

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
 Data File : VU027276.D
 Acq On : 28 Sep 2018 17:01
 Operator : MD/SY
 Sample : J5041-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 S13-0250

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	2.324	348	358	368	rVB2	5335	9124	1.04%	0.183%
2	2.443	384	395	410	rBV	17329	30684	3.50%	0.614%
3	2.710	463	478	489	rBV2	4594	9610	1.10%	0.192%
4	3.996	864	878	891	rVB5	3522	8941	1.02%	0.179%
5	4.884	1137	1154	1171	rBV	117172	265025	30.27%	5.301%
6	4.987	1171	1186	1202	rVV	169804	378530	43.24%	7.572%
7	5.083	1203	1216	1233	rVB2	25453	61827	7.06%	1.237%
8	5.311	1268	1287	1308	rBV	147565	307099	35.08%	6.143%
9	5.540	1346	1358	1375	rVB2	35870	87034	9.94%	1.741%
10	5.887	1452	1466	1485	rBV	255931	501471	57.28%	10.031%
11	6.401	1613	1626	1642	rBV6	17479	48168	5.50%	0.963%
12	6.591	1673	1685	1697	rVB	4148	8805	1.01%	0.176%
13	6.742	1720	1732	1745	rBV3	13919	27126	3.10%	0.543%
14	6.929	1774	1790	1805	rBV	31205	62086	7.09%	1.242%
15	7.051	1813	1828	1842	rBV	56412	112606	12.86%	2.252%
16	7.565	1965	1988	2022	rBV	485887	875509	100.00%	17.512%
17	7.713	2022	2034	2047	rVB2	20998	40005	4.57%	0.800%
18	7.919	2085	2098	2112	rBV	52898	94229	10.76%	1.885%
19	8.048	2126	2138	2147	rVB5	5677	9634	1.10%	0.193%
20	8.491	2258	2276	2289	rBV3	11051	22092	2.52%	0.442%
21	8.848	2377	2387	2398	rBV5	6263	10535	1.20%	0.211%
22	9.089	2450	2462	2488	rBV	365079	615692	70.32%	12.315%
23	9.385	2538	2554	2567	rVB6	11993	30357	3.47%	0.607%
24	9.739	2645	2664	2677	rBV6	8594	25406	2.90%	0.508%
25	10.308	2827	2841	2856	rBV	323232	519420	59.33%	10.390%
26	10.494	2891	2899	2909	rVB6	7519	11964	1.37%	0.239%
27	11.292	3135	3147	3156	rBV3	6768	12000	1.37%	0.240%
28	11.485	3194	3207	3228	rBV	385718	606408	69.26%	12.130%
29	12.295	3450	3459	3469	rVB5	11597	19580	2.24%	0.392%
30	12.539	3528	3535	3549	rVB3	8056	12273	1.40%	0.245%
31	13.578	3842	3858	3863	rVV5	8455	23900	2.73%	0.478%
32	13.610	3863	3868	3881	rVB2	9813	16180	1.85%	0.324%
33	14.018	3986	3995	4004	rBV4	5521	9949	1.14%	0.199%
34	14.549	4150	4160	4171	rVB7	6096	10996	1.26%	0.220%

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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	14.883	4253	4264	4272	rBV	12871	22301	2.55%	0.446%
36	14.932	4272	4279	4287	rVB5	5878	9608	1.10%	0.192%
37	15.067	4310	4321	4335	rBV5	16306	36987	4.22%	0.740%
38	15.922	4576	4587	4597	rBV4	8803	17177	1.96%	0.344%
39	16.063	4621	4631	4638	rBV2	11791	19397	2.22%	0.388%
40	16.102	4638	4643	4651	rVB5	6878	9626	1.10%	0.193%

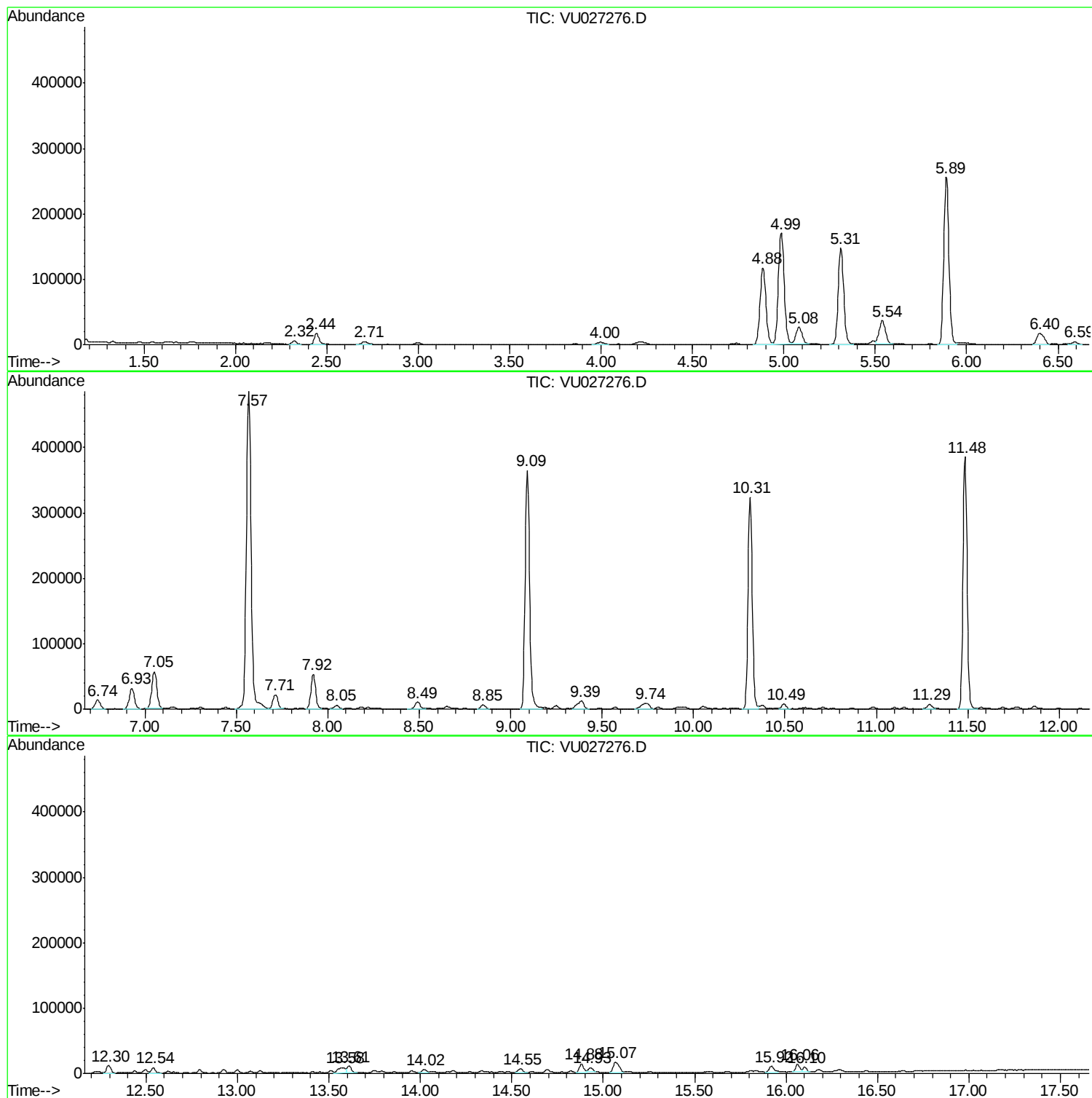
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ClientSampled :
S13-0250

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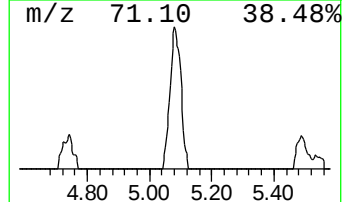
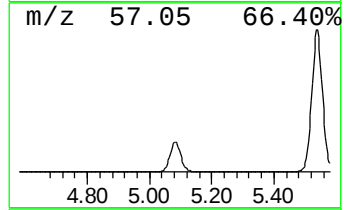
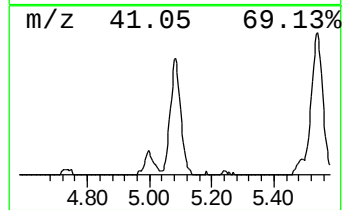
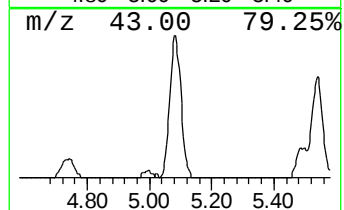
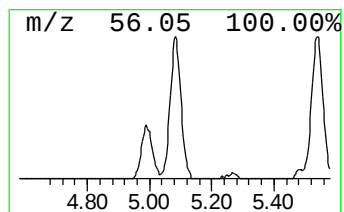
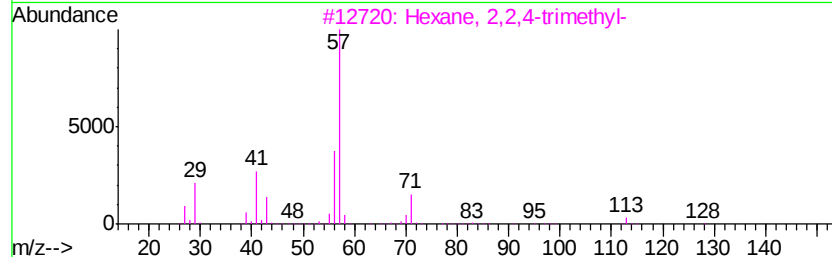
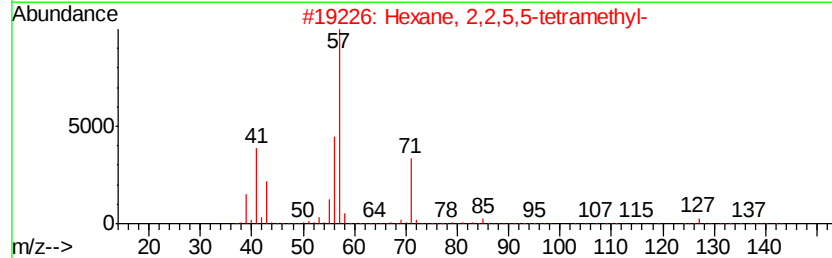
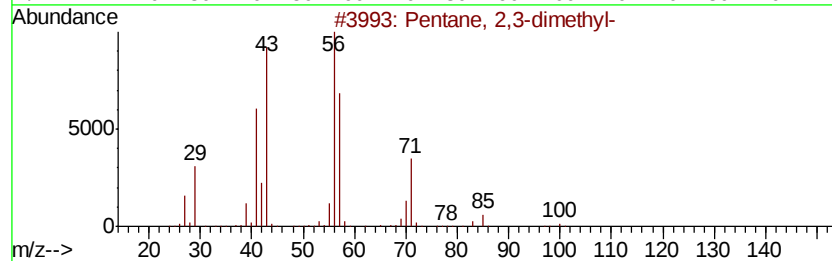
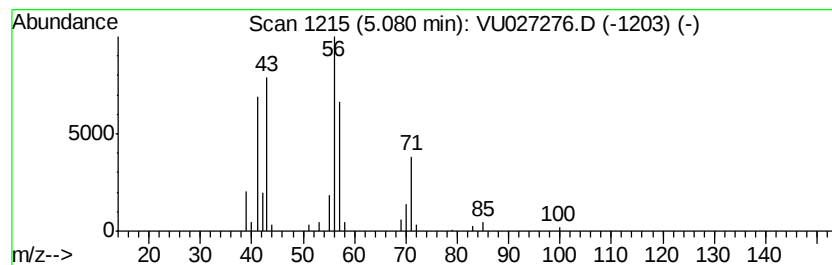
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	8.17 ug/l	61827	Pentafluorobenzene	4.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2		Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
3		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40
5		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	40



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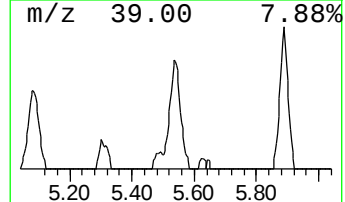
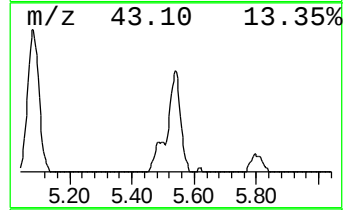
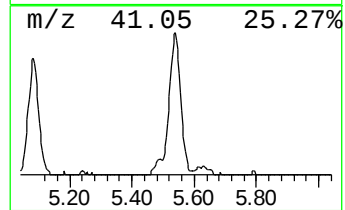
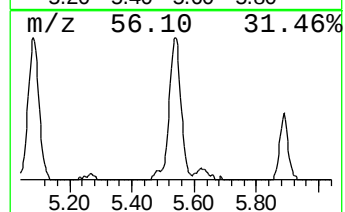
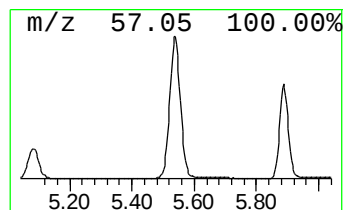
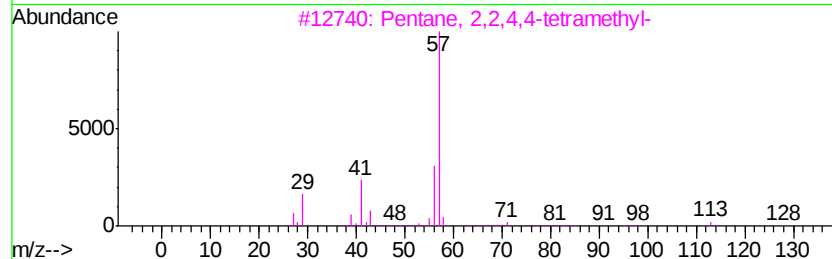
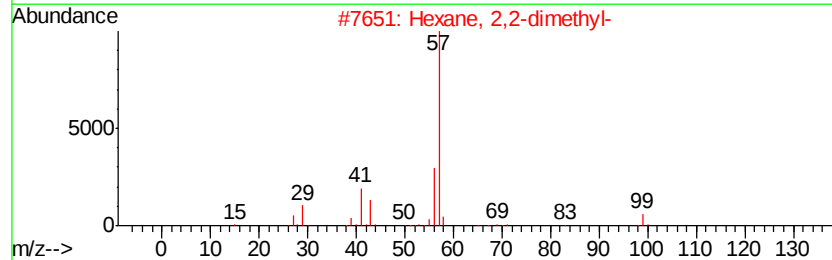
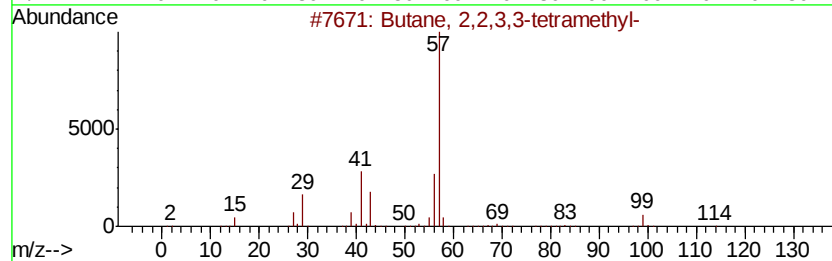
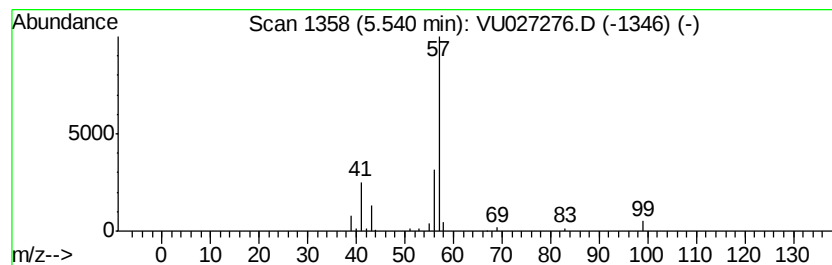
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	8.68 ug/l	87034	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
4		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	56
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



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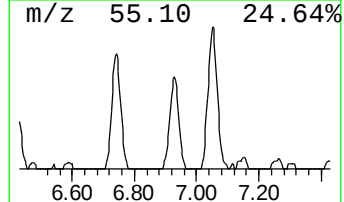
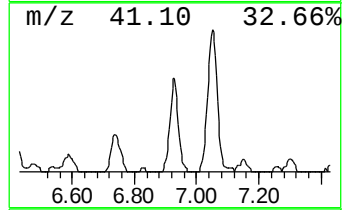
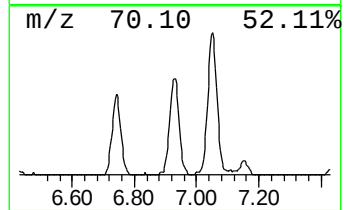
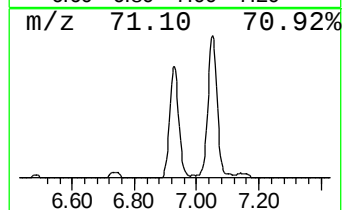
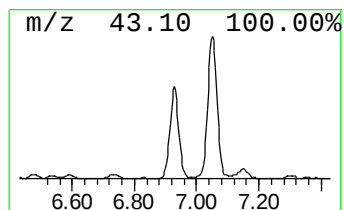
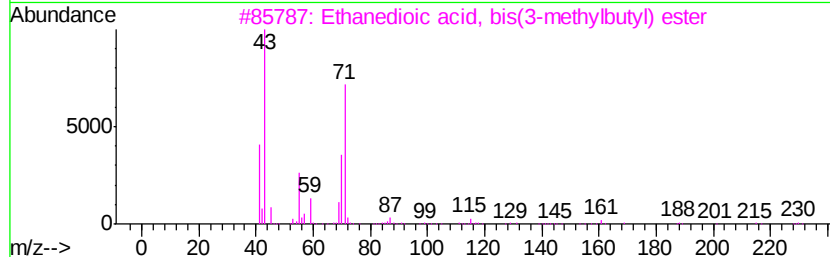
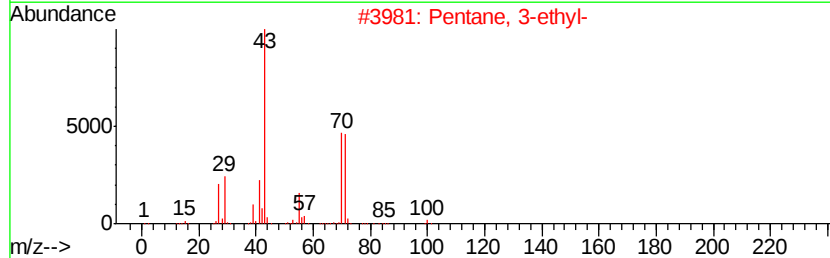
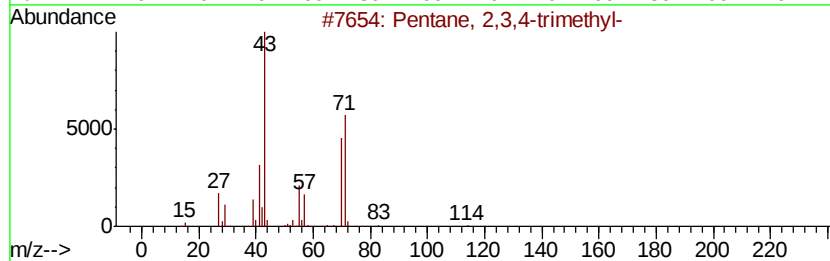
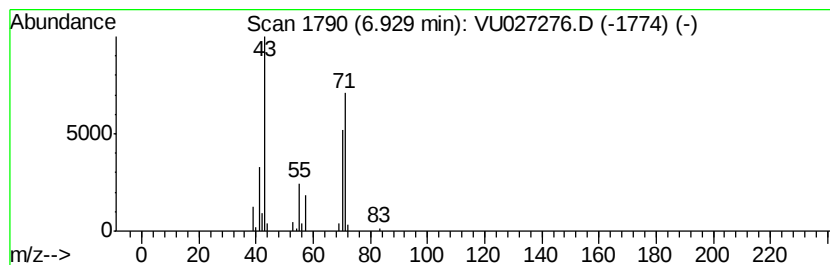
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	6.19 ug/l	62086	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
3		Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	59
4		Pentane, 2-nitro-	117	C5H11NO2	004609-89-6	50
5		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50



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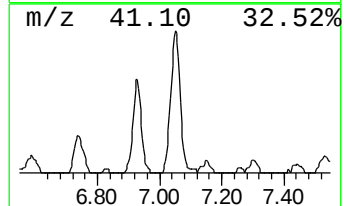
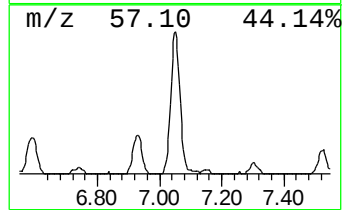
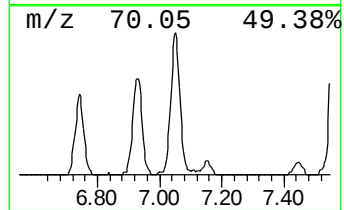
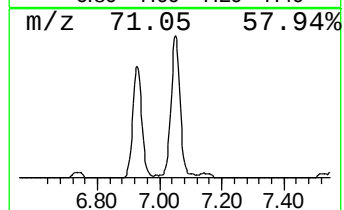
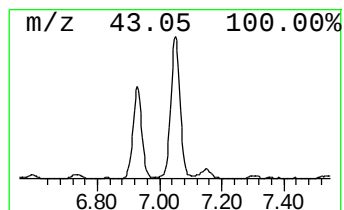
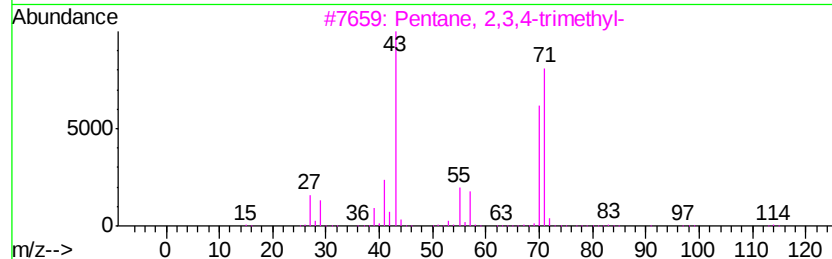
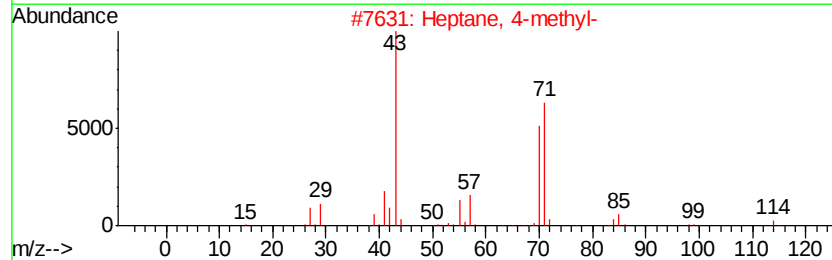
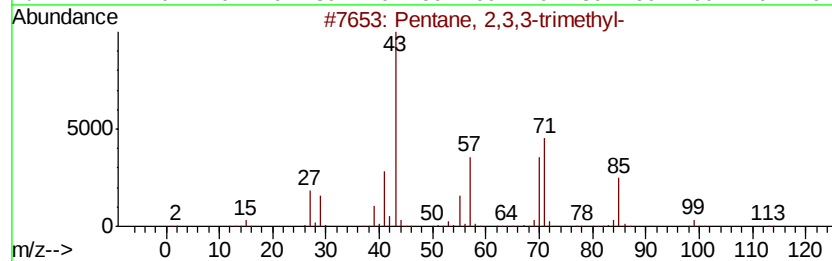
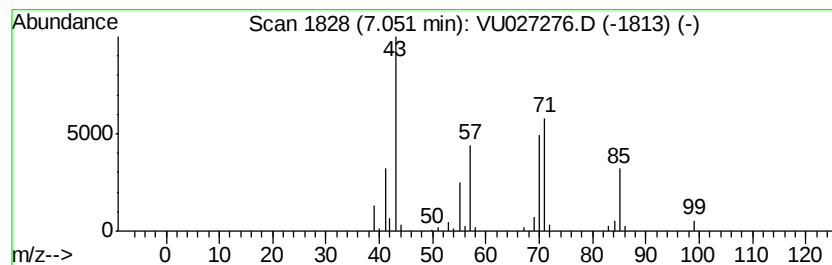
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	11.23 ug/l	112606	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		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4		Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	53
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	45



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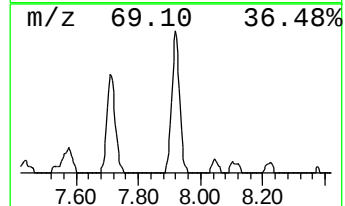
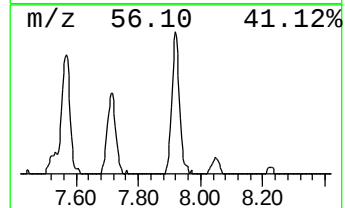
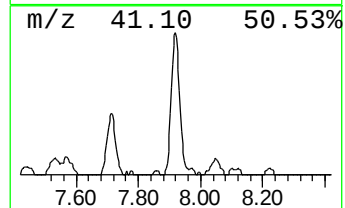
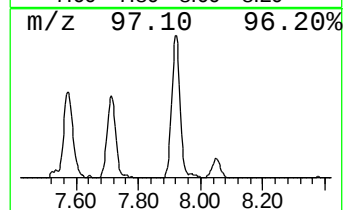
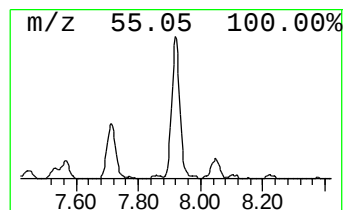
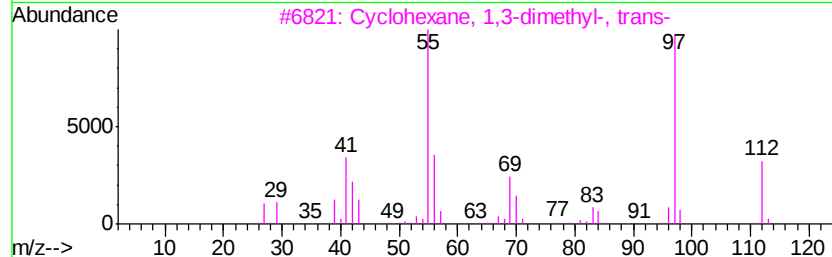
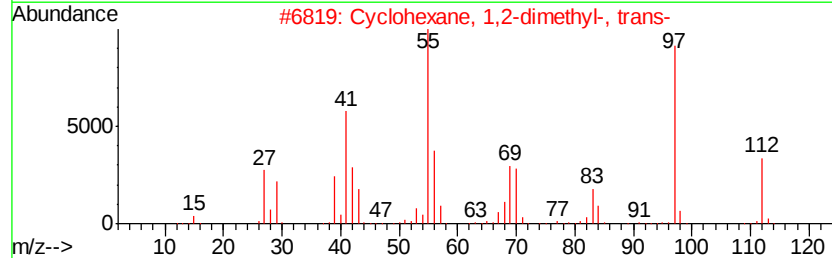
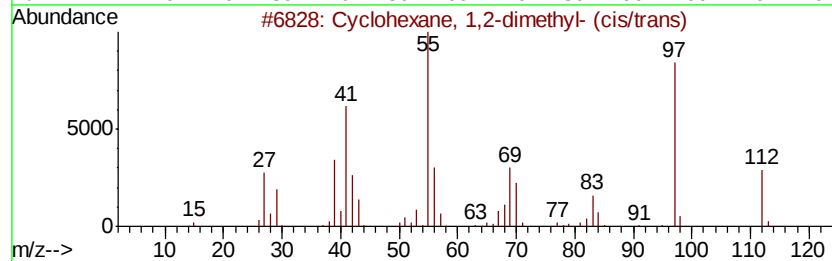
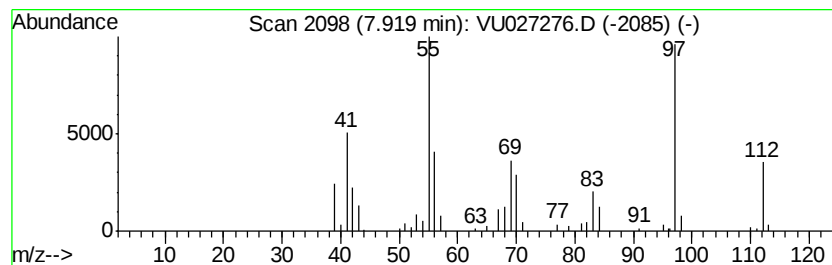
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexane, 1,2-dimethyl- ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.92	7.65 ug/l	94229	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	97
2		Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	97
3		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	87
4		Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	72
5		Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027276.D
Acq On : 28 Sep 2018 17:01
Operator : MD/SY
Sample : J5041-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
S13-0250

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
Pentane, 2,3-dime...	5.08	8.2	ug/l	61827	1	4.99	378530	50.0
Butane, 2,2,3,3-t...	5.54	8.7	ug/l	87034	2	5.89	501471	50.0
Pentane, 2,3,4-tr...	6.93	6.2	ug/l	62086	2	5.89	501471	50.0
Pentane, 2,3,3-tr...	7.05	11.2	ug/l	112606	2	5.89	501471	50.0
Cyclohexane, 1,2-...	7.92	7.7	ug/l	94229	3	9.09	615692	50.0