

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070051.D
 Acq On : 14 Dec 2021 00:33
 Operator : JC/MD
 Sample : M5007-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-06

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.443	160	169	191	rVB	291651	485032	6.23%	1.063%
2	4.588	951	969	990	rVB3	27284	81456	1.05%	0.178%
3	5.079	1121	1152	1175	rBV3	82264	320039	4.11%	0.701%
4	5.618	1327	1353	1381	rBV2	121813	441914	5.68%	0.968%
5	7.045	1860	1885	1908	rBV5	92164	288783	3.71%	0.633%
6	7.321	1968	1988	2015	rBV5	31997	93586	1.20%	0.205%
7	8.021	2222	2249	2260	rBV2	864285	2053529	26.39%	4.499%
8	8.086	2261	2273	2295	rVB	1410895	3157959	40.59%	6.919%
9	8.437	2383	2404	2436	rBV	967421	2270475	29.18%	4.974%
10	8.614	2451	2470	2495	rBV	558960	1343860	17.27%	2.944%
11	8.968	2582	2602	2631	rBV	2443790	5059975	65.04%	11.086%
12	9.593	2822	2835	2855	rVB2	51705	113746	1.46%	0.249%
13	9.883	2923	2943	2965	rBV2	299820	613899	7.89%	1.345%
14	10.014	2972	2992	3014	rBV	642645	1333086	17.13%	2.921%
15	10.371	3110	3125	3135	rBV3	59048	110859	1.42%	0.243%
16	10.441	3135	3151	3183	rVV	3937319	7404347	95.17%	16.223%
17	11.744	3618	3637	3676	rBV	4266747	7780112	100.00%	17.046%
18	12.731	3987	4005	4030	rBV	3336170	5992601	77.02%	13.129%
19	13.039	4102	4120	4138	rBV	25340	84894	1.09%	0.186%
20	13.675	4340	4357	4393	rBV	3791117	6612272	84.99%	14.487%

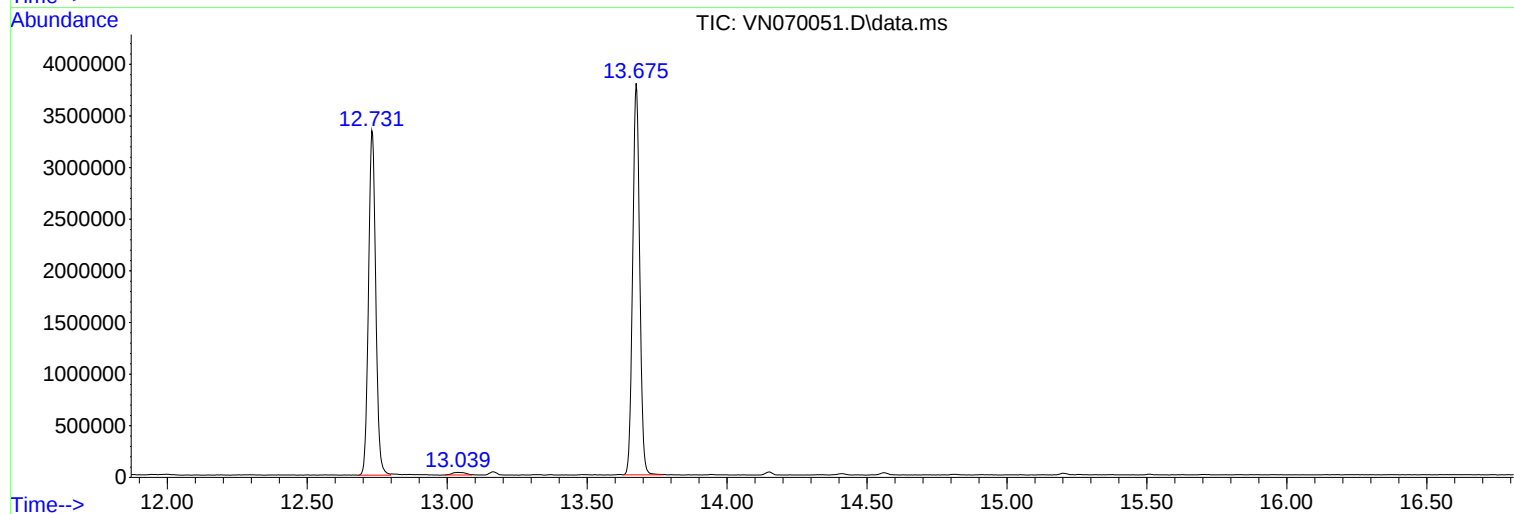
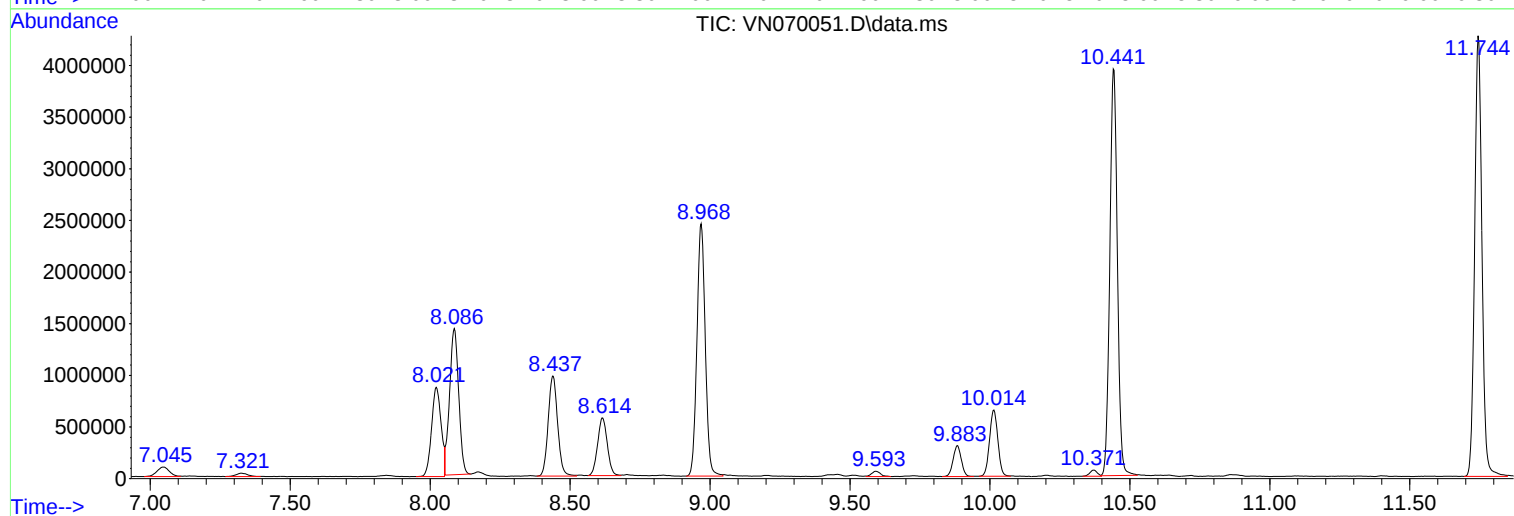
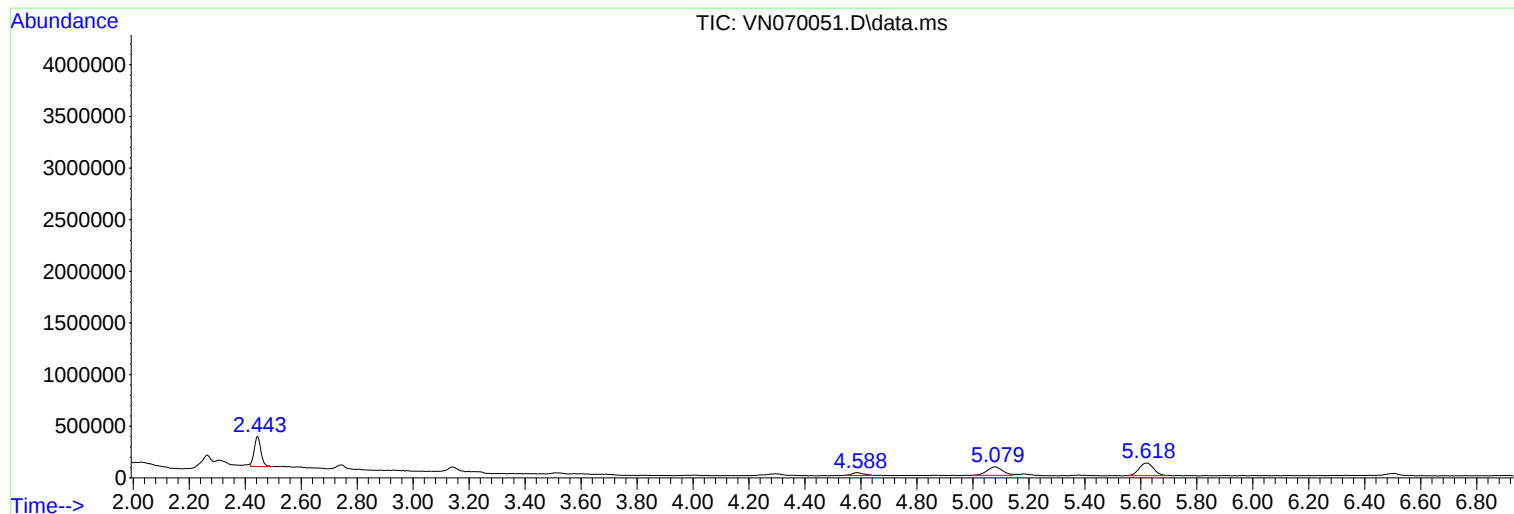
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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Operator : JC/MD
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Instrument :
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ClientSampleId :
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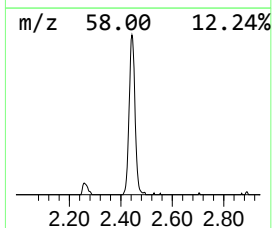
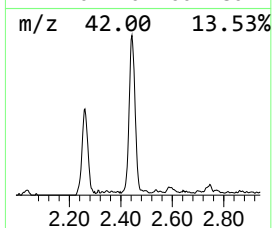
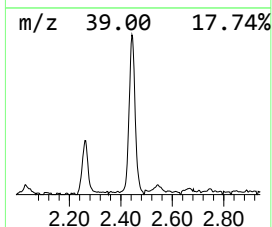
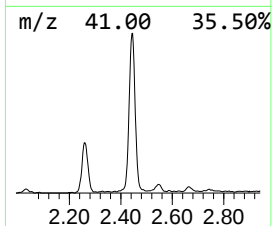
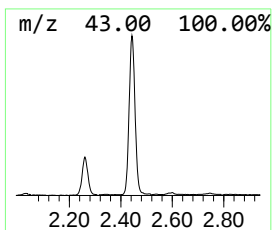
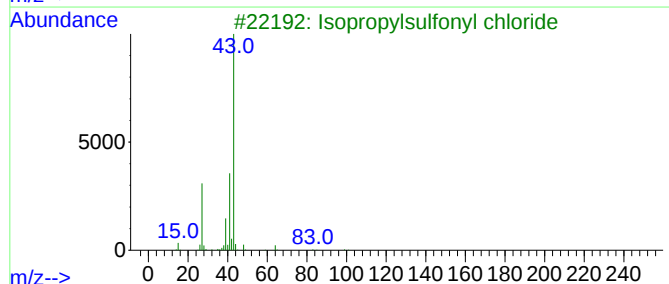
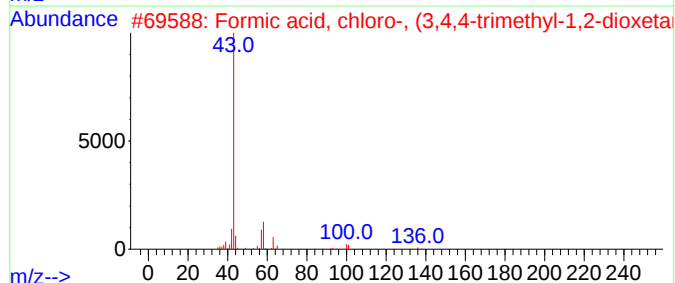
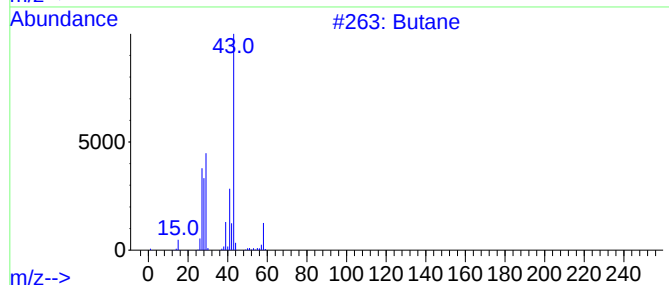
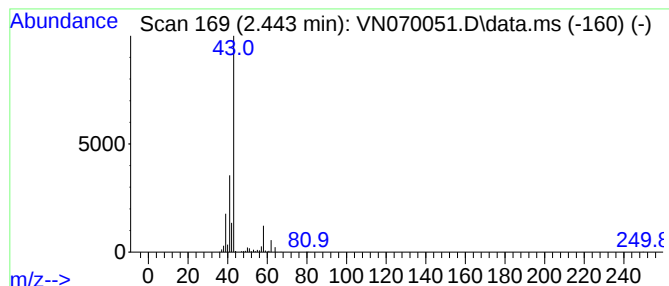
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.443	7.68 ug/l	485032	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	53
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	38
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Acetone	58	C3H6O	000067-64-1	4
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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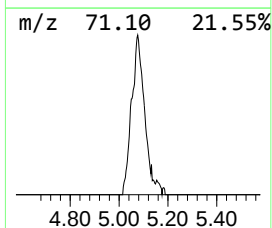
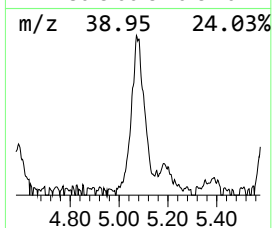
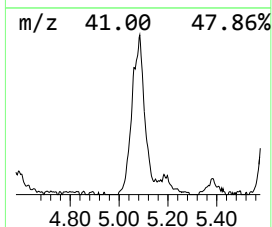
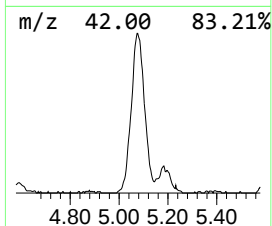
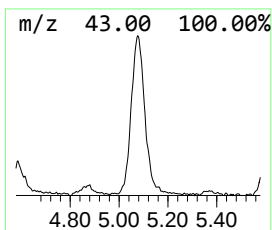
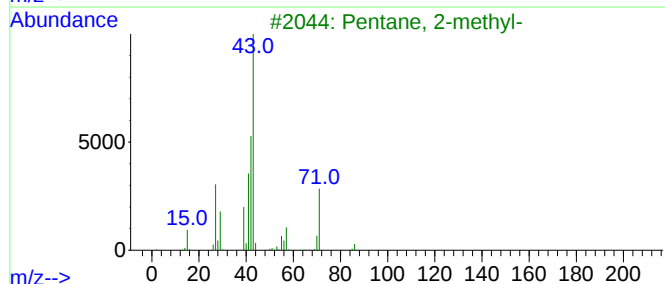
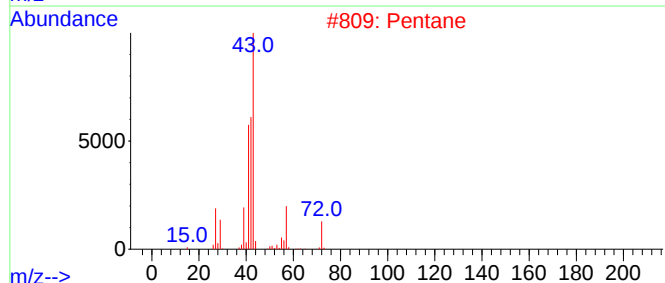
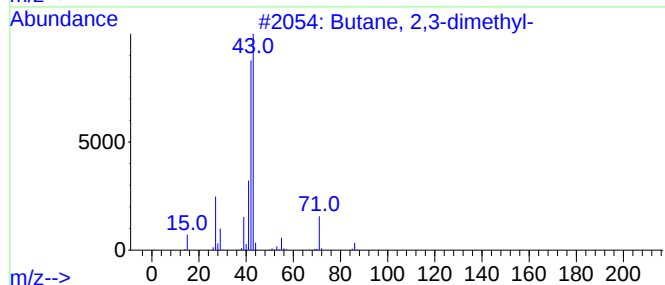
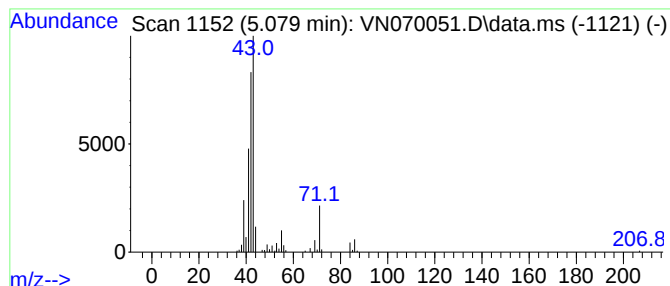
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.079	5.07 ug/l	320039	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
2			Pentane	72	C5H12	000109-66-0	33
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	28
4			Propenal dimethylhydrazone	98	C5H10N2	025368-52-9	9
5			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9



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Instrument :
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TOLL-MW-06

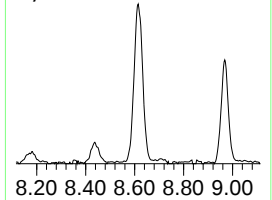
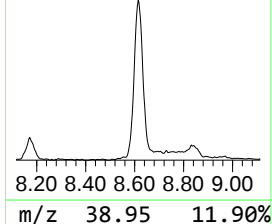
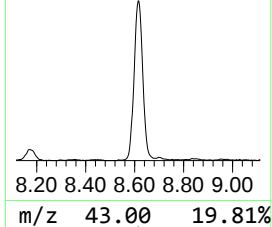
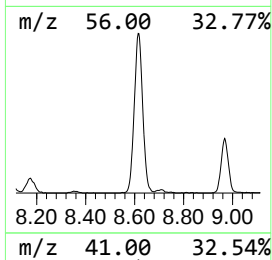
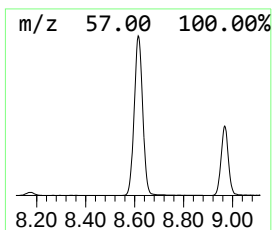
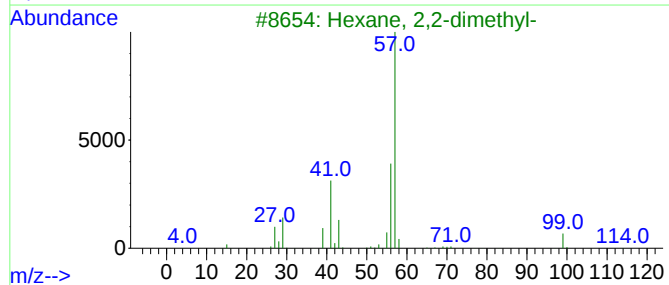
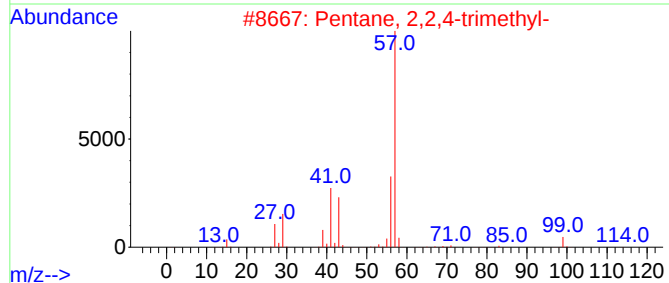
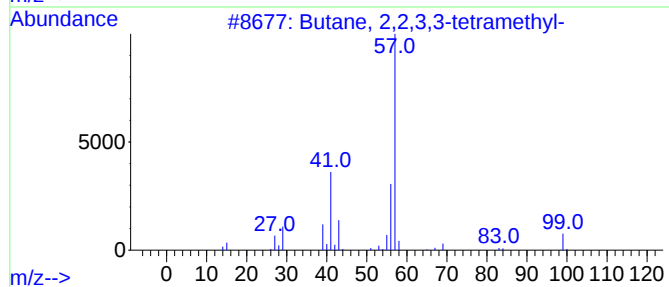
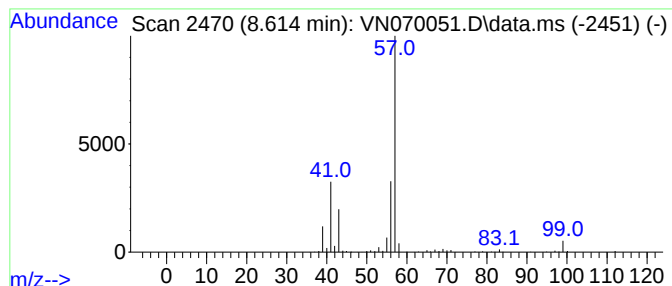
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	13.28 ug/l	1343860	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-dimethyl-	114	C8H18	000590-73-8	59
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50



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Instrument :
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ClientSampleId :
TOLL-MW-06

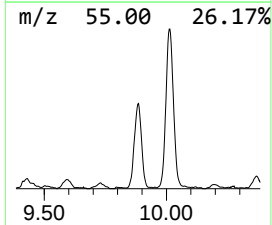
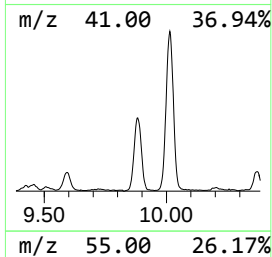
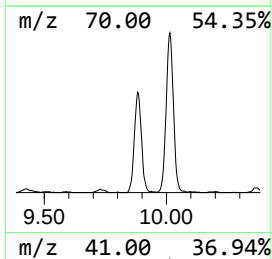
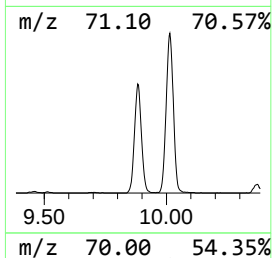
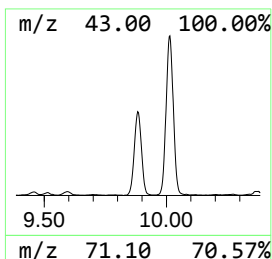
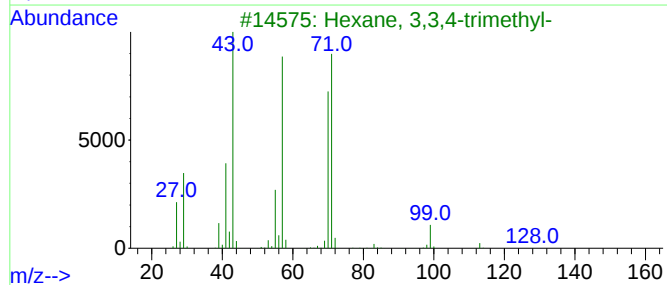
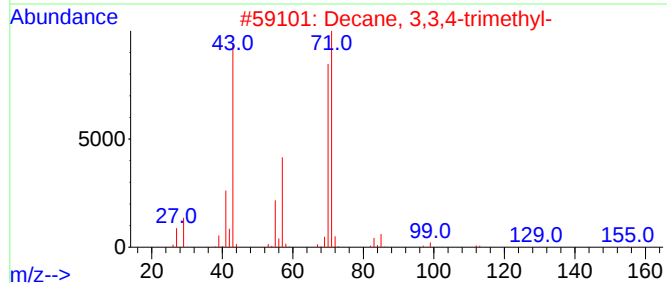
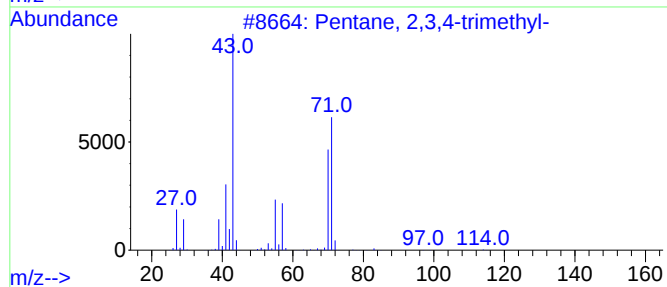
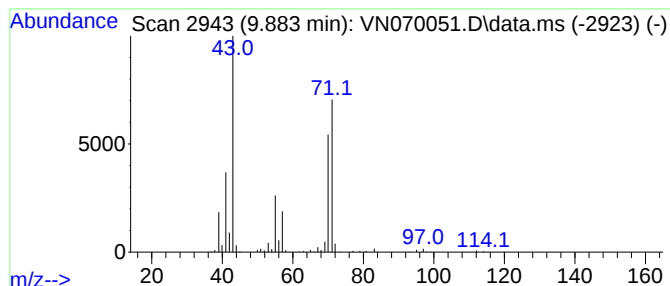
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	6.07 ug/l	613899	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	91
2			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	72
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	72
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	64



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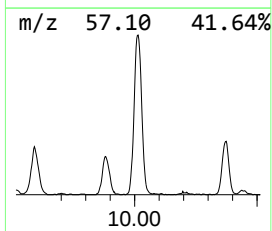
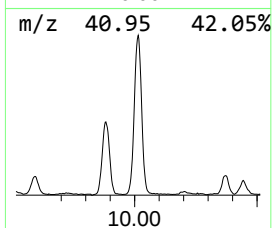
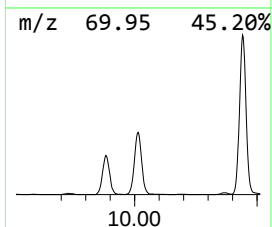
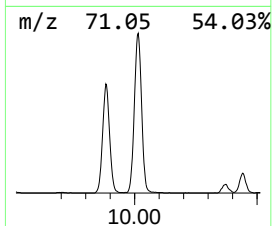
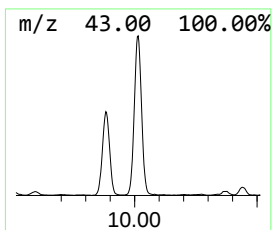
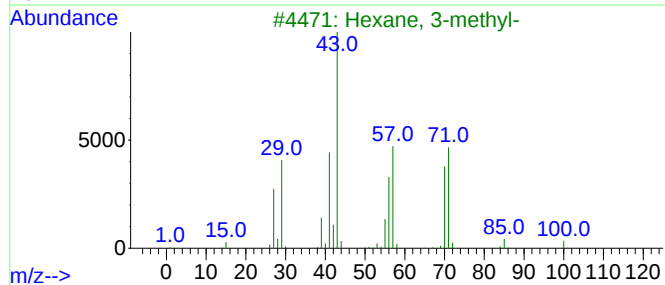
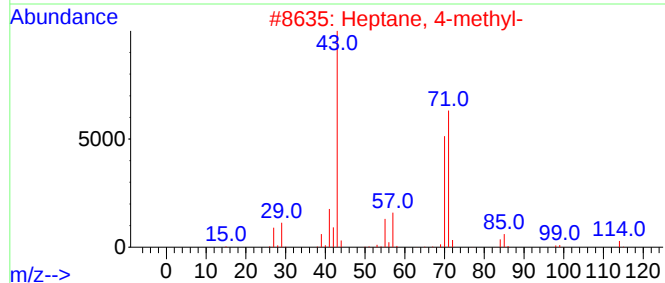
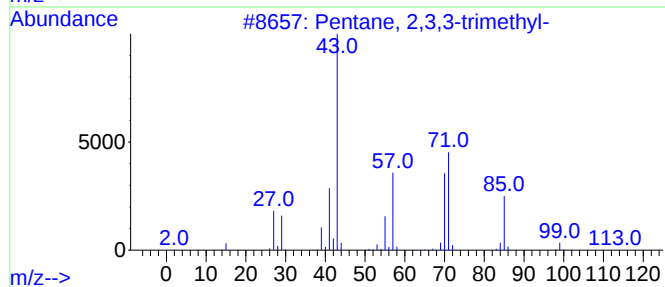
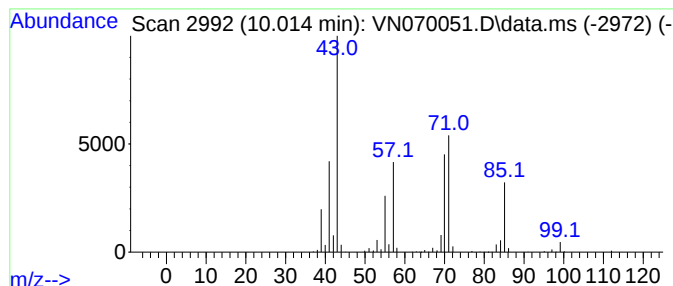
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	13.17 ug/l	1333090	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	78
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53



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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
Butane	2.443	7.7	ug/l	485032	1	8.086	3157960	50.0
Butane, 2,3-dim...	5.079	5.1	ug/l	320039	1	8.086	3157960	50.0
Butane, 2,2,3,3...	8.614	13.3	ug/l	1343860	2	8.968	5059980	50.0
Pentane, 2,3,4-...	9.883	6.1	ug/l	613899	2	8.968	5059980	50.0
Pentane, 2,3,3-...	10.014	13.2	ug/l	1333090	2	8.968	5059980	50.0