

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070054.D
 Acq On : 14 Dec 2021 1:50
 Operator : JC/MD
 Sample : M5007-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-09

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: VN070054.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.143	415	430	458	rVB2	358930	827832	7.93%	1.009%
2	5.079	1127	1152	1180	rBV3	139862	543053	5.20%	0.662%
3	5.380	1239	1264	1288	rBV3	91591	322203	3.08%	0.393%
4	5.621	1324	1354	1388	rBV3	206896	727503	6.96%	0.887%
5	7.048	1857	1886	1914	rBV2	663001	2024125	19.38%	2.467%
6	7.847	2164	2184	2206	rVB3	63402	178463	1.71%	0.217%
7	8.024	2228	2250	2261	rBV	843288	2030032	19.43%	2.474%
8	8.086	2261	2273	2289	rVV	1400225	3200349	30.64%	3.900%
9	8.174	2289	2306	2339	rVB	2960777	7372524	70.58%	8.985%
10	8.440	2386	2405	2429	rBV	954779	2182077	20.89%	2.659%
11	8.617	2434	2471	2496	rBV	4191996	10445501	100.00%	12.730%
12	8.968	2583	2602	2636	rBV	2386968	4976469	47.64%	6.065%
13	9.513	2796	2805	2819	rVB3	94030	182358	1.75%	0.222%
14	9.593	2820	2835	2862	rVV	369501	776709	7.44%	0.947%
15	9.730	2865	2886	2904	rVB6	93284	268800	2.57%	0.328%
16	9.883	2924	2943	2966	rBV	3052253	6040114	57.83%	7.361%
17	10.014	2969	2992	3024	rVV	4886214	10049440	96.21%	12.247%
18	10.199	3045	3061	3074	rBV3	170857	333939	3.20%	0.407%
19	10.368	3101	3124	3136	rBV4	306417	627355	6.01%	0.765%
20	10.441	3136	3151	3184	rVB	4053434	7594167	72.70%	9.255%
21	10.610	3205	3214	3238	rVB10	62937	201707	1.93%	0.246%
22	10.784	3266	3279	3294	rBV3	68887	134591	1.29%	0.164%
23	10.872	3295	3312	3330	rVV9	199206	530147	5.08%	0.646%
24	11.259	3437	3456	3467	rBV3	82188	173153	1.66%	0.211%
25	11.744	3620	3637	3668	rBV	4192816	7698059	73.70%	9.381%
26	11.993	3716	3730	3752	rVB	39206	117840	1.13%	0.144%
27	12.734	3988	4006	4027	rBV	3229391	5735858	54.91%	6.990%
28	13.675	4340	4357	4388	rBV	3564092	6209928	59.45%	7.568%
29	14.150	4518	4534	4548	rBV2	162789	287829	2.76%	0.351%
30	14.407	4614	4630	4642	rVB9	70812	148174	1.42%	0.181%
31	14.812	4770	4781	4795	rVB7	69352	116066	1.11%	0.141%

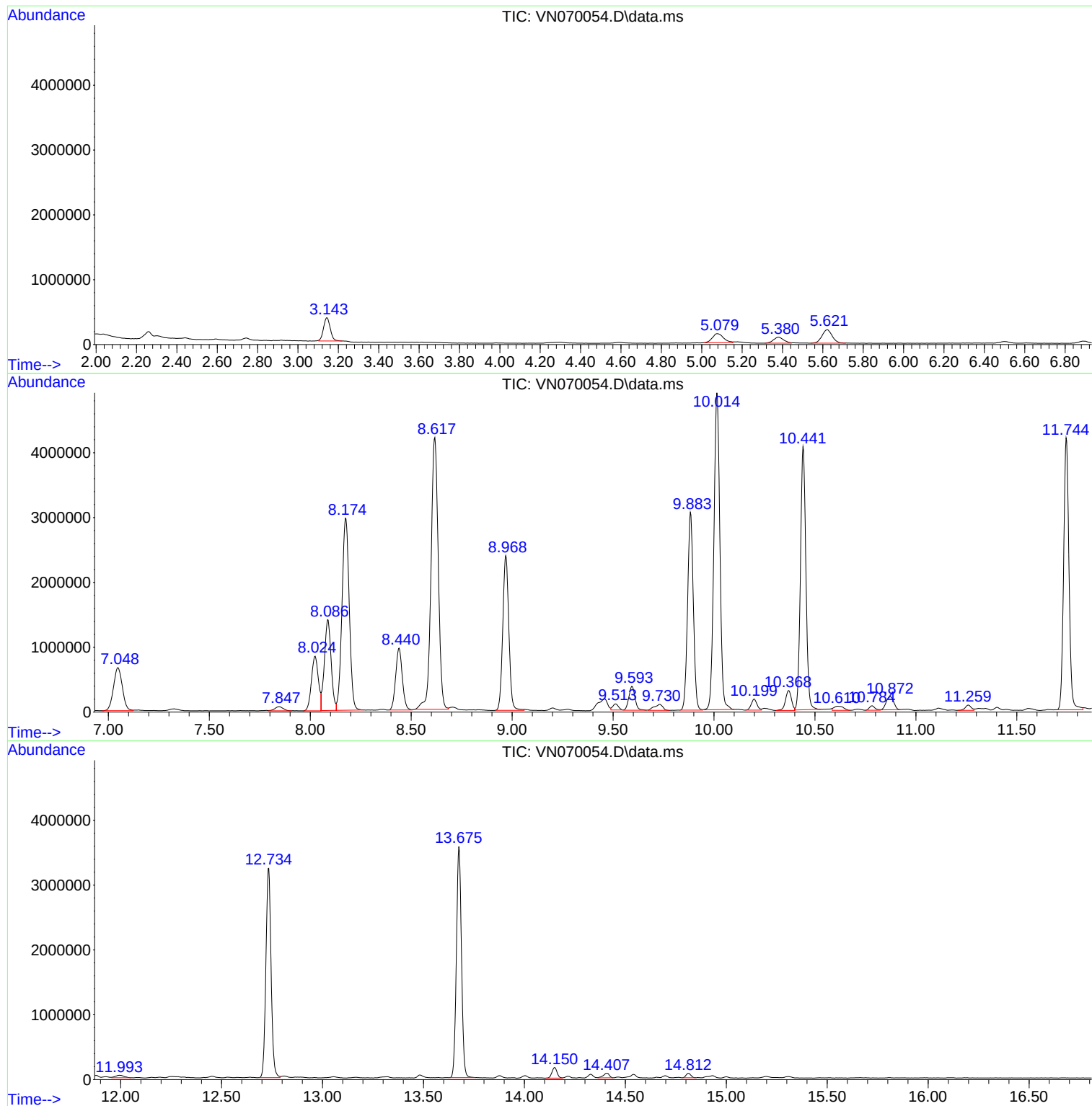
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Instrument :
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ClientSampleId :
TOLL-MW-09

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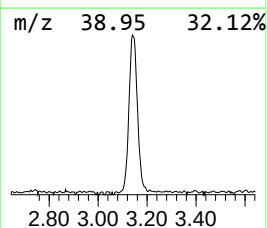
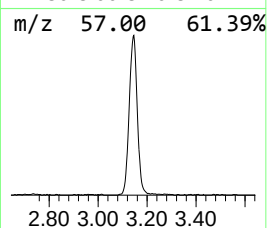
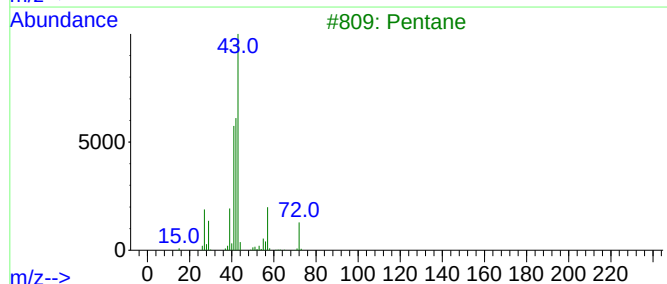
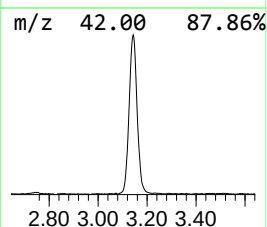
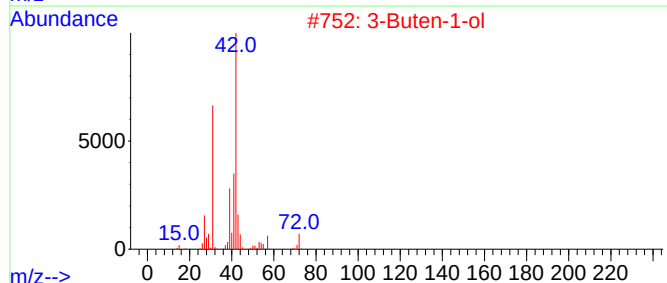
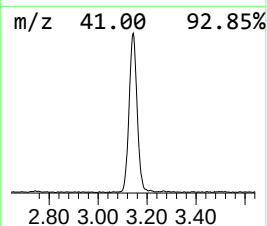
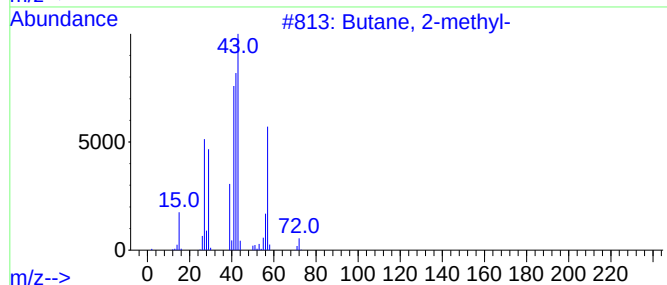
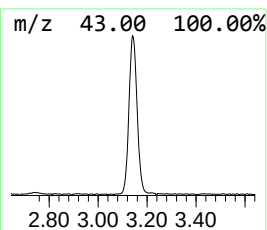
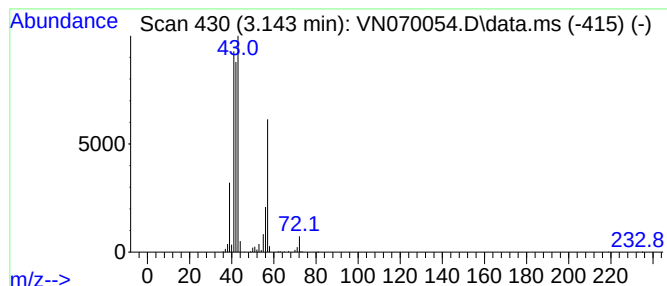
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	12.93 ug/l	827832	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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TOLL-MW-09

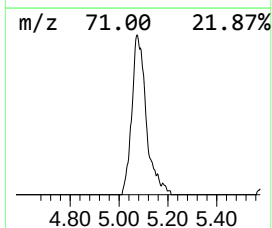
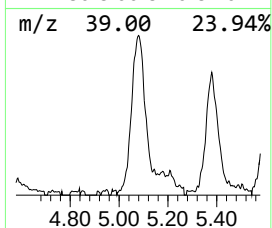
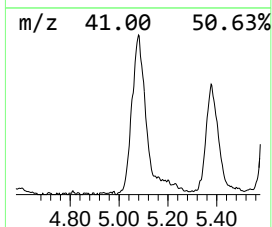
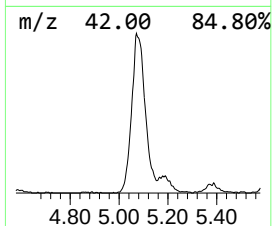
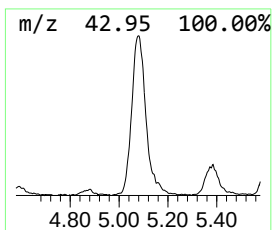
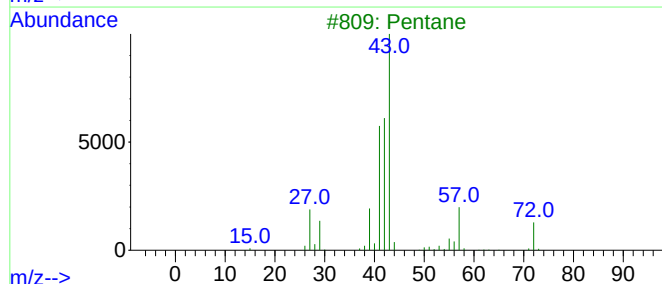
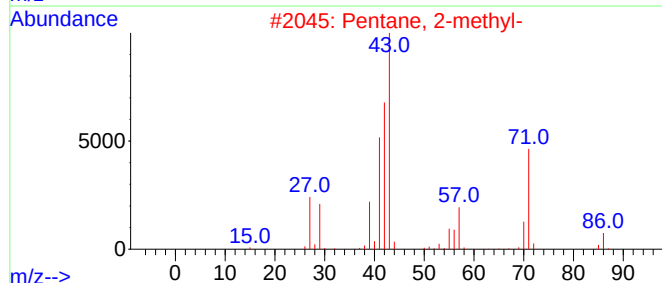
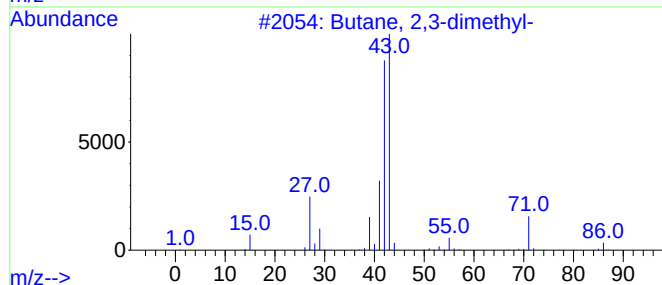
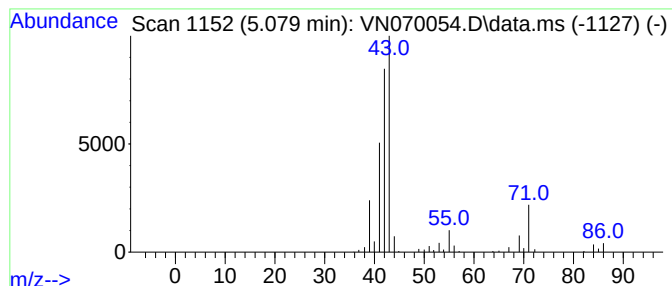
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.079	8.48 ug/l	543053	Pentafluorobenzene	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	56
3		Pentane	72	C5H12	000109-66-0	36
4		1-Pentene	70	C5H10	000109-67-1	28
5		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	12



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

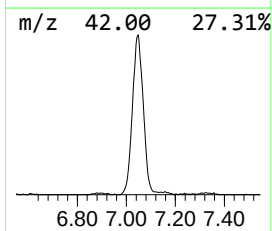
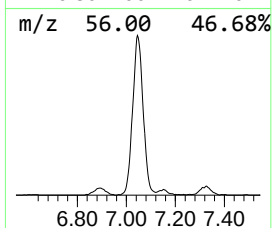
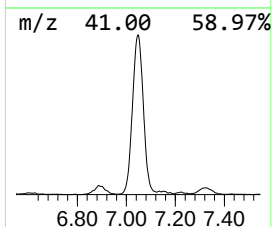
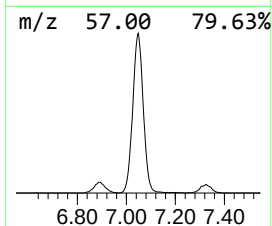
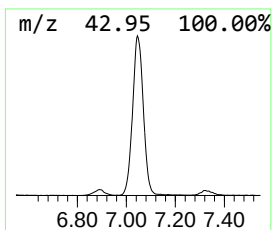
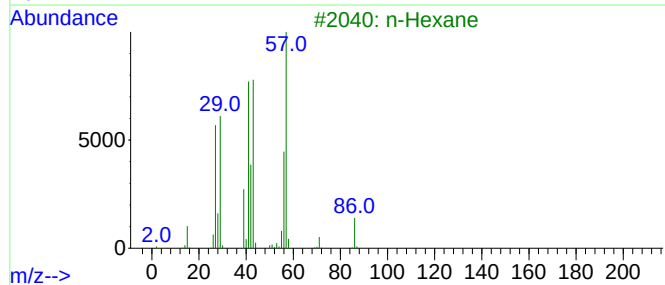
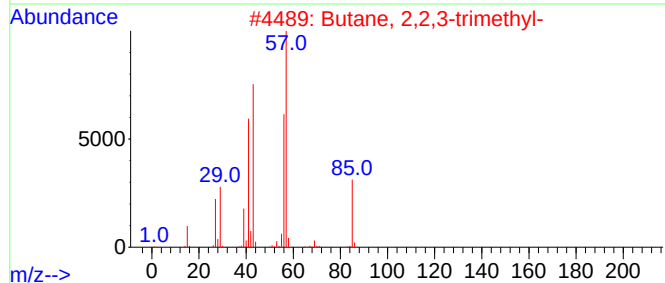
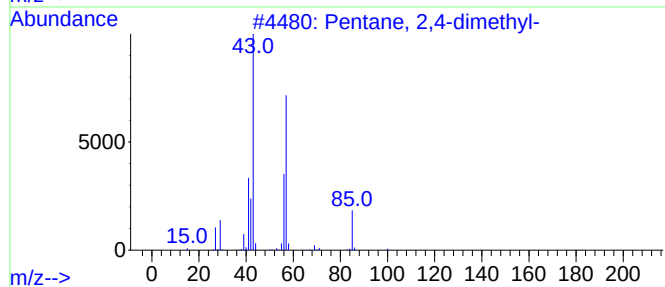
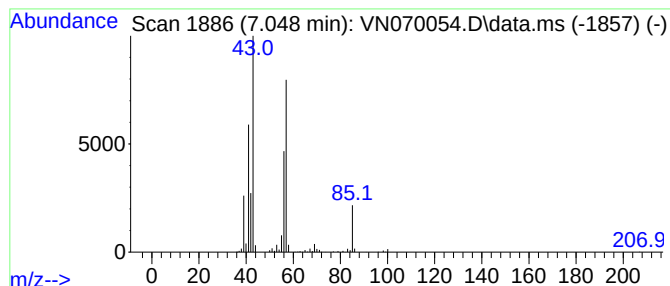
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.048	31.62 ug/l	2024130	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3			n-Hexane	86	C6H14	000110-54-3	53
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	47



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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TOLL-MW-09

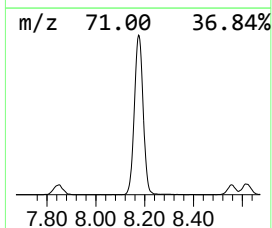
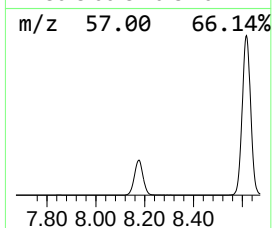
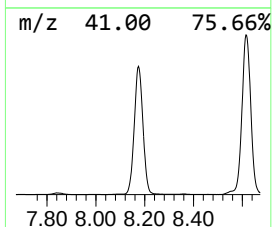
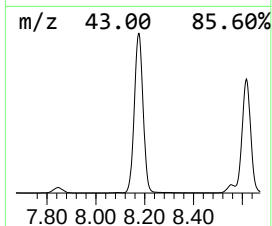
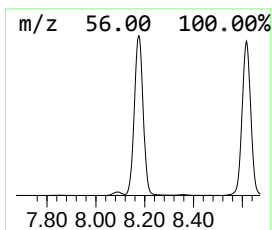
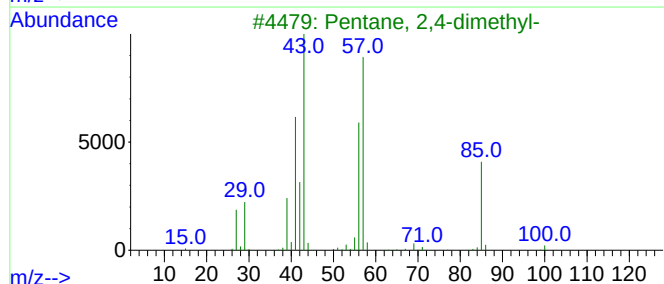
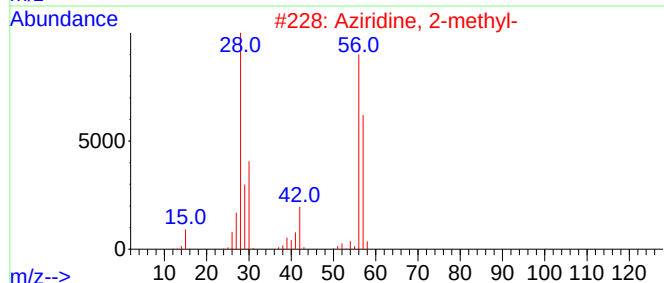
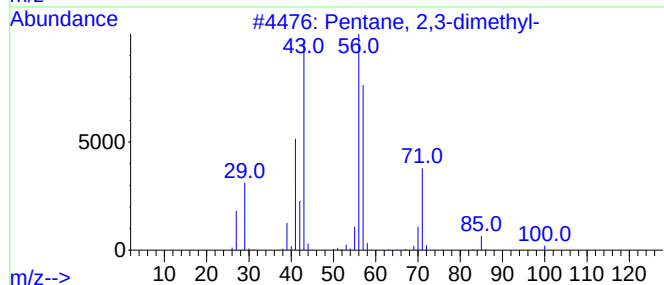
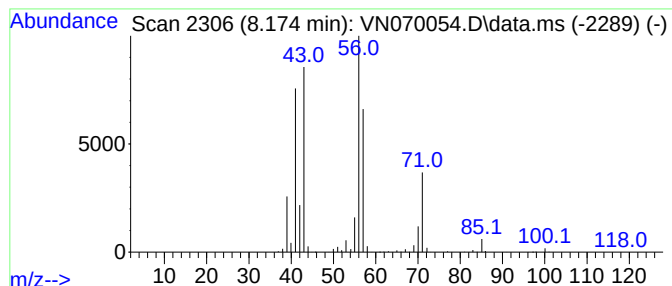
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	115.18 ug/l	7372520	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
3			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	43
4			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	38
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38



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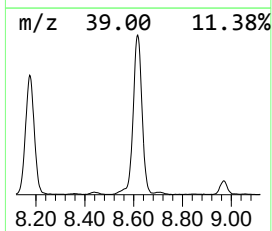
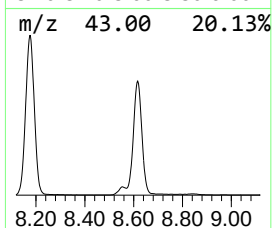
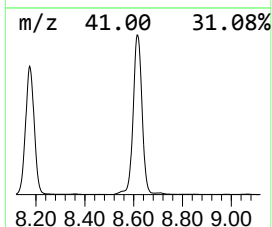
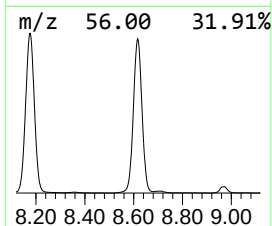
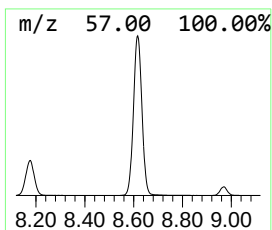
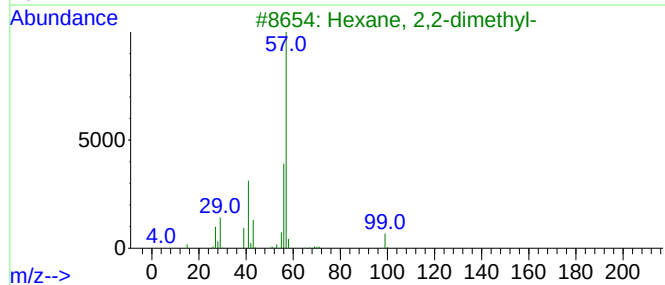
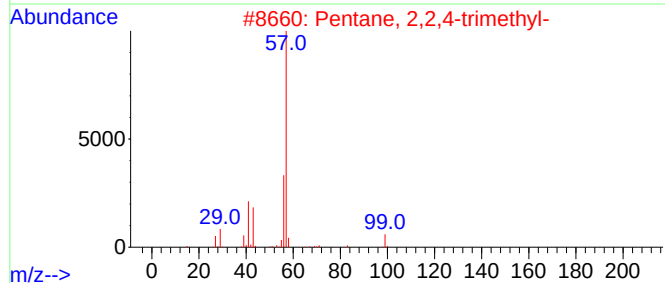
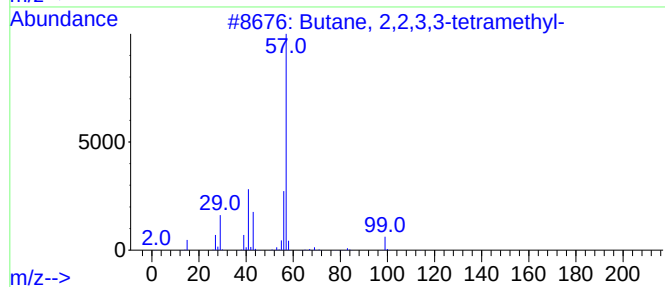
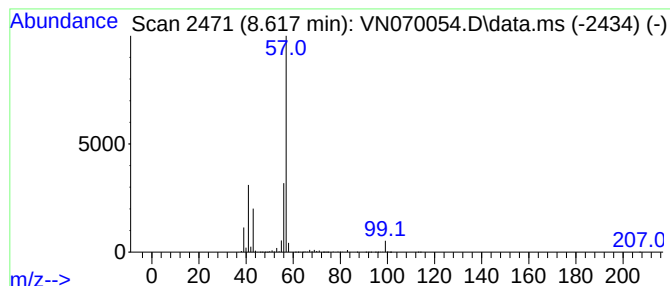
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	104.95 ug/l	10445500	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	83
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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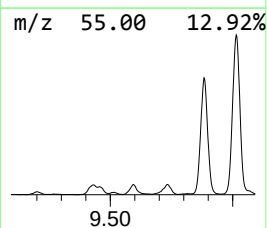
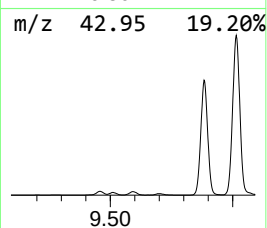
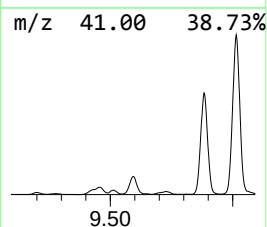
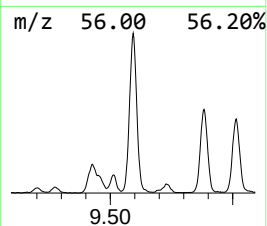
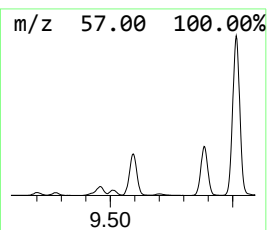
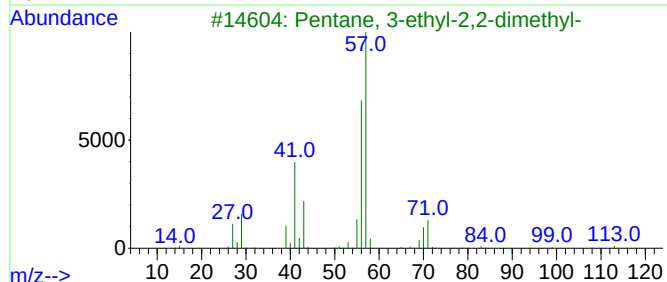
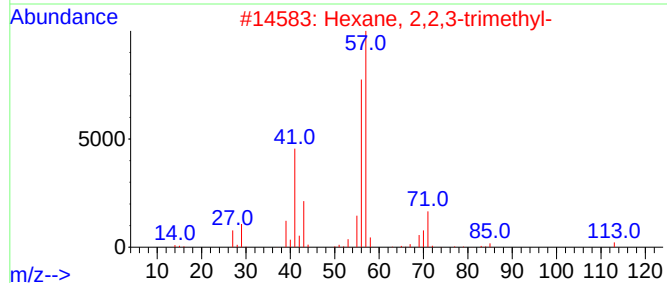
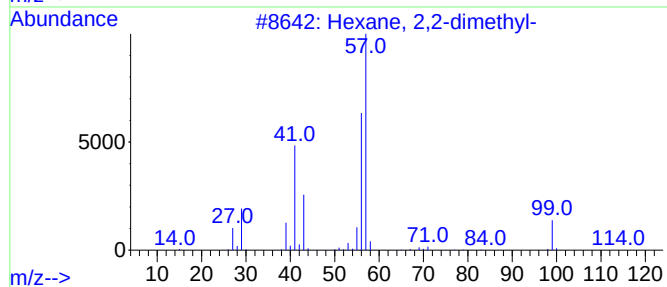
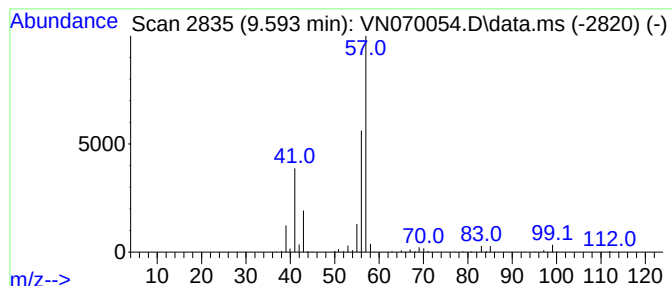
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Quant Title : SW846 8260

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

Peak Number 6 Hexane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.593	7.80 ug/l	776709	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	72
4			Pentane, 3-methyl-	86	C6H14	000096-14-0	72
5			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070054.D
Acq On : 14 Dec 2021 1:50
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

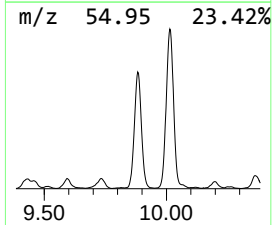
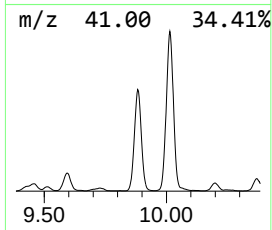
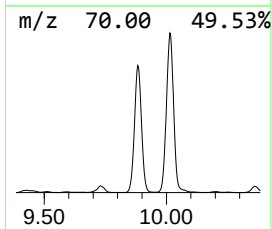
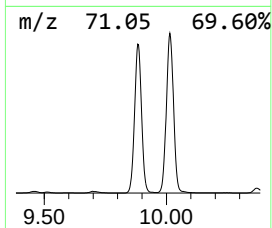
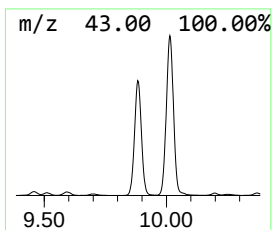
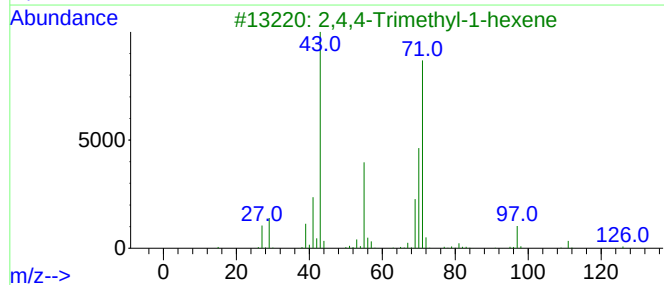
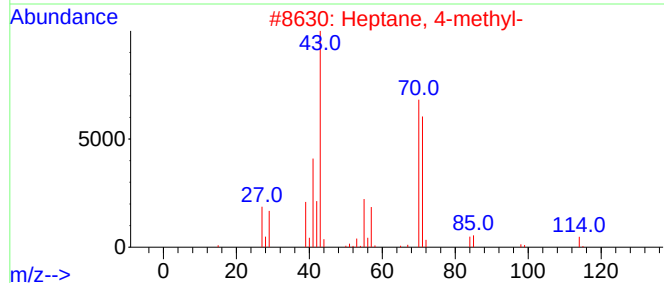
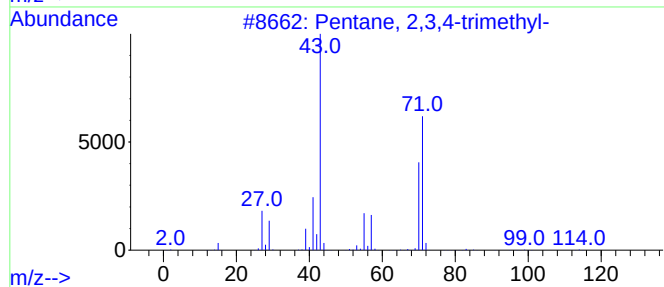
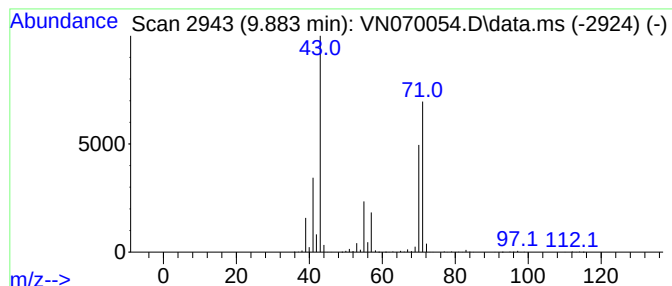
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	60.69 ug/l	6040110	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	83
3			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070054.D
Acq On : 14 Dec 2021 1:50
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

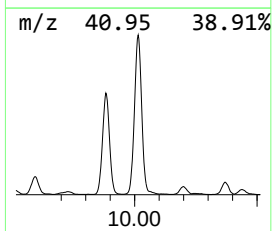
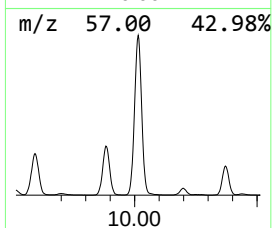
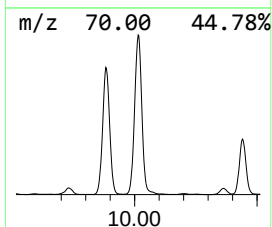
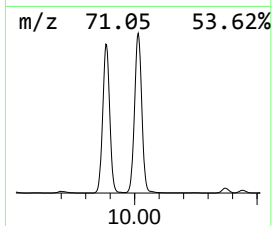
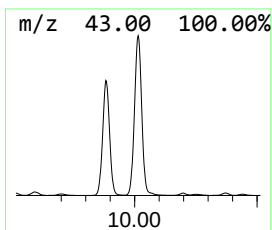
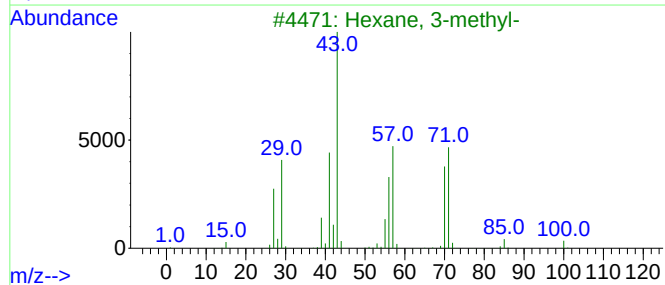
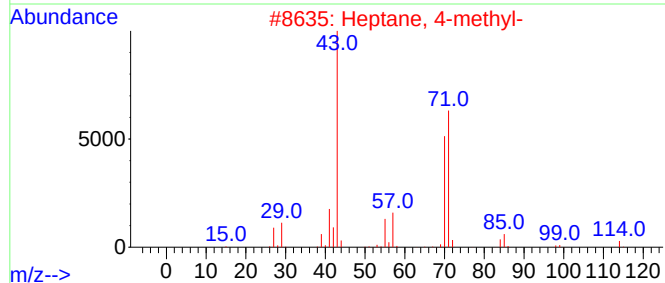
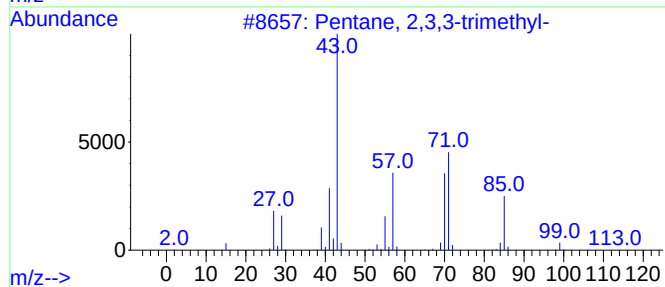
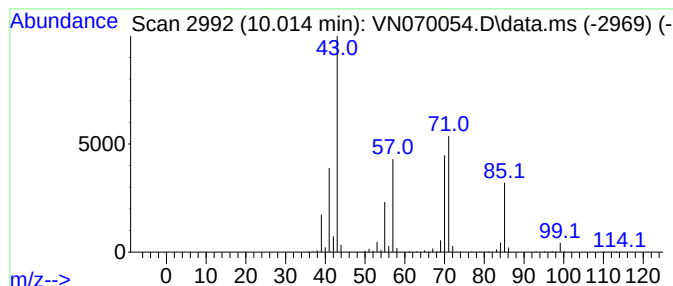
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	100.97 ug/l	10049400	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	64
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070054.D
Acq On : 14 Dec 2021 1:50
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.143	12.9	ug/l	827832	1	8.088	3200350	50.0
Butane, 2,3-dim...	5.079	8.5	ug/l	543053	1	8.088	3200350	50.0
Pentane, 2,4-di...	7.048	31.6	ug/l	2024130	1	8.088	3200350	50.0
Pentane, 2,3-di...	8.174	115.2	ug/l	7372520	1	8.088	3200350	50.0
Butane, 2,2,3,3...	8.617	105.0	ug/l	10445500	2	8.968	4976470	50.0
Hexane, 2,2-dim...	9.593	7.8	ug/l	776709	2	8.968	4976470	50.0
Pentane, 2,3,4-...	9.883	60.7	ug/l	6040110	2	8.968	4976470	50.0
Pentane, 2,3,3-...	10.014	101.0	ug/l	10049400	2	8.968	4976470	50.0