

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
 Data File : VN070378.D
 Acq On : 30 Dec 2021 5:27
 Operator : JC/MD
 Sample : M5007-11
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-10RE

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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.446	161	170	193	rVB3	223629	386376	7.68%	1.246%
2	5.624	1328	1355	1384	rBV2	101276	352198	7.00%	1.136%
3	7.048	1864	1886	1902	rBV3	48432	142797	2.84%	0.461%
4	7.327	1971	1990	2016	rBV2	157034	429595	8.54%	1.386%
5	8.021	2226	2249	2261	rBV2	637325	1565173	31.11%	5.048%
6	8.086	2261	2273	2291	rVV	1133905	2614271	51.96%	8.432%
7	8.174	2291	2306	2332	rVB3	292121	750683	14.92%	2.421%
8	8.440	2385	2405	2430	rBV	800933	1846657	36.70%	5.956%
9	8.617	2451	2471	2492	rBV2	410516	1025271	20.38%	3.307%
10	8.968	2583	2602	2637	rBV	1771911	3708699	73.71%	11.962%
11	9.456	2754	2784	2795	rBV10	44486	156646	3.11%	0.505%
12	9.513	2795	2805	2821	rVB5	28556	59537	1.18%	0.192%
13	9.593	2821	2835	2850	rBV2	47344	97061	1.93%	0.313%
14	9.883	2923	2943	2966	rBV	404501	816477	16.23%	2.633%
15	10.014	2972	2992	3010	rBV	626024	1292333	25.69%	4.168%
16	10.196	3045	3060	3074	rBV5	30842	65581	1.30%	0.212%
17	10.371	3097	3125	3135	rBV2	68950	143118	2.84%	0.462%
18	10.443	3135	3152	3186	rVB	2651463	5031361	100.00%	16.228%
19	10.642	3204	3226	3241	rVB4	68493	157240	3.13%	0.507%
20	10.717	3241	3254	3269	rVB3	59316	107324	2.13%	0.346%
21	10.872	3296	3312	3329	rVB3	29875	87046	1.73%	0.281%
22	11.747	3618	3638	3681	rBV	2323722	4261726	84.70%	13.745%
23	12.734	3988	4006	4031	rBV	1746517	3099785	61.61%	9.998%
24	13.675	4341	4357	4379	rBV	1603079	2807790	55.81%	9.056%

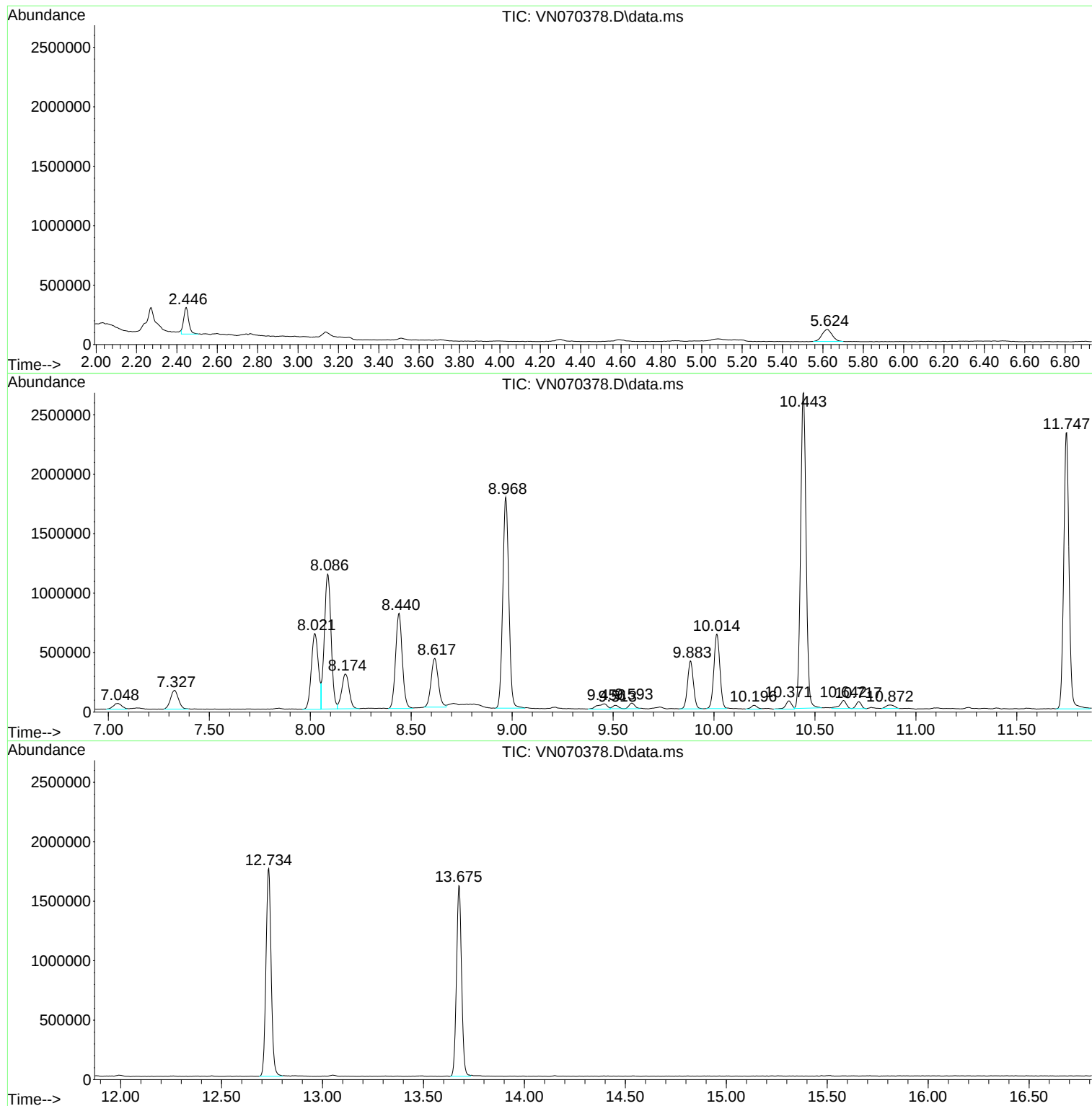
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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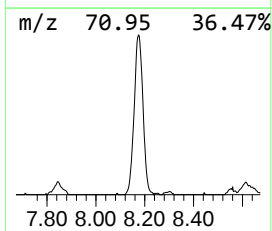
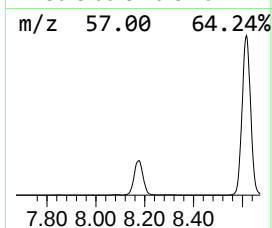
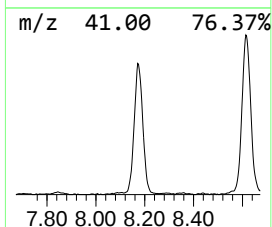
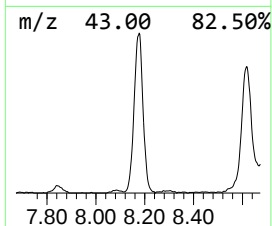
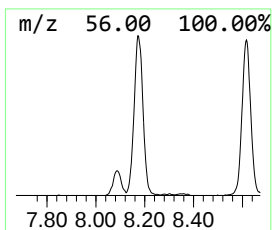
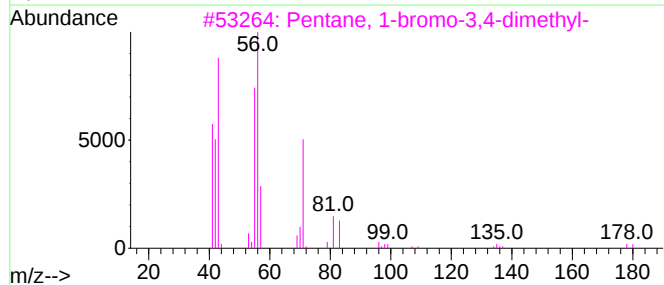
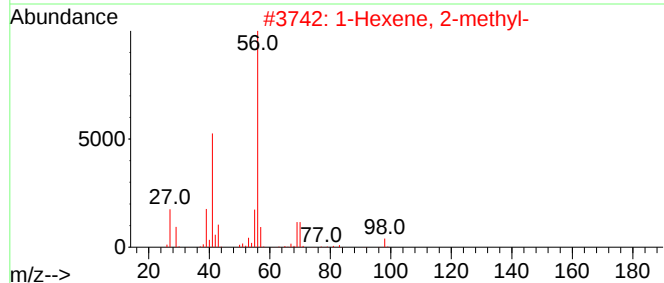
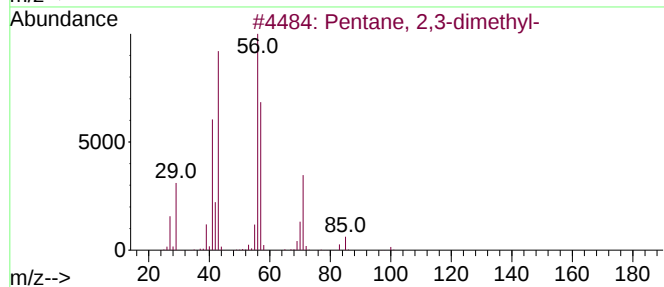
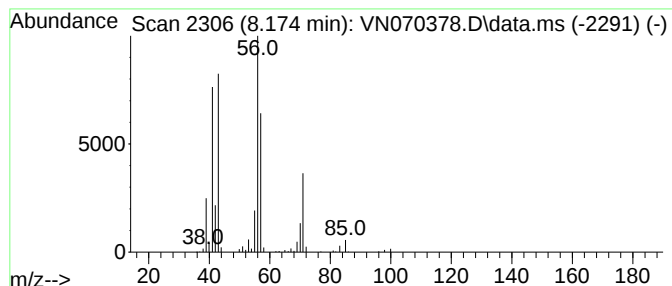
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	14.36 ug/l	750683	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	50
3			Pentane, 1-bromo-3,4-dimethyl-	178	C7H15Br	006570-92-9	42
4			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	40
5			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	38



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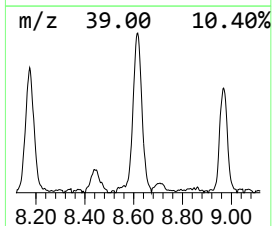
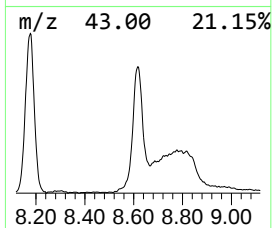
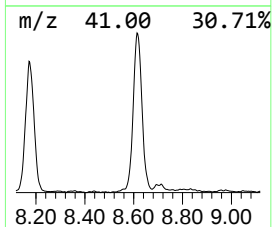
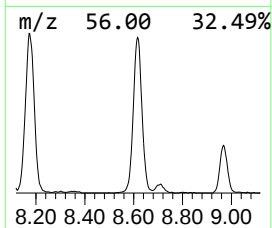
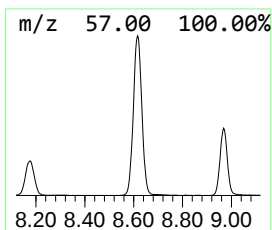
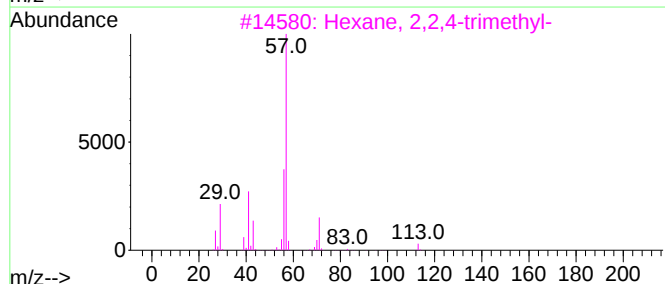
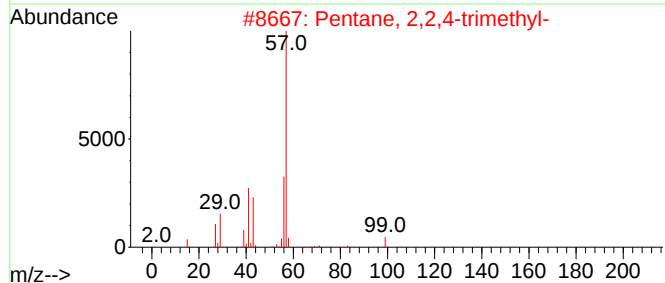
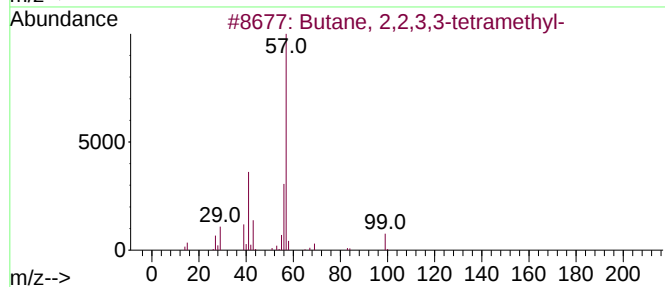
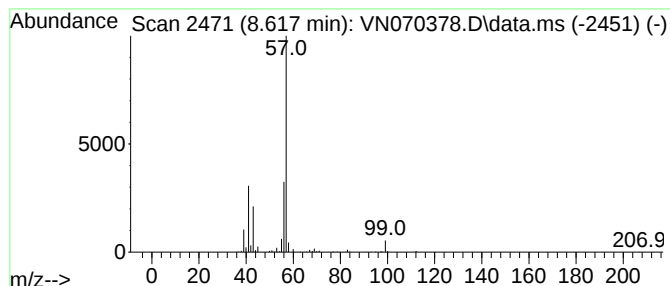
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	13.82 ug/l	1025270	1,4-Difluorobenzene	8.968

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



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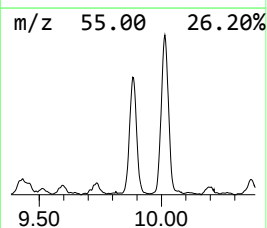
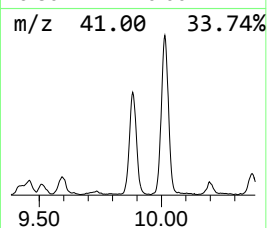
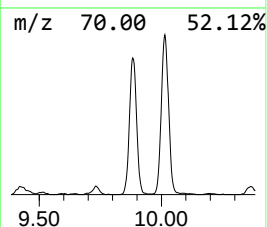
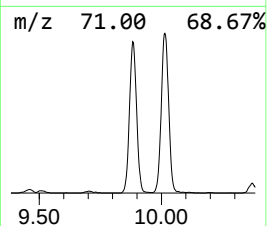
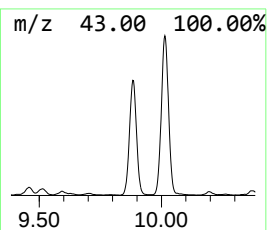
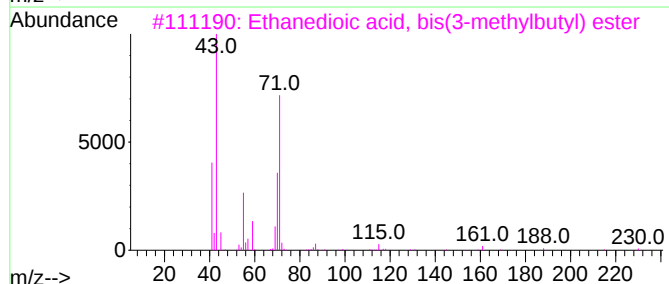
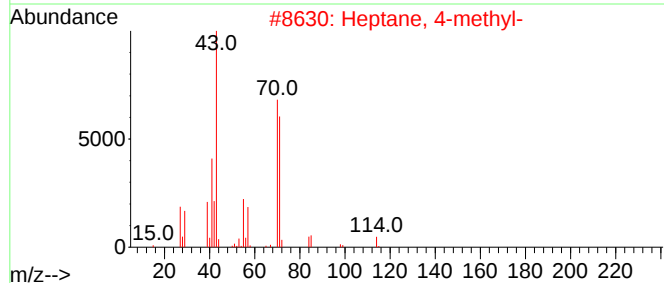
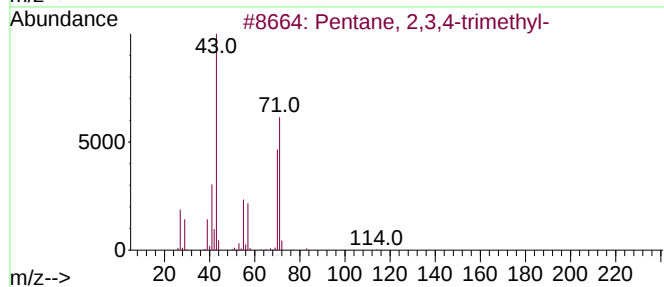
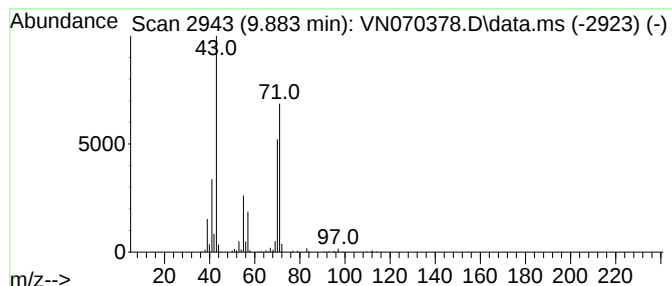
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	11.01 ug/l	816477	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	59
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	59
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56



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ALS Vial : 44 Sample Multiplier: 1

Instrument :
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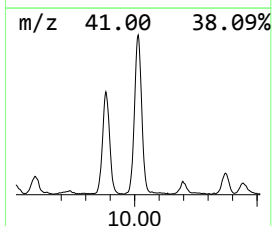
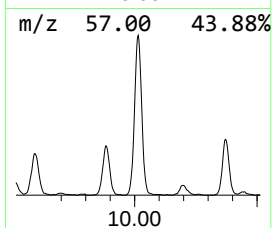
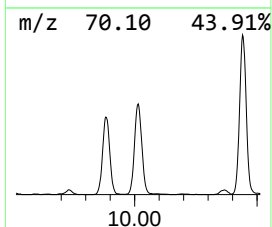
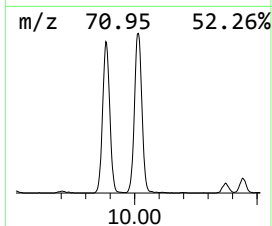
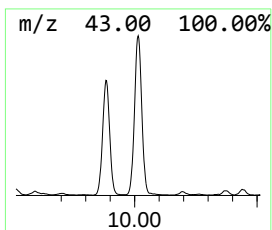
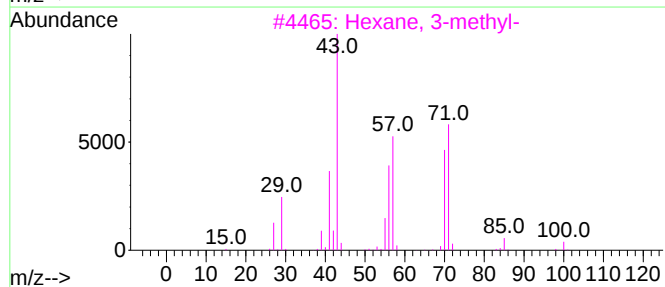
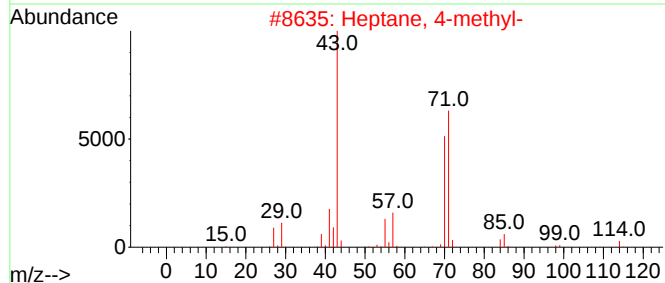
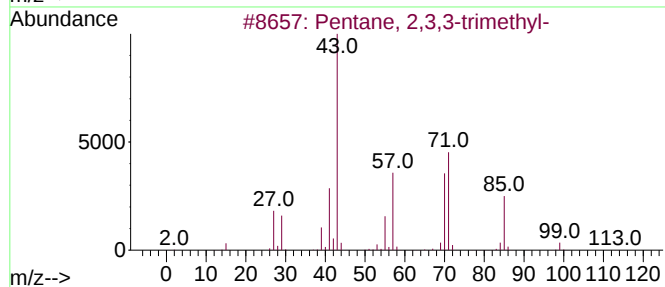
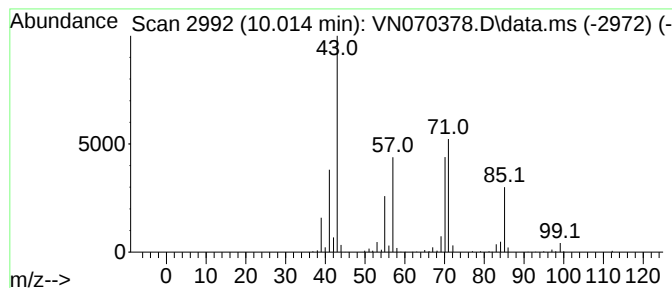
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Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	17.42 ug/l	1292330	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.174	14.4	ug/l	750683	1	8.086	2614270	50.0
Butane, 2,2,3,3...	8.617	13.8	ug/l	1025270	2	8.968	3708700	50.0
Pentane, 2,3,4-...	9.883	11.0	ug/l	816477	2	8.968	3708700	50.0
Pentane, 2,3,3-...	10.014	17.4	ug/l	1292330	2	8.968	3708700	50.0