

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
 Data File : VN072987.D
 Acq On : 21 Jun 2022 16:44
 Operator : JC\MD
 Sample : N3379-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-10

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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN072987.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	55	60	65	rVB	51817	67610	5.09%	0.721%
2	2.404	81	88	94	rBV2	41183	68428	5.15%	0.729%
3	3.081	197	203	213	rVB7	8103	17206	1.29%	0.183%
4	5.539	609	621	634	rBV4	27646	99529	7.49%	1.061%
5	6.963	854	863	873	rBV2	11291	33099	2.49%	0.353%
6	7.251	903	912	924	rVB3	42192	115640	8.70%	1.233%
7	7.951	1021	1031	1036	rBV2	201416	477460	35.91%	5.089%
8	8.016	1036	1042	1050	rVV	383756	893443	67.20%	9.524%
9	8.104	1050	1057	1068	rVB2	73106	181058	13.62%	1.930%
10	8.369	1093	1102	1115	rBV	205502	478167	35.97%	5.097%
11	8.545	1123	1132	1141	rBV	107967	260015	19.56%	2.772%
12	8.904	1183	1193	1211	rVB	517238	1107882	83.33%	11.809%
13	9.363	1263	1271	1273	rBV5	9563	19539	1.47%	0.208%
14	9.392	1273	1276	1281	rVV2	10466	19149	1.44%	0.204%
15	9.451	1281	1286	1291	rVV3	8098	15468	1.16%	0.165%
16	9.522	1293	1298	1307	rVB2	13003	26861	2.02%	0.286%
17	9.816	1340	1348	1359	rVB	113727	230110	17.31%	2.453%
18	9.945	1359	1370	1379	rBV	181366	376594	28.33%	4.014%
19	10.133	1395	1402	1411	rBV4	8414	19411	1.46%	0.207%
20	10.304	1424	1431	1436	rBV2	19939	36361	2.73%	0.388%
21	10.374	1436	1443	1460	rVB	715149	1329498	100.00%	14.172%
22	10.574	1468	1477	1483	rVB5	19890	46812	3.52%	0.499%
23	10.651	1485	1490	1496	rVB3	17795	30331	2.28%	0.323%
24	10.804	1512	1516	1526	rVB10	12599	35110	2.64%	0.374%
25	11.680	1657	1665	1676	rBV	730381	1282112	96.44%	13.666%
26	12.668	1824	1833	1844	rBV	572175	968348	72.84%	10.322%
27	13.610	1985	1993	2001	rBV	697590	1146199	86.21%	12.218%

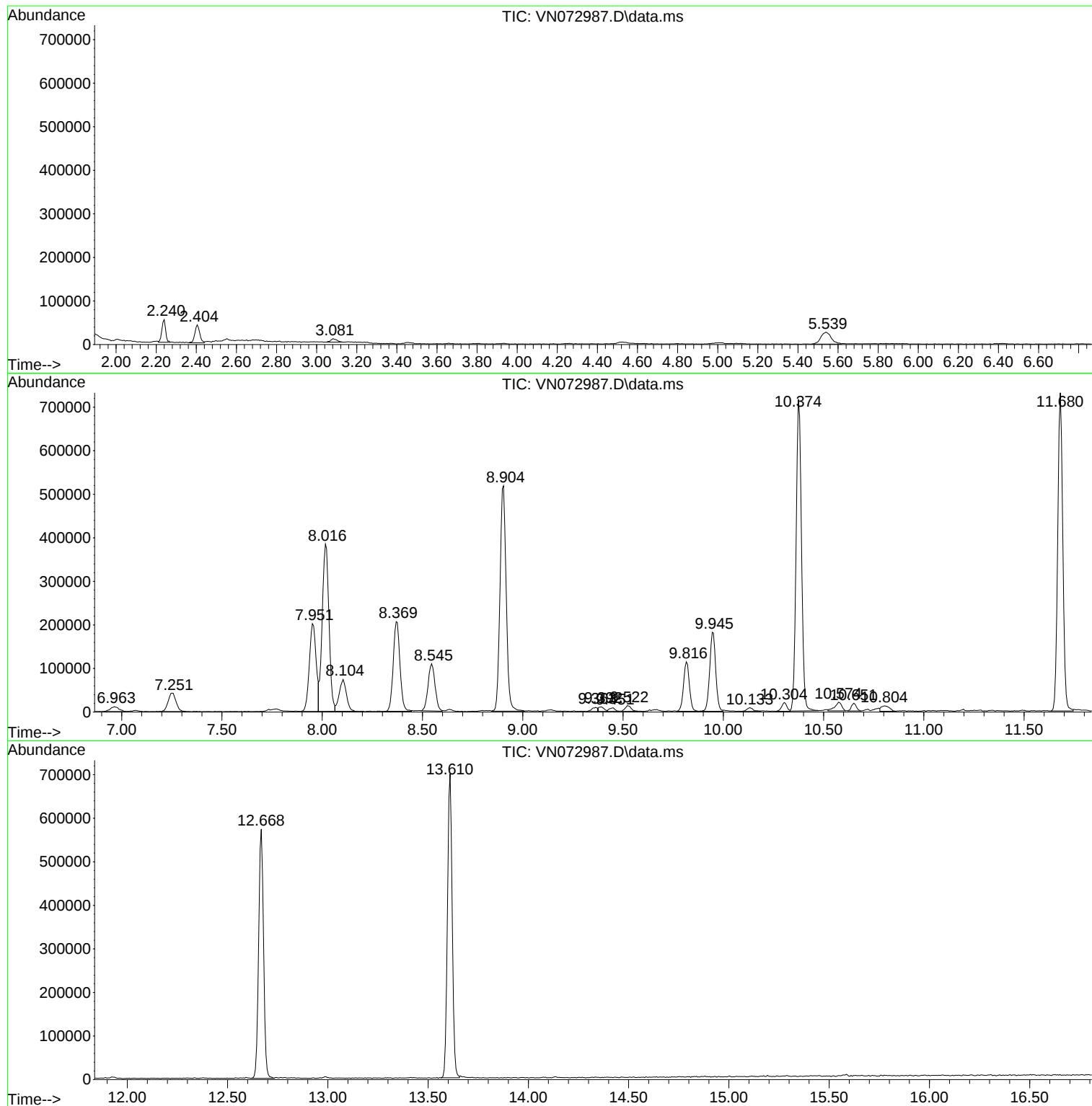
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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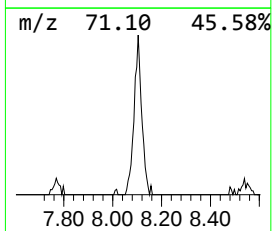
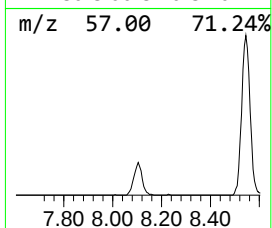
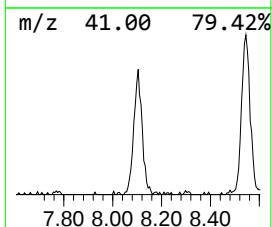
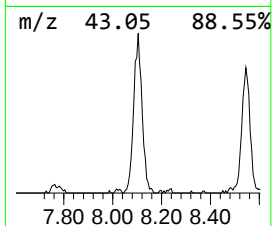
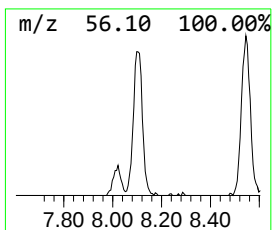
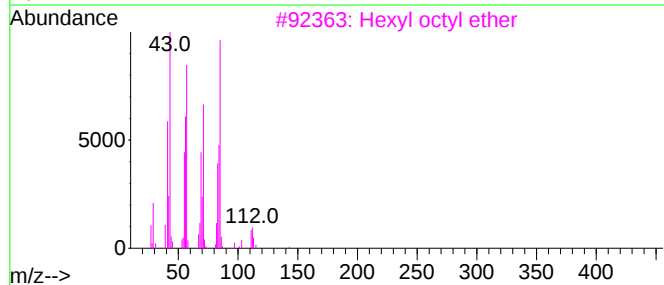
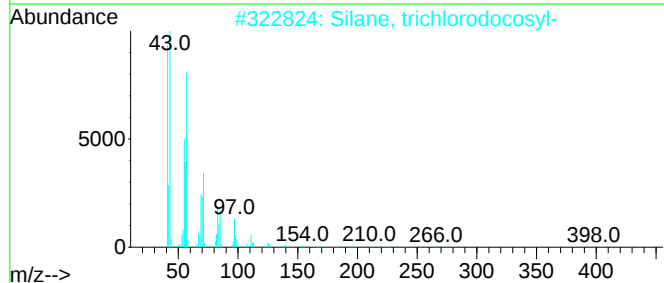
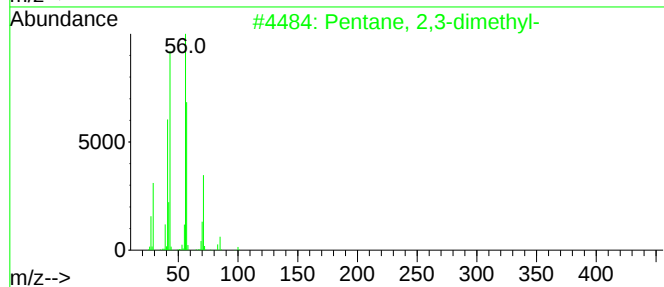
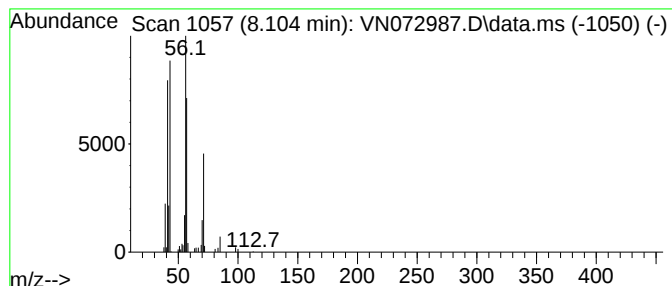
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	10.13 ug/l	181058	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	47
3			Hexyl octyl ether	214	C14H30O	017071-54-4	43
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
5			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	42



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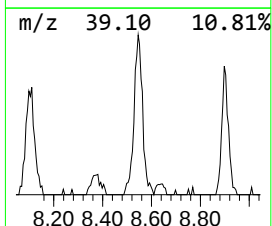
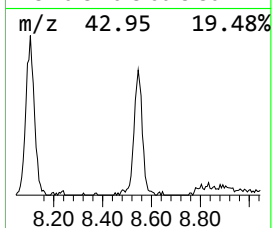
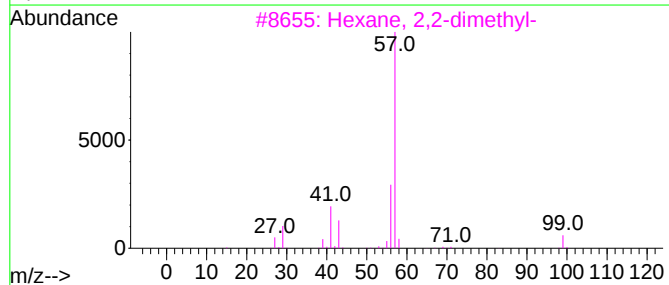
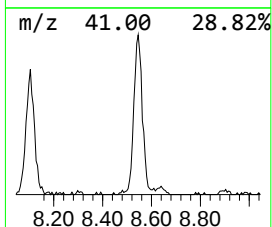
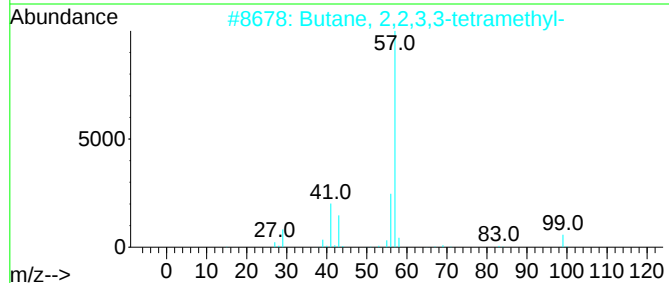
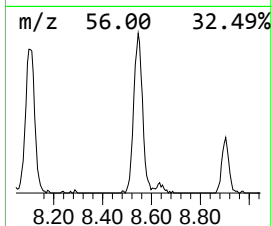
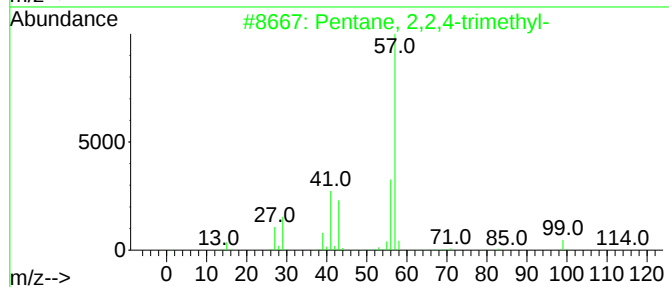
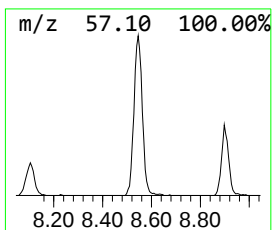
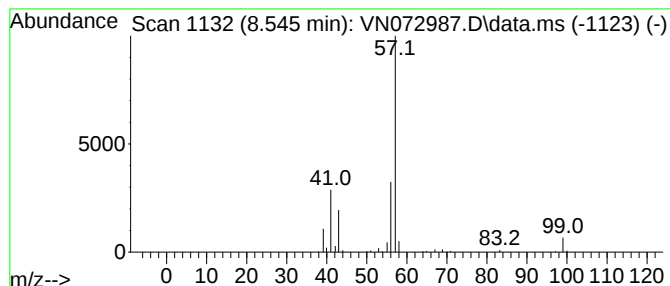
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	11.73 ug/l	260015	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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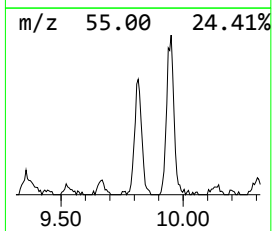
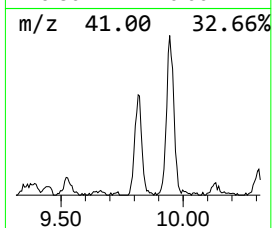
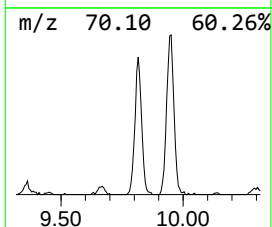
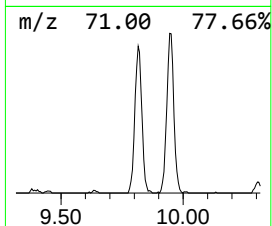
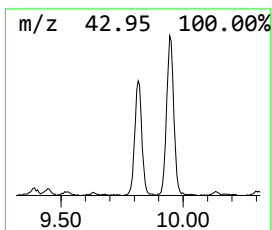
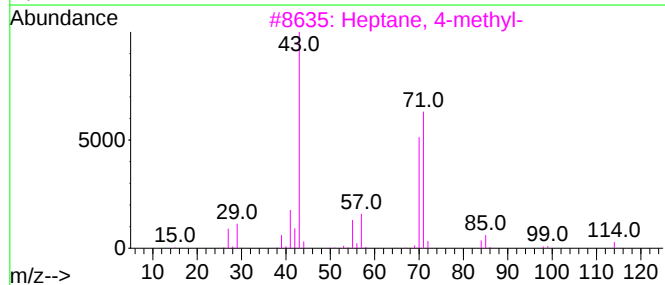
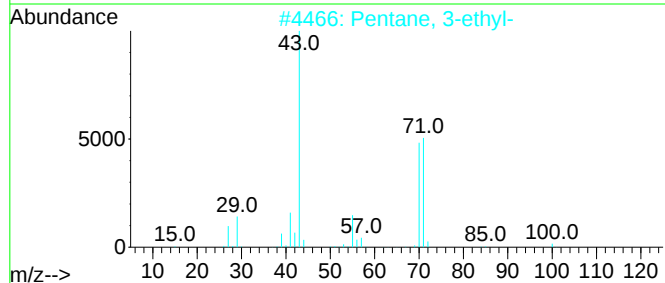
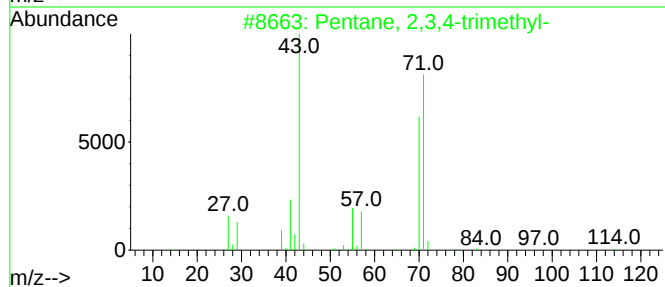
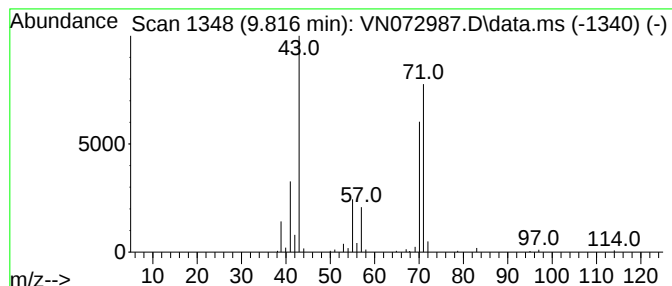
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	10.39 ug/l	230110	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74
5			Diisooamyl ether	158	C10H22O	000544-01-4	64



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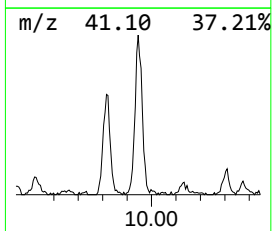
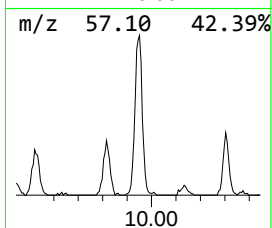
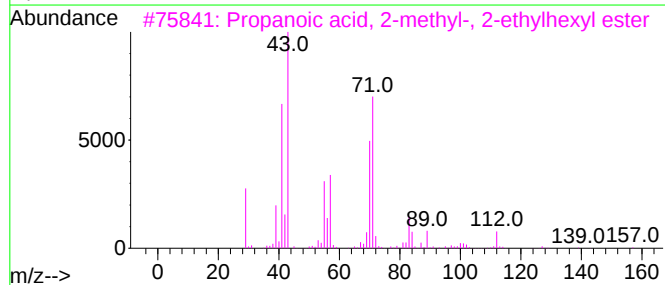
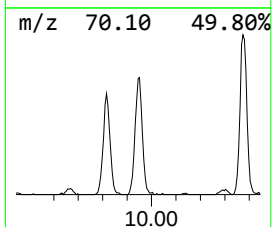
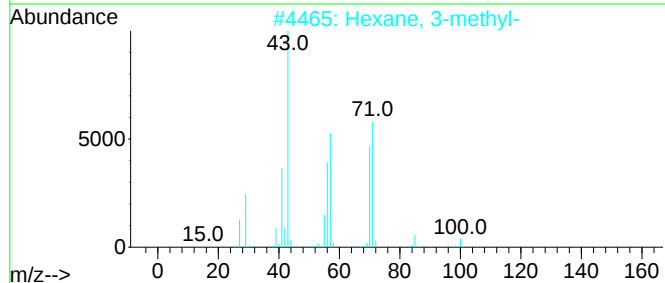
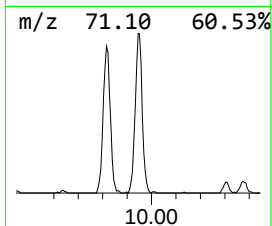
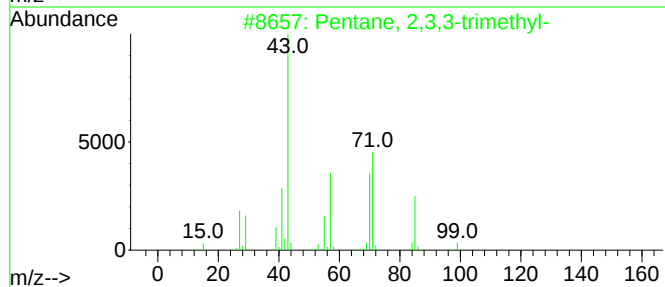
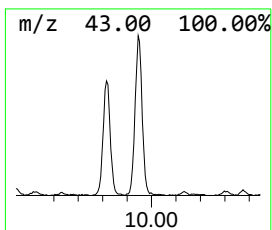
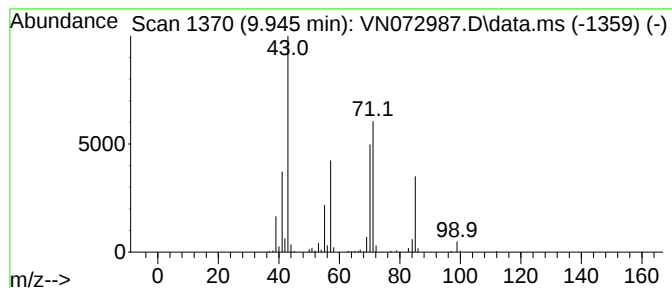
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	17.00 ug/l	376594	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	64
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59



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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...	8.104	10.1	ug/l	181058	1	8.022	893443	50.0
Pentane, 2,2,4-...	8.545	11.7	ug/l	260015	2	8.904	1107880	50.0
Pentane, 2,3,4-...	9.816	10.4	ug/l	230110	2	8.904	1107880	50.0
Pentane, 2,3,3-...	9.945	17.0	ug/l	376594	2	8.904	1107880	50.0