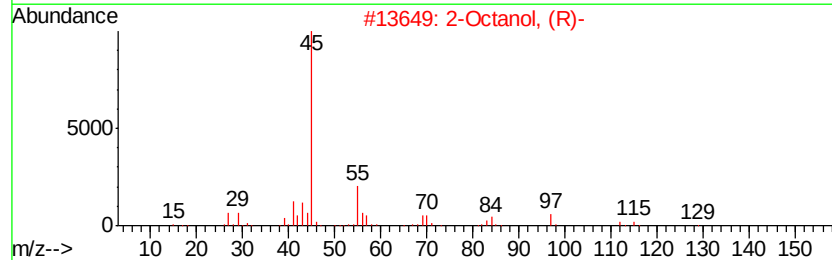
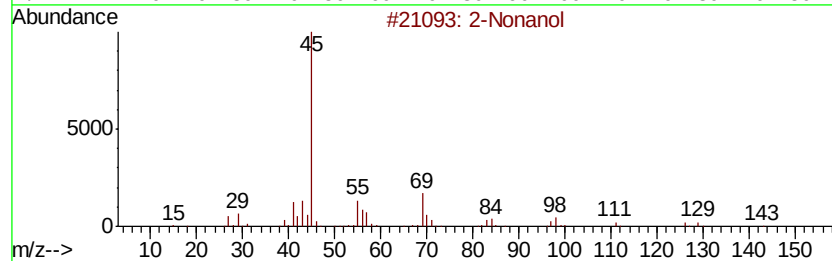
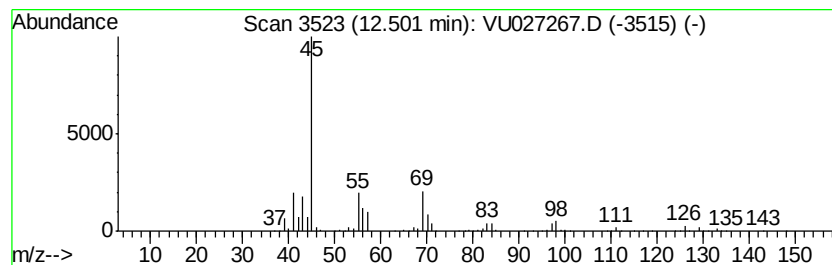
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Quant Title : SW846 8260

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

Peak Number 10 2-Nonanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	48.19 ug/l	580912	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Nonanol	144	C9H20O	000628-99-9	90
2		2-Octanol, (R)-	130	C8H18O	005978-70-1	78
3		2-Octanol	130	C8H18O	000123-96-6	78
4		2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	78
5		2-Decanol	158	C10H22O	001120-06-5	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027267.D
Acq On : 28 Sep 2018 13:32
Operator : MD/SY
Sample : J5104-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FA18-JEB5-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.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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Pentane, 2,2,4-tr...	5.54	76.3	ug/l	623456	2	5.89	408270	50.0
2-Pentanol	6.78	39.1	ug/l	319460	2	5.89	408270	50.0
Pentane, 2,3,3-tr...	7.05	46.0	ug/l	375904	2	5.89	408270	50.0
2-Heptanone	9.92	121.2	ug/l	1265090	3	9.09	522098	50.0
2-Heptanol	10.05	95.5	ug/l	997313	3	9.09	522098	50.0
2-Octanone	11.26	241.3	ug/l	2908750	4	11.48	602683	50.0
2-Octanol, (R)-	11.34	248.2	ug/l	2992170	4	11.48	602683	50.0
2-Nonanone	12.45	38.7	ug/l	466618	4	11.48	602683	50.0
2-Nonanol	12.50	48.2	ug/l	580912	4	11.48	602683	50.0