

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
 Data File : VN072985.D
 Acq On : 21 Jun 2022 15:55
 Operator : JC\MD
 Sample : N3379-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-04

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: VN072985.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	69	rVB	50526	70139	5.08%	0.696%
2	2.405	82	88	95	rBV2	41569	73644	5.33%	0.731%
3	3.087	199	204	211	rVB6	8007	16229	1.17%	0.161%
4	5.540	610	621	632	rBV4	26172	93773	6.79%	0.931%
5	6.969	854	864	874	rVB5	12736	40117	2.90%	0.398%
6	7.251	901	912	921	rBV	42512	113568	8.22%	1.127%
7	7.951	1020	1031	1036	rBV2	210774	493733	35.74%	4.900%
8	8.016	1036	1042	1051	rVV	405801	919473	66.56%	9.126%
9	8.104	1051	1057	1067	rVB2	74585	185984	13.46%	1.846%
10	8.369	1092	1102	1113	rBV	221541	509918	36.91%	5.061%
11	8.545	1122	1132	1143	rVB	123518	300264	21.74%	2.980%
12	8.898	1184	1192	1205	rBV	541694	1142139	82.68%	11.335%
13	9.392	1270	1276	1280	rVV7	11096	28336	2.05%	0.281%
14	9.445	1280	1285	1290	rVB5	9399	16599	1.20%	0.165%
15	9.528	1290	1299	1305	rBV2	14419	30862	2.23%	0.306%
16	9.816	1338	1348	1359	rVB	129947	255585	18.50%	2.537%
17	9.945	1359	1370	1381	rBV	194797	406231	29.41%	4.032%
18	10.133	1396	1402	1410	rBV4	9639	20701	1.50%	0.205%
19	10.304	1422	1431	1436	rBV3	22924	44262	3.20%	0.439%
20	10.375	1436	1443	1459	rVB	735172	1375503	99.57%	13.651%
21	10.580	1468	1478	1484	rVB4	19194	46059	3.33%	0.457%
22	10.651	1484	1490	1497	rVB2	17497	30558	2.21%	0.303%
23	10.798	1504	1515	1516	rBV5	10878	22637	1.64%	0.225%
24	11.680	1656	1665	1676	rBV	773159	1381466	100.00%	13.711%
25	12.669	1824	1833	1843	rBV	635086	1079258	78.12%	10.711%
26	13.610	1985	1993	2003	rBV	806193	1378818	99.81%	13.684%

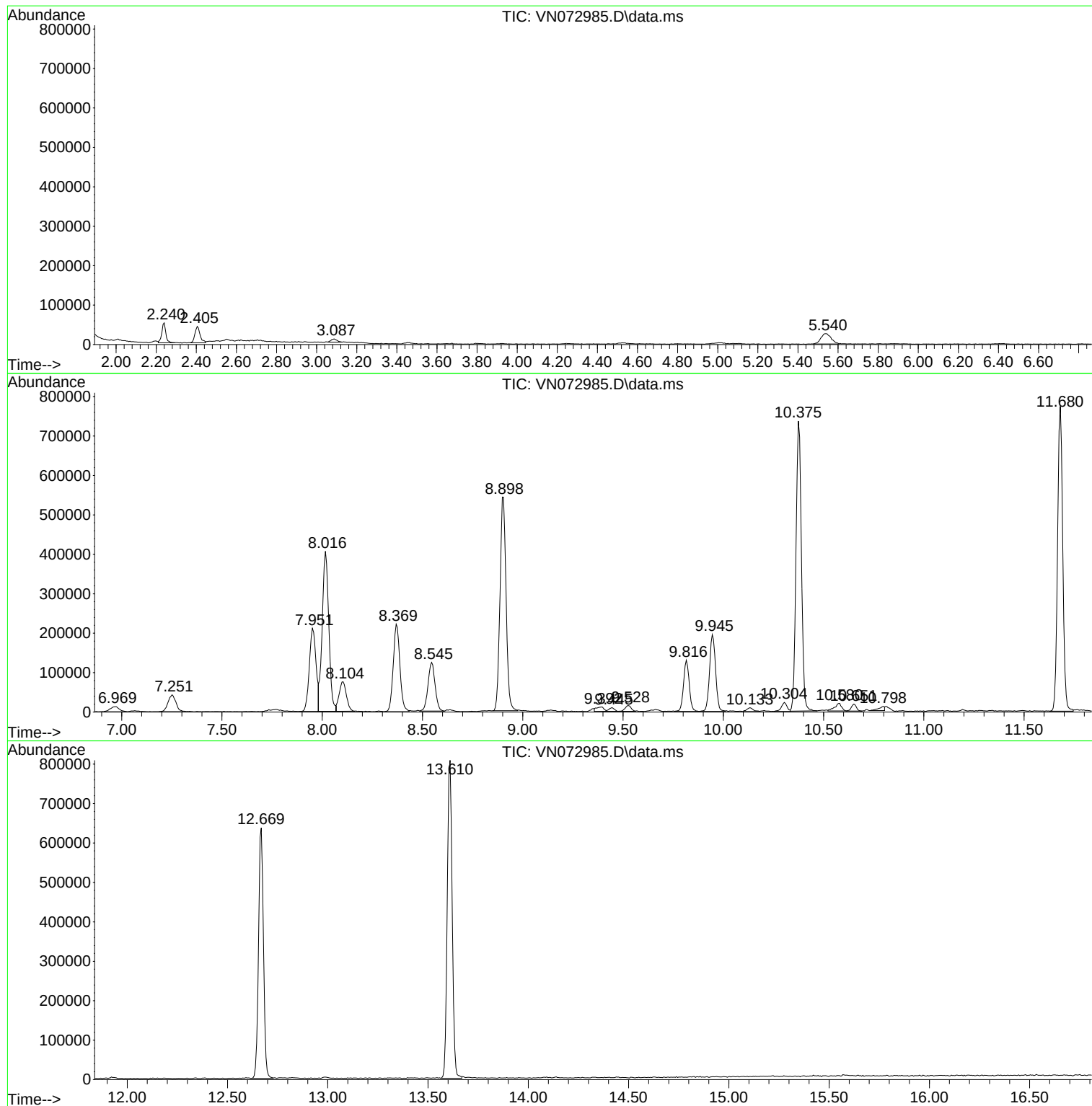
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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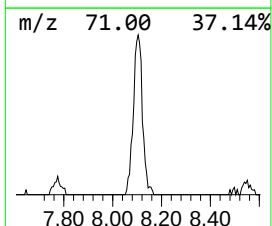
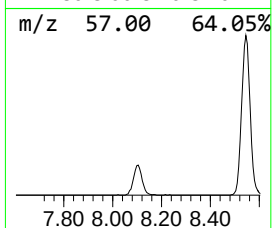
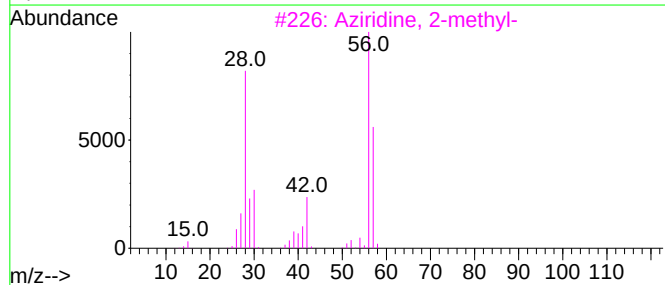
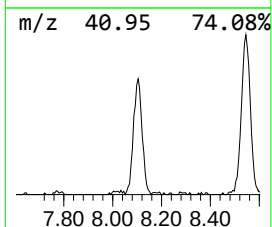
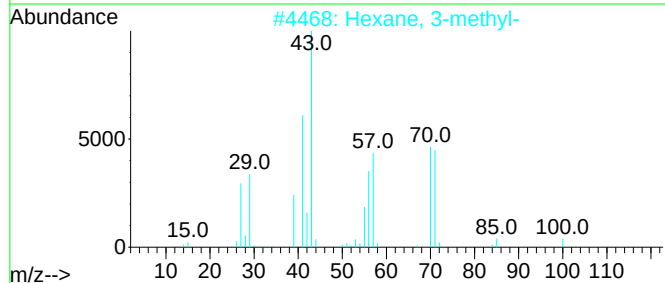
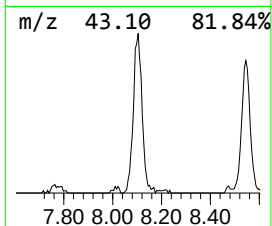
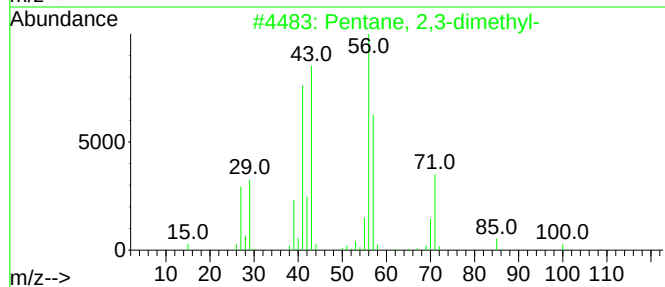
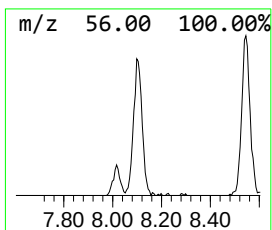
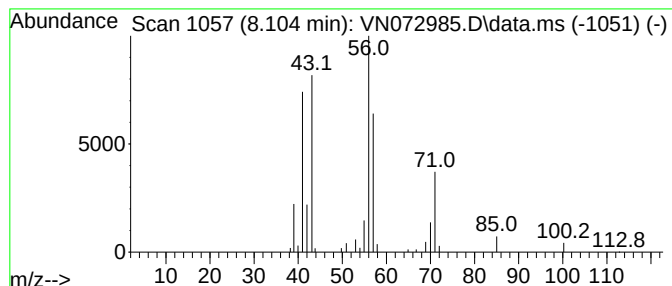
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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	10.11 ug/l	185984	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	40



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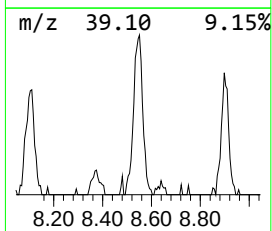
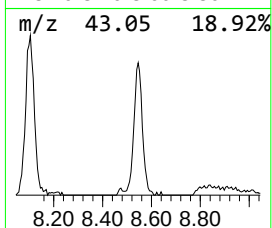
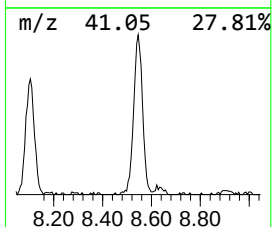
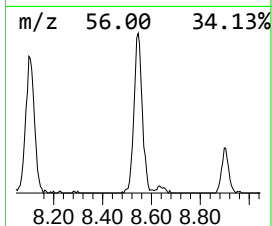
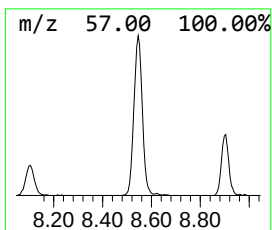
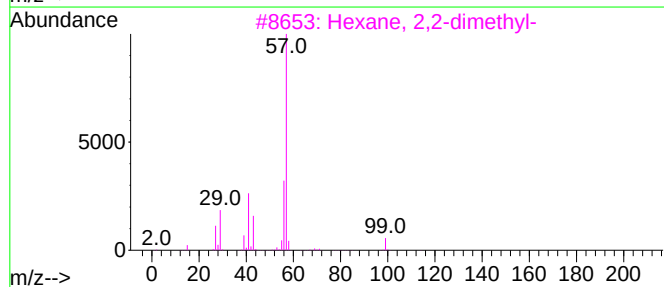
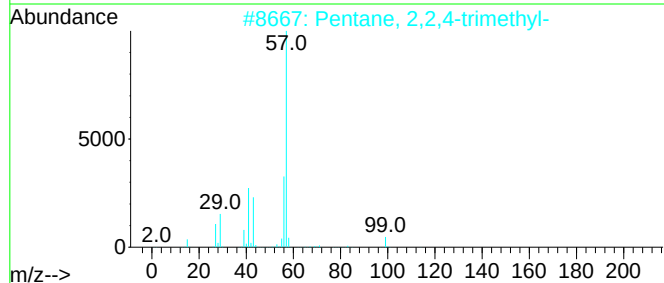
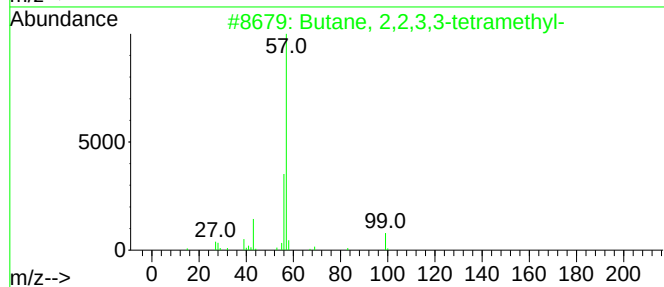
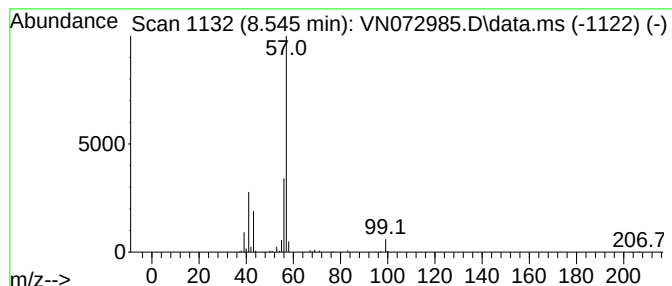
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	13.14 ug/l	300264	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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Instrument :
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ClientSampleId :
TOLL-MW-04

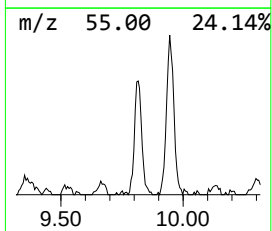
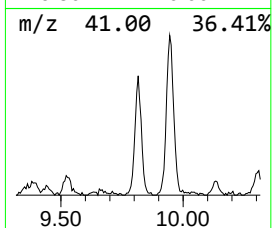
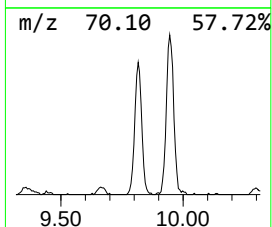
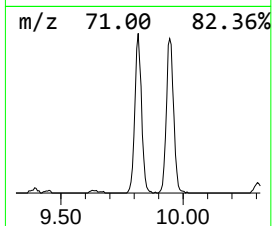
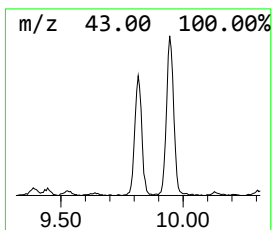
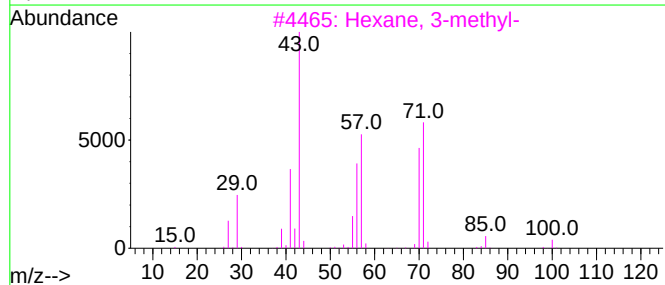
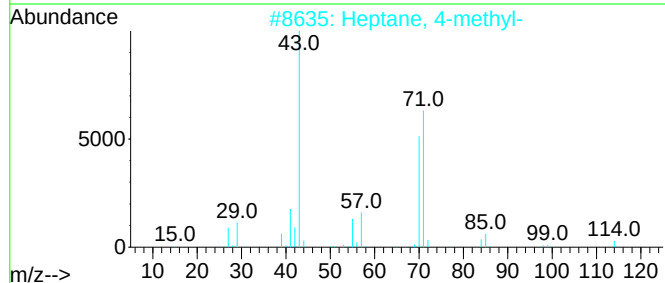
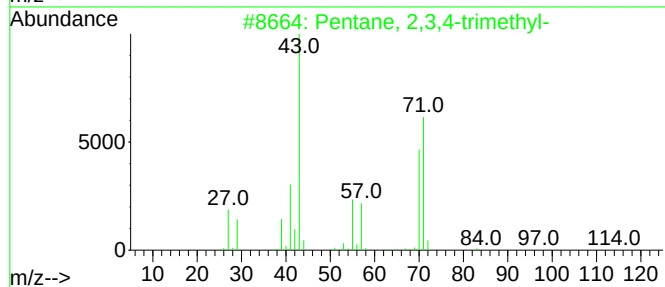
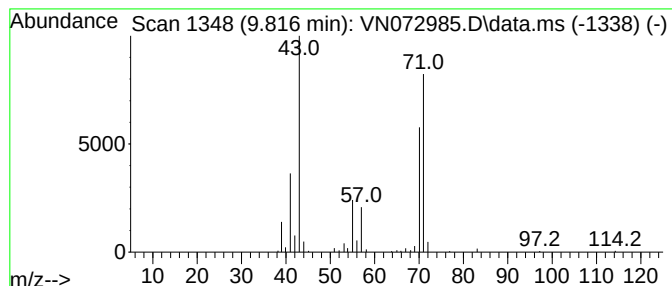
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	11.19 ug/l	255585	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78



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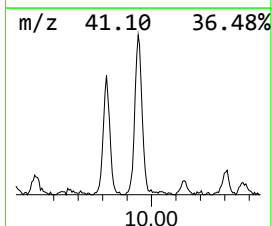
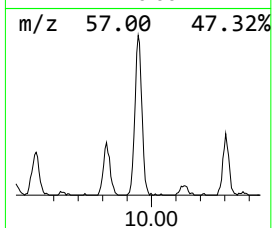
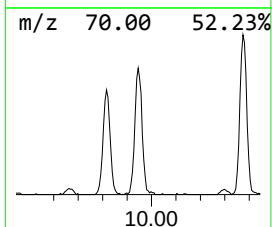
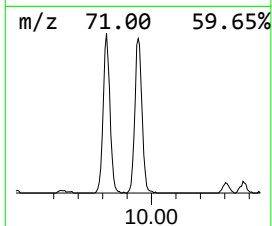
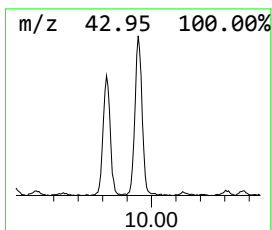
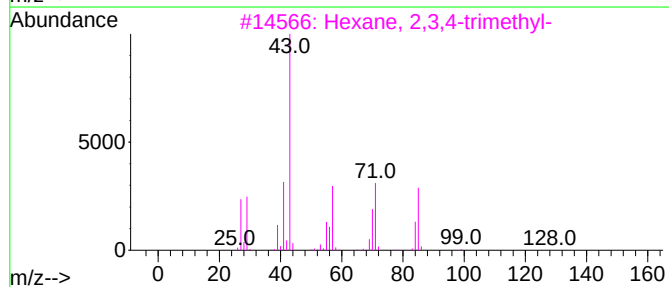
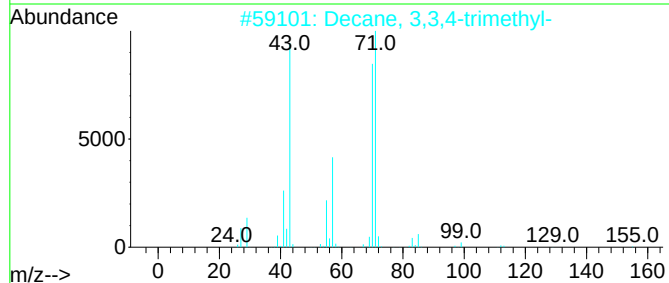
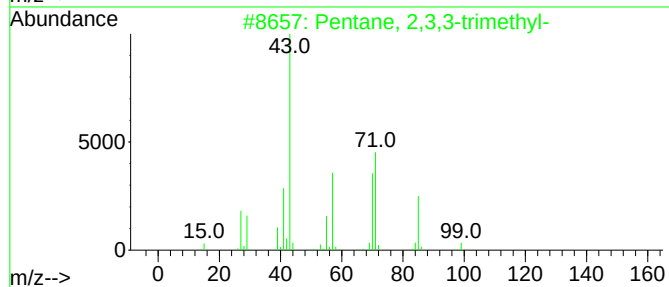
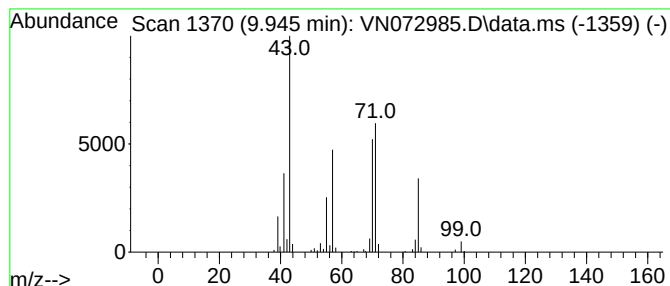
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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	17.78 ug/l	406231	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59



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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...	8.104	10.1	ug/l	185984	1	8.016	919473	50.0
Butane, 2,2,3,3...	8.545	13.1	ug/l	300264	2	8.898	1142140	50.0
Pentane, 2,3,4-...	9.816	11.2	ug/l	255585	2	8.898	1142140	50.0
Pentane, 2,3,3-...	9.945	17.8	ug/l	406231	2	8.898	1142140	50.0