

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN062520\
 Data File : VN062112.D
 Acq On : 25 Jun 2020 15:41
 Operator : JC/MD
 Sample : L3071-04 100X
 Misc : 10.62g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SB-B

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_N\METHODS\82N062420W.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	2.420	192	201	211	rVB	12962	25937	1.81%	0.289%
2	2.773	301	311	323	rVB3	13185	27047	1.89%	0.302%
3	6.477	1444	1463	1477	rBV8	6248	20382	1.43%	0.227%
4	6.776	1535	1556	1572	rBV2	9887	29853	2.09%	0.333%
5	7.548	1778	1796	1807	rBV	176543	442785	30.97%	4.940%
6	7.625	1808	1820	1836	rVB	294360	710144	49.66%	7.922%
7	7.837	1873	1886	1904	rVB3	18792	44519	3.11%	0.497%
8	7.989	1915	1933	1954	rBV2	189365	445492	31.16%	4.970%
9	8.169	1962	1989	2011	rBV	79680	212598	14.87%	2.372%
10	8.397	2047	2060	2078	rBV6	11496	27061	1.89%	0.302%
11	8.548	2090	2107	2132	rBV	479787	1019833	71.32%	11.377%
12	9.050	2241	2263	2274	rBV7	23043	59956	4.19%	0.669%
13	9.107	2274	2281	2294	rVB3	14609	28231	1.97%	0.315%
14	9.487	2386	2399	2416	rBV3	53666	109141	7.63%	1.218%
15	9.622	2422	2441	2455	rBV2	75910	173890	12.16%	1.940%
16	9.699	2455	2465	2472	rBV5	9728	18106	1.27%	0.202%
17	9.841	2488	2509	2529	rBV7	12749	37882	2.65%	0.423%
18	9.992	2545	2556	2564	rBV3	26806	47576	3.33%	0.531%
19	10.059	2564	2577	2591	rVV	793028	1429918	100.00%	15.952%
20	10.127	2591	2598	2607	rVB	20728	35864	2.51%	0.400%
21	10.255	2632	2638	2650	rVB5	10415	17860	1.25%	0.199%
22	11.381	2973	2988	3005	rBV	730208	1269158	88.76%	14.159%
23	11.484	3010	3020	3032	rVV	49062	87203	6.10%	0.973%
24	11.596	3036	3055	3077	rBV3	62590	133227	9.32%	1.486%
25	12.223	3240	3250	3261	rBV2	26040	42442	2.97%	0.473%
26	12.377	3283	3298	3324	rVB	526297	906809	63.42%	10.116%
27	12.567	3344	3357	3367	rVB2	36491	58997	4.13%	0.658%
28	12.631	3367	3377	3382	rVV	25925	41861	2.93%	0.467%
29	12.664	3382	3387	3393	rVV	27464	42376	2.96%	0.473%
30	12.705	3393	3400	3417	rVB2	35998	61786	4.32%	0.689%
31	12.866	3442	3450	3463	rVB2	14663	21692	1.52%	0.242%
32	13.014	3486	3496	3508	rVB2	64465	104967	7.34%	1.171%
33	13.319	3578	3591	3609	rBV	614030	1063322	74.36%	11.863%
34	13.519	3646	3653	3659	rBV2	17903	25020	1.75%	0.279%

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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

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Peak separation: 5

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Title : SW846 8260

35	13.561	3659	3666	3687	rVB5	20213	47324	3.31%	0.528%
36	13.863	3751	3760	3772	rVB	20256	29567	2.07%	0.330%
37	14.184	3849	3860	3866	rBV2	10788	17709	1.24%	0.198%
38	14.223	3866	3872	3880	rVB3	10026	14497	1.01%	0.162%
39	14.561	3965	3977	3989	rBV9	13663	31635	2.21%	0.353%

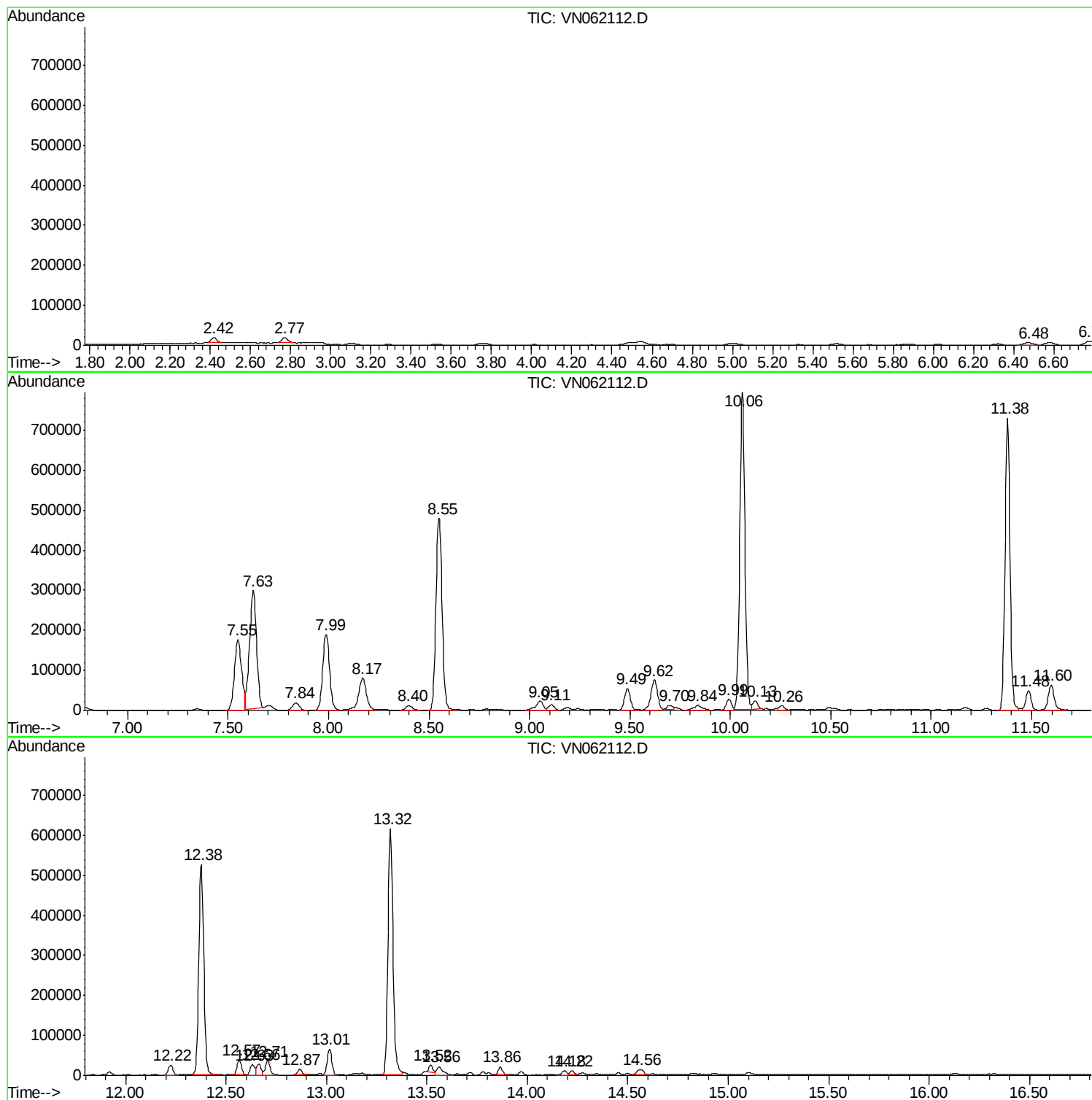
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

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



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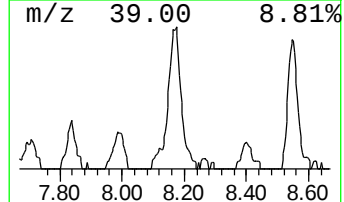
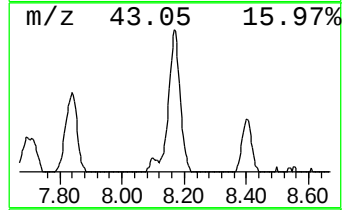
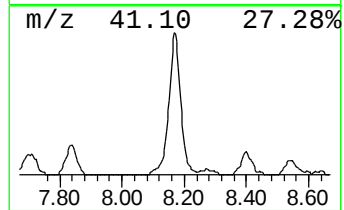
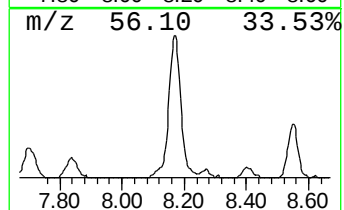
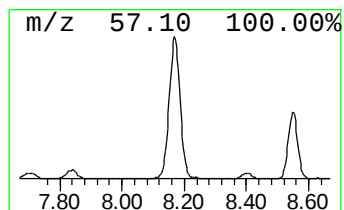
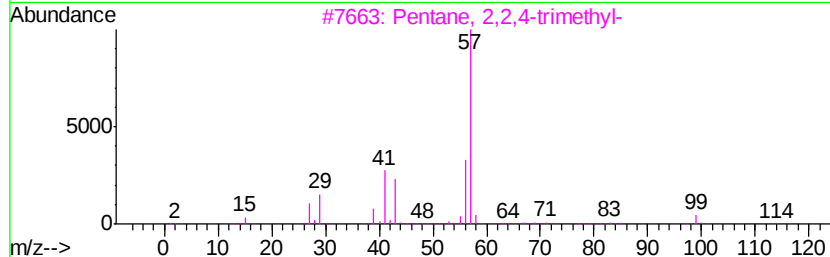
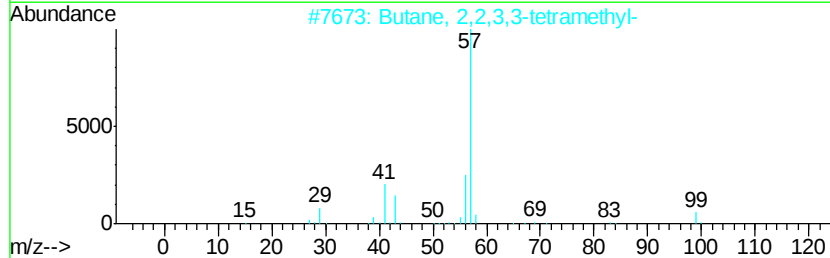
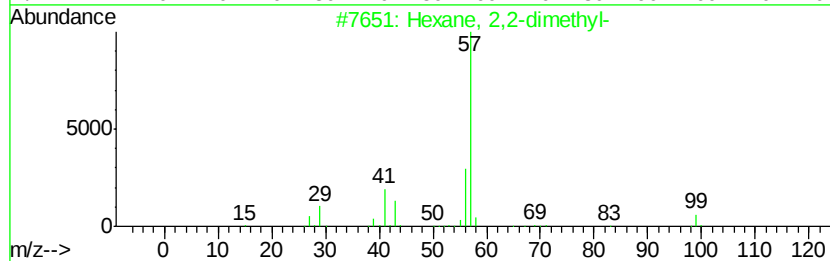
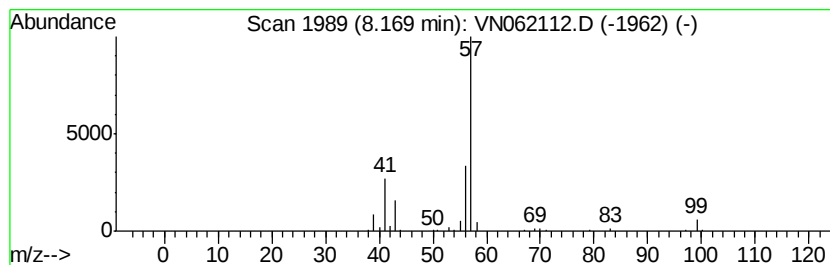
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	10.42 ug/l	212598	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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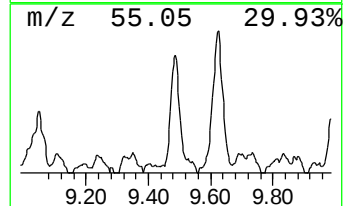
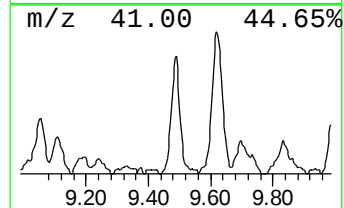
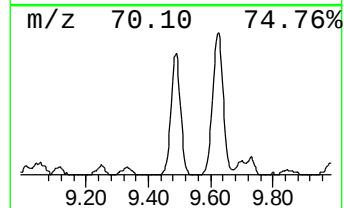
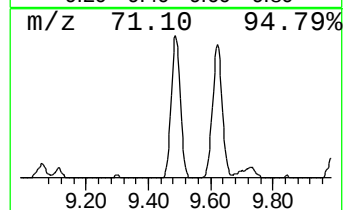
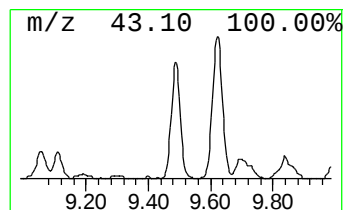
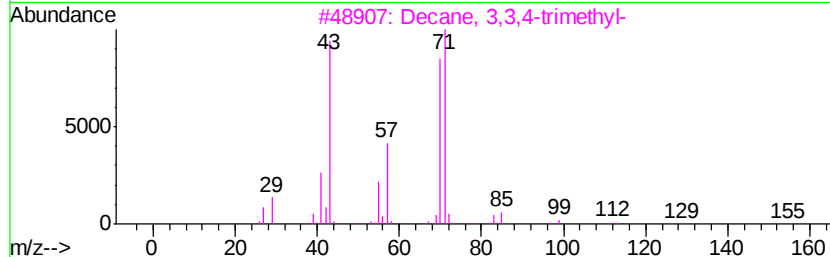
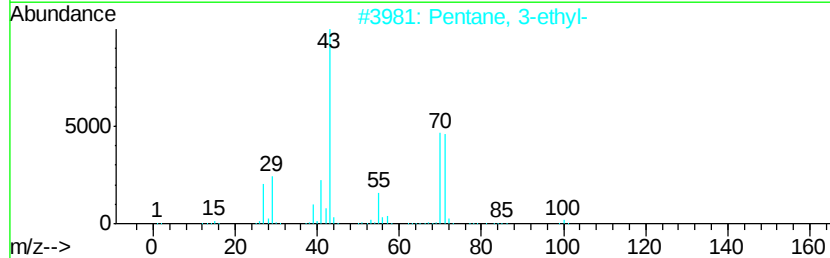
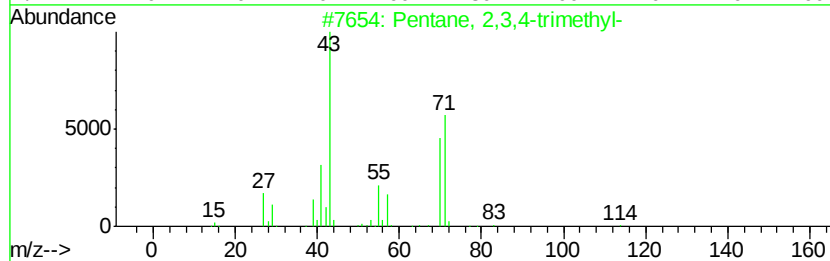
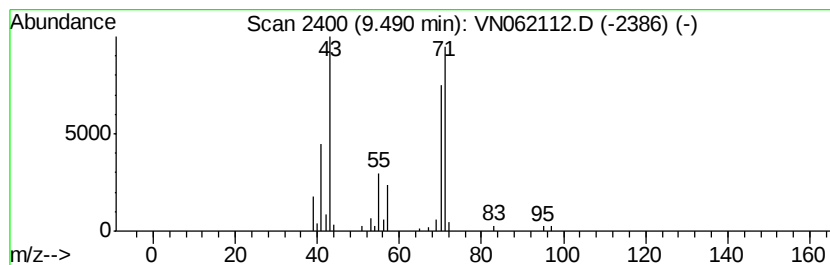
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Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.49	5.35 ug/l	109141	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	74
5		Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	53



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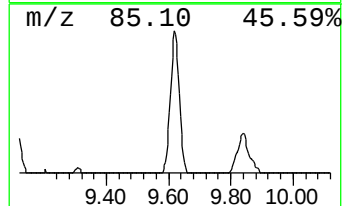
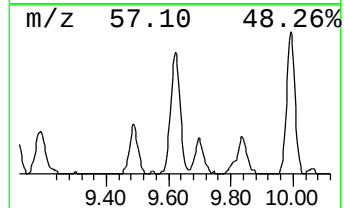
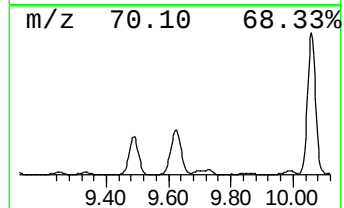
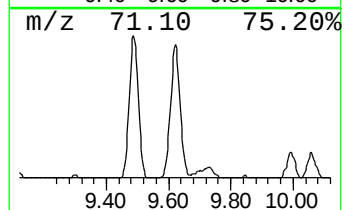
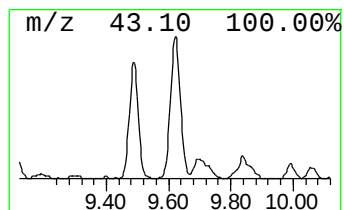
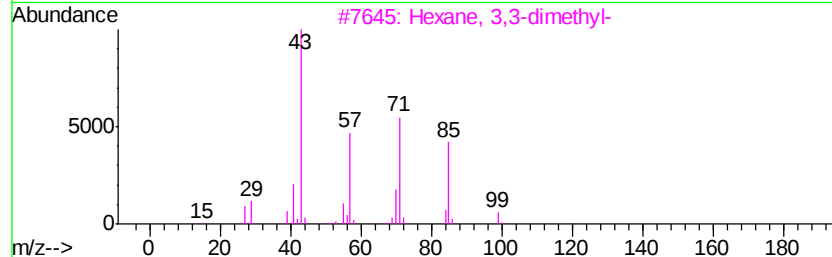
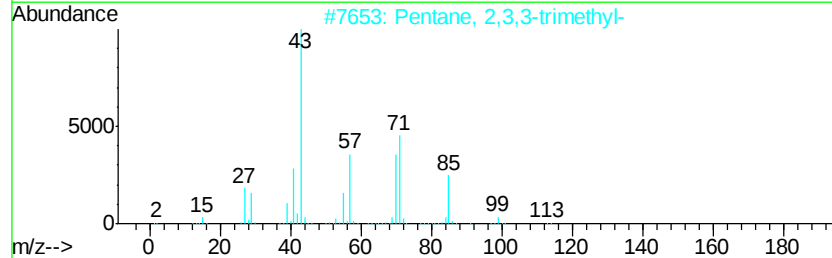
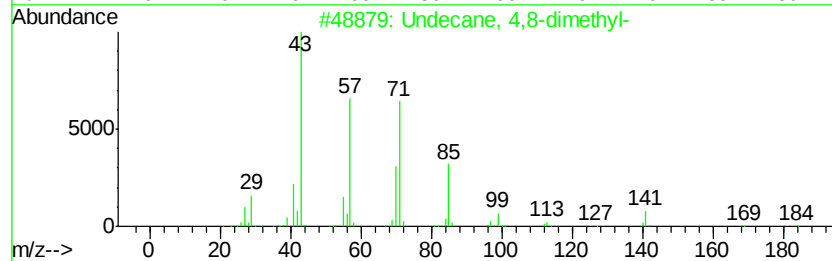
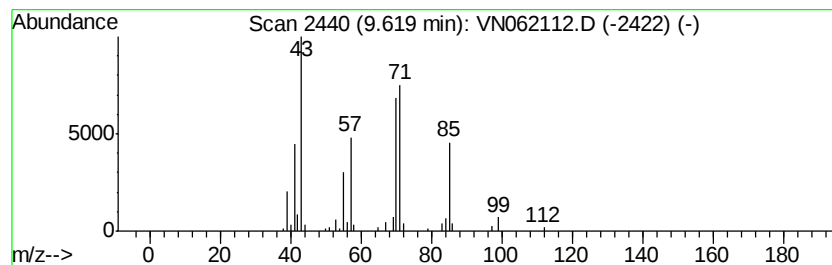
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Quant Title : SW846 8260

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

Peak Number 3 Undecane, 4,8-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	8.53 ug/l	173890	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	72
2		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	72
4		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 2,2-dimet...	8.17	10.4	ug/l	212598	2	8.55	1019830	50.0
Pentane, 2,3,4-tr...	9.49	5.3	ug/l	109141	2	8.55	1019830	50.0
Undecane, 4,8-dim...	9.62	8.5	ug/l	173890	2	8.55	1019830	50.0