

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
 Data File : VN070384.D
 Acq On : 30 Dec 2021 8:00
 Operator : JC/MD
 Sample : M5007-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-09RE

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: VN070384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	413	429	451	rVB	287853	661353	7.53%	1.089%
2	4.291	844	858	880	rVB2	42369	116281	1.32%	0.192%
3	5.076	1121	1151	1180	rBV4	120968	481194	5.48%	0.793%
4	5.379	1234	1264	1297	rBV2	106092	389586	4.44%	0.642%
5	5.621	1328	1354	1384	rVB4	189688	655227	7.46%	1.079%
6	7.045	1858	1885	1914	rBV3	515025	1580840	18.00%	2.604%
7	7.327	1974	1990	2016	rVB7	27711	90350	1.03%	0.149%
8	7.847	2165	2184	2202	rVB3	53730	145744	1.66%	0.240%
9	8.024	2224	2250	2261	rBV	628233	1521670	17.33%	2.507%
10	8.086	2261	2273	2288	rVV	1140128	2619278	29.82%	4.315%
11	8.174	2289	2306	2334	rVB	2442845	6061790	69.02%	9.985%
12	8.440	2386	2405	2430	rBV	764191	1753804	19.97%	2.889%
13	8.617	2432	2471	2495	rBV	3335109	8370888	95.31%	13.789%
14	8.968	2584	2602	2631	rBV	1784974	3734164	42.52%	6.151%
15	9.199	2677	2688	2701	rBV3	42079	91808	1.05%	0.151%
16	9.512	2797	2805	2819	rVB6	72087	138626	1.58%	0.228%
17	9.595	2819	2836	2862	rVV	310626	663463	7.55%	1.093%
18	9.730	2865	2886	2901	rVB5	77205	224516	2.56%	0.370%
19	9.882	2924	2943	2966	rBV	2527160	5050815	57.51%	8.320%
20	10.014	2967	2992	3024	rVV	4249204	8783039	100.00%	14.468%
21	10.199	3046	3061	3074	rBV3	142260	286094	3.26%	0.471%
22	10.368	3100	3124	3136	rBV4	235271	483868	5.51%	0.797%
23	10.443	3136	3152	3183	rVB	2719260	5139078	58.51%	8.465%
24	10.781	3267	3278	3292	rBV3	59464	111400	1.27%	0.184%
25	10.869	3294	3311	3330	rVV6	194322	524516	5.97%	0.864%
26	11.258	3438	3456	3467	rBV5	77323	157140	1.79%	0.259%
27	11.744	3621	3637	3666	rBV	2355659	4269499	48.61%	7.033%
28	12.001	3719	3733	3752	rVB	32130	90767	1.03%	0.150%
29	12.731	3988	4005	4028	rBV	1756729	3152227	35.89%	5.193%
30	13.675	4342	4357	4385	rVB	1624701	2854299	32.50%	4.702%
31	14.149	4520	4534	4547	rBV3	144991	257151	2.93%	0.424%
32	14.407	4613	4630	4643	rVB7	66989	131531	1.50%	0.217%
33	14.812	4769	4781	4796	rBV8	65362	114423	1.30%	0.188%

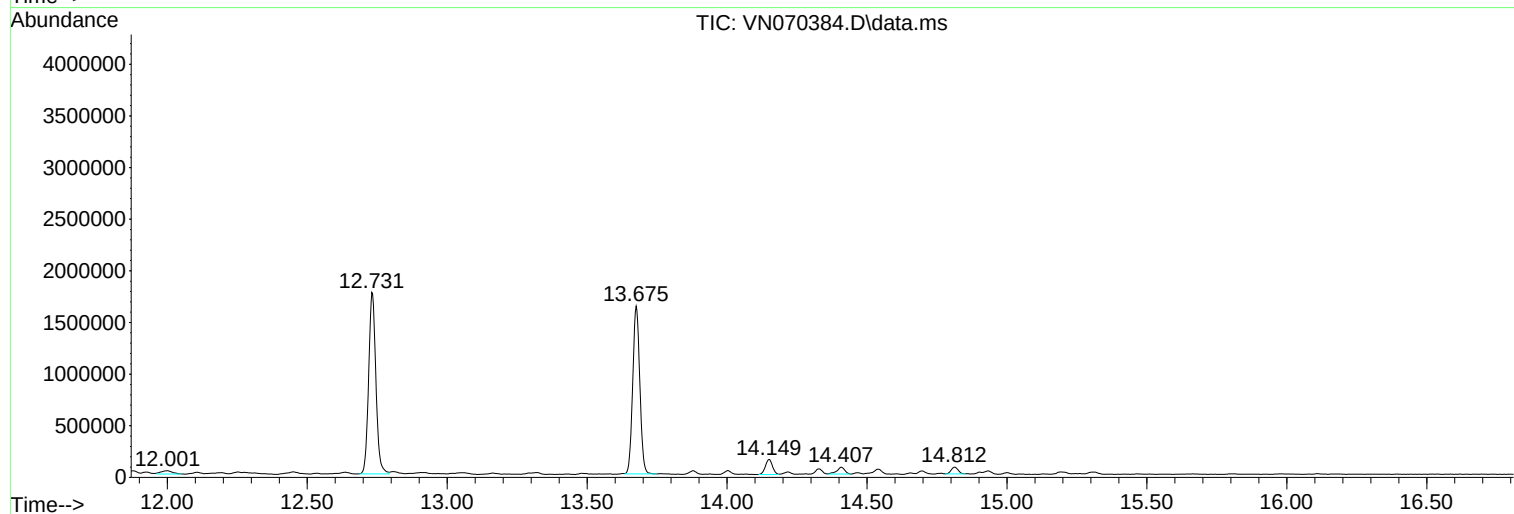
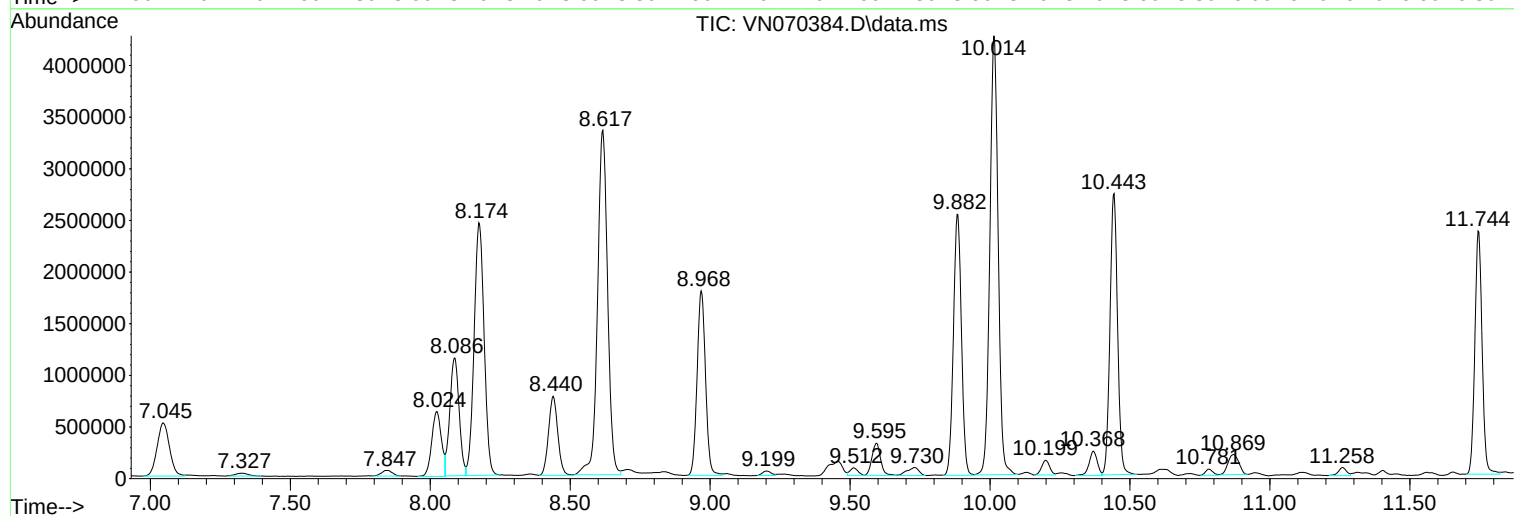
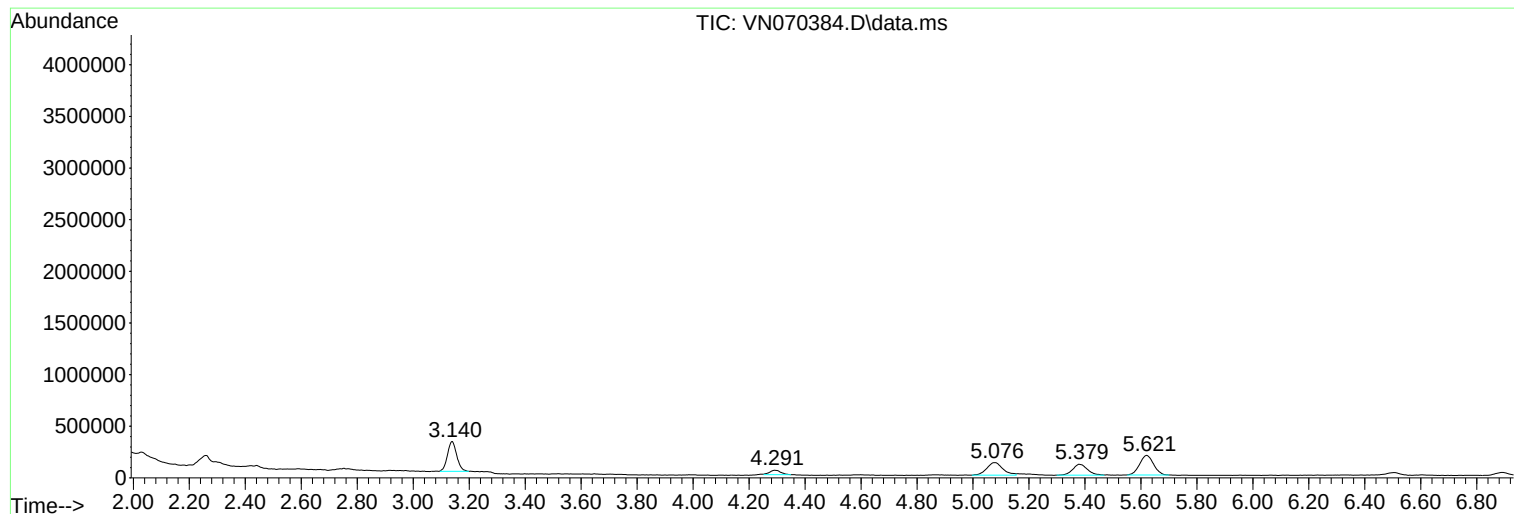
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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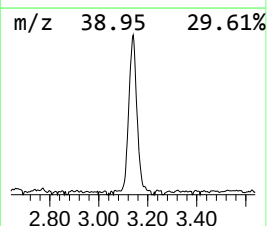
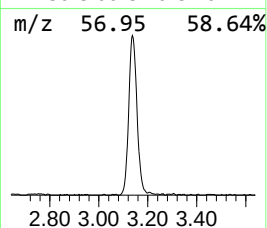
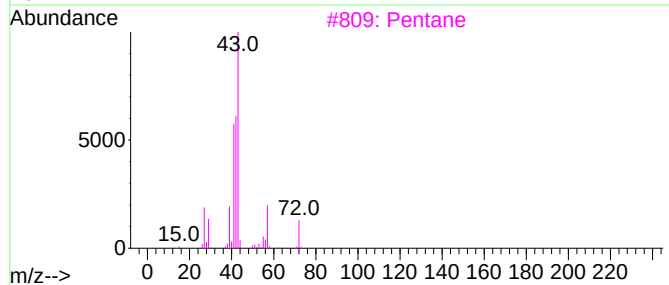
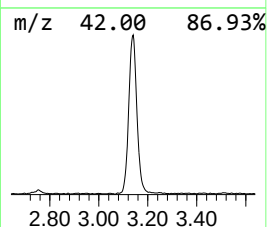
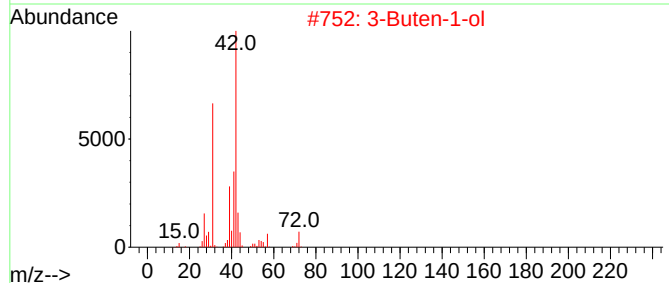
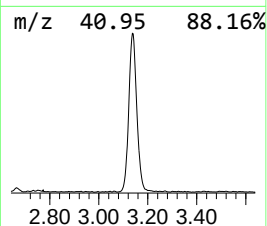
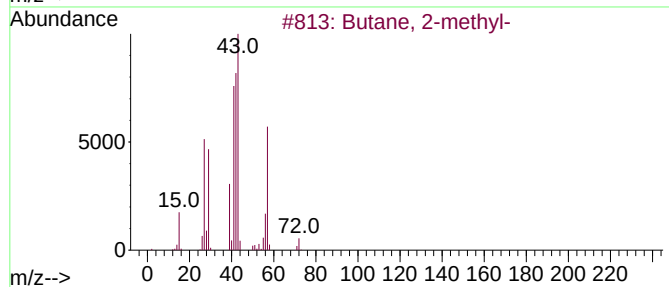
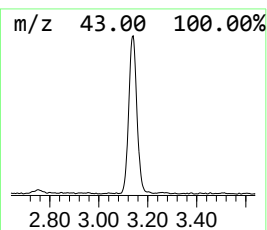
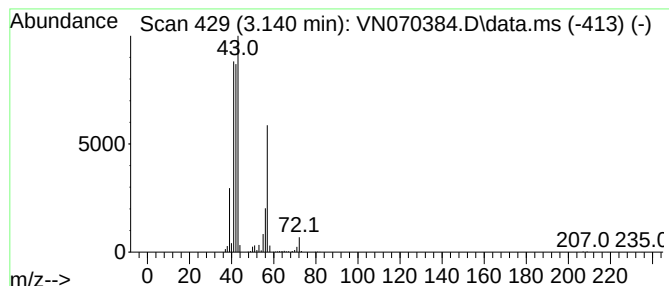
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	12.62 ug/l	661353	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	3-Buten-1-ol			72	C4H8O	000627-27-0	47
3	Pentane			72	C5H12	000109-66-0	36
4	1-Pentene, 4-methyl-			84	C6H12	000691-37-2	12
5	2-Butene			56	C4H8	000107-01-7	9



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ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

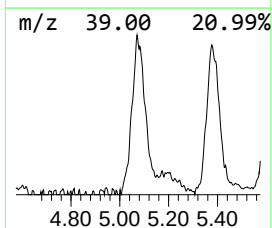
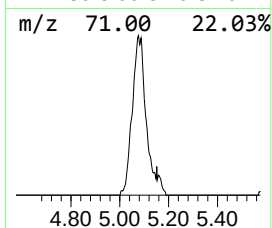
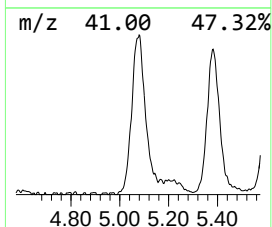
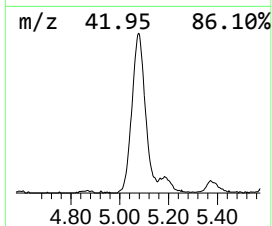
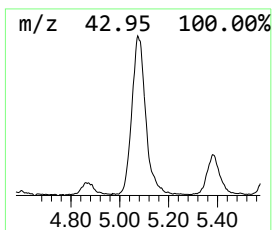
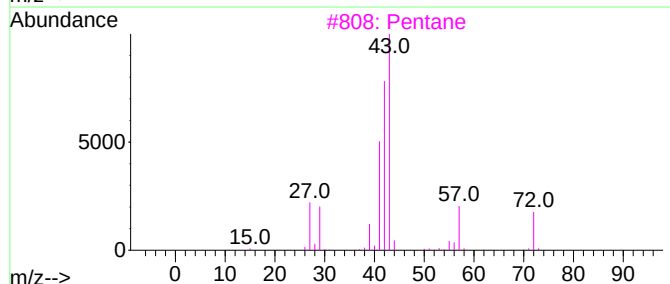
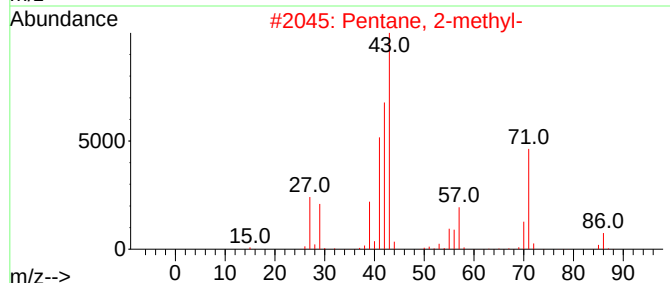
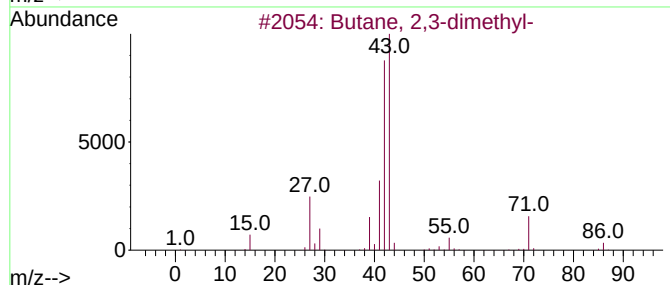
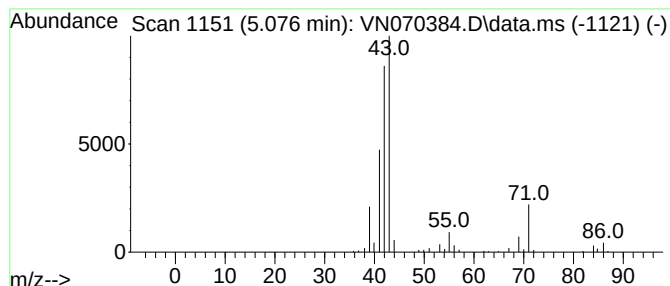
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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.
5.076	9.19 ug/l	481194	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	72
3		Pentane	72	C5H12	000109-66-0	42
4		1-Pentene	70	C5H10	000109-67-1	28
5		Butanal, 2-ethyl-	100	C6H12O	000097-96-1	10



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ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

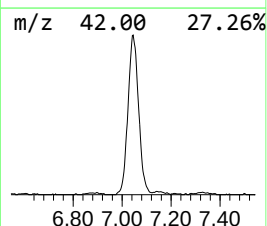
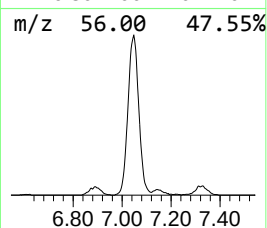
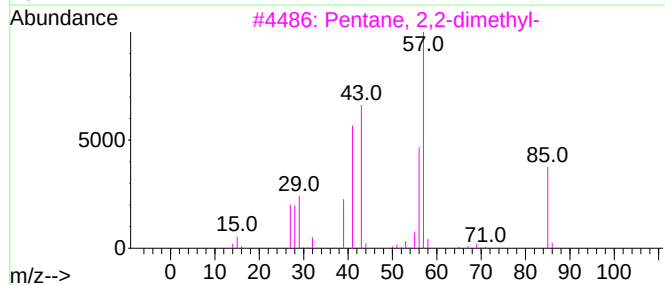
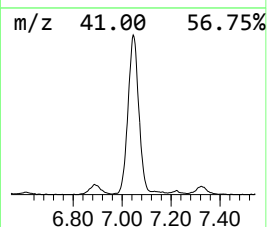
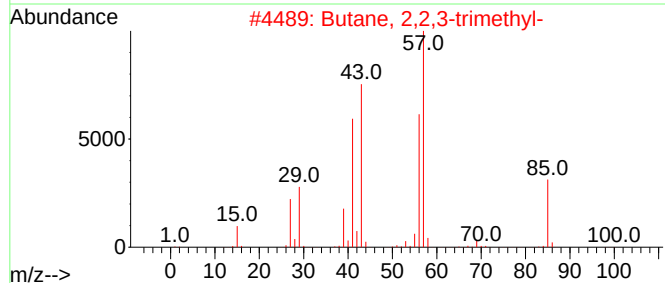
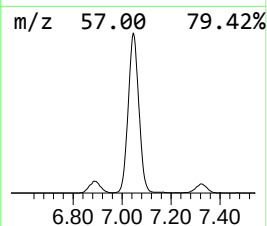
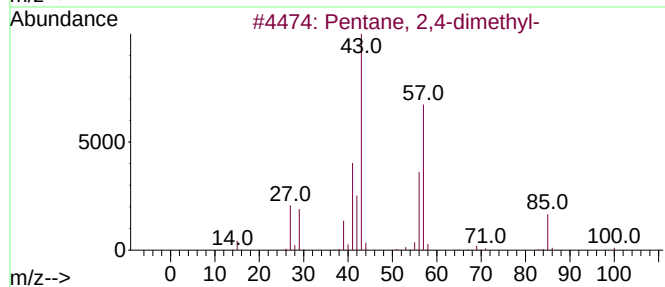
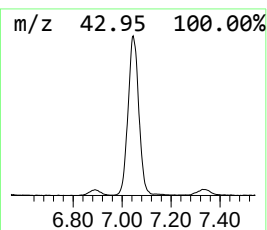
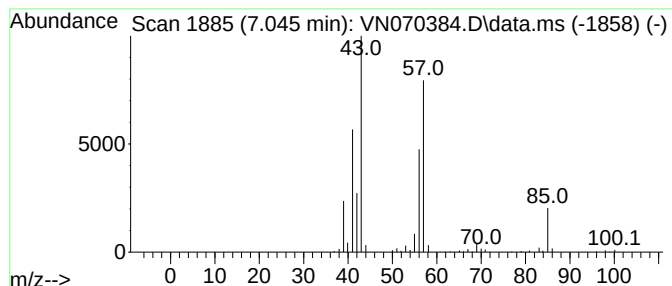
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	30.18 ug/l	1580840	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			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	50
5			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	50



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 50 Sample Multiplier: 1

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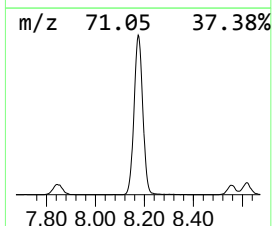
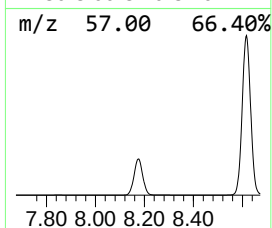
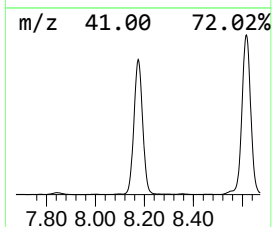
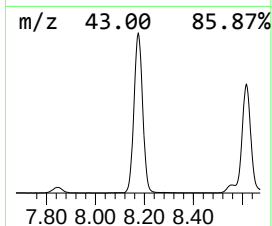
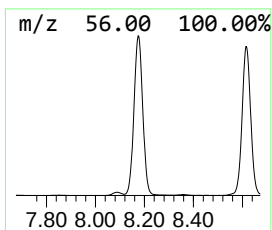
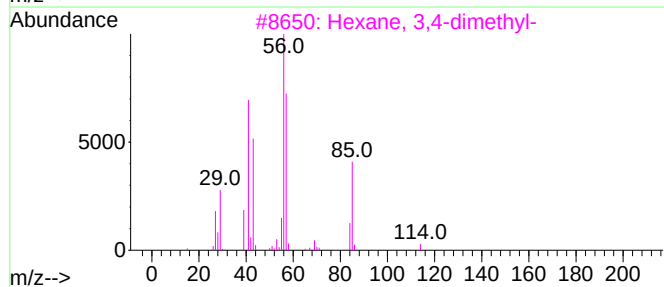
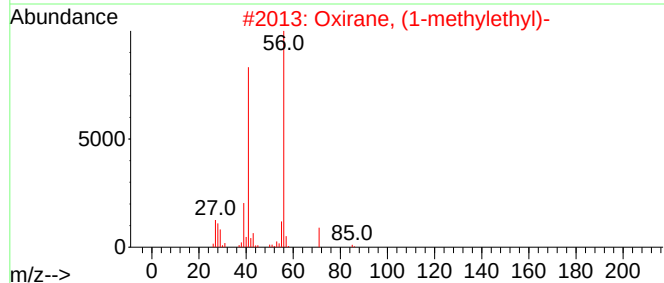
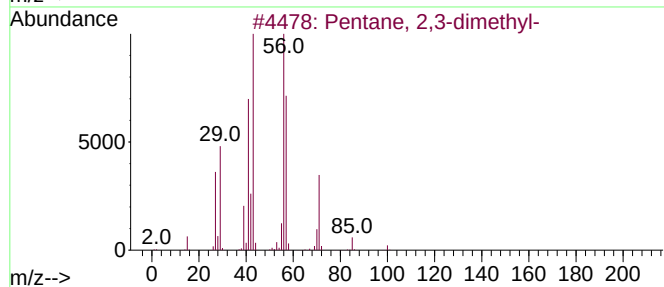
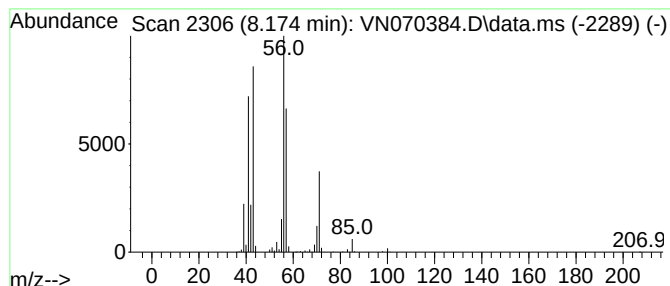
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	115.72 ug/l	6061790	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43
3			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	40
4			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	38



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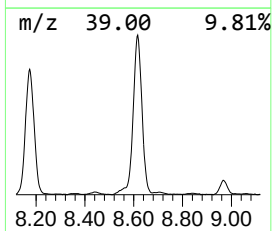
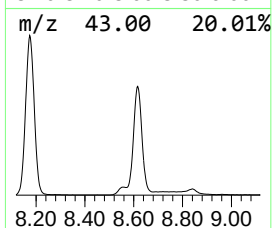
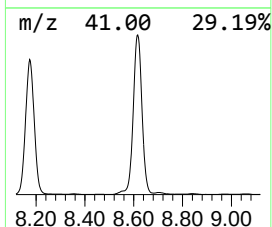
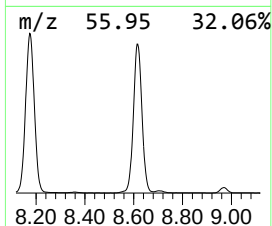
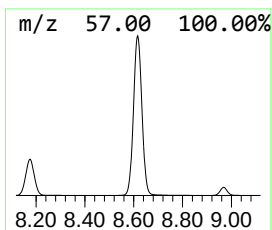
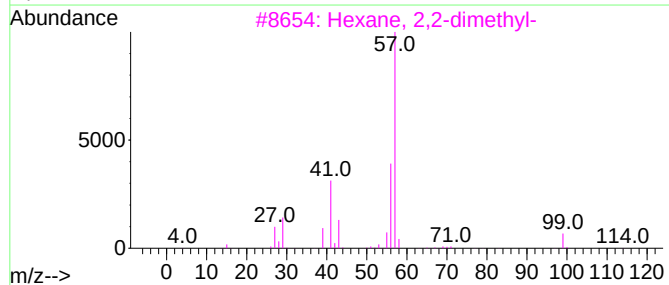
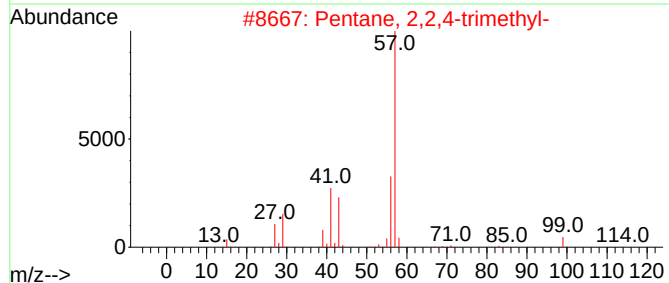
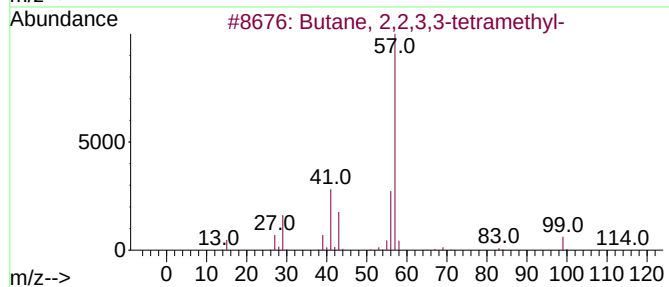
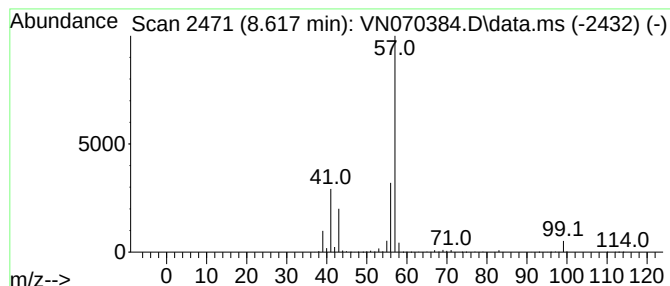
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	112.08 ug/l	8370890	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	83
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	64



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TOLL-MW-09RE

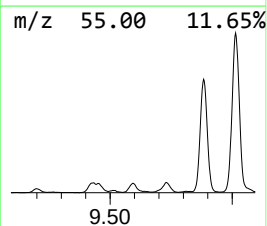
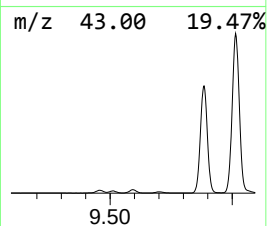
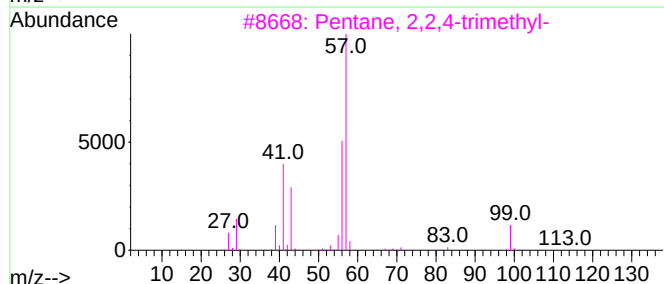
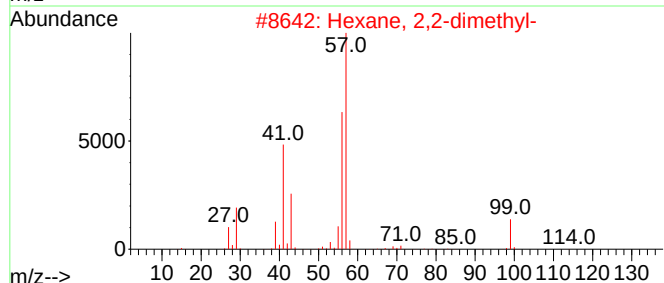
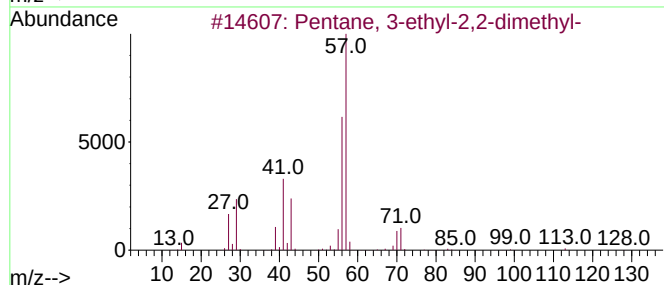
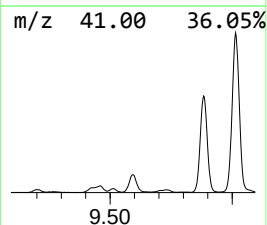
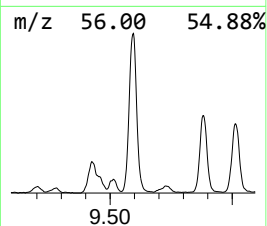
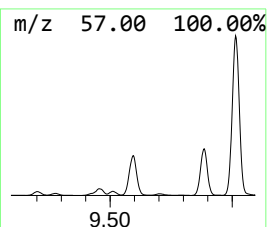
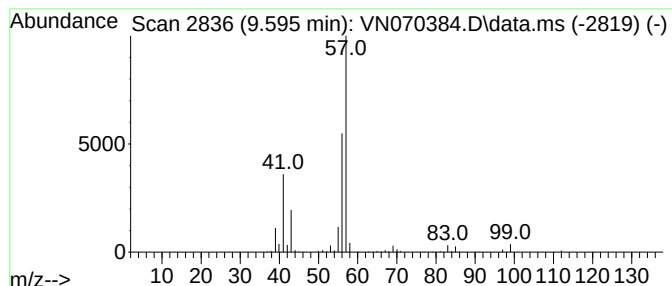
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-ethyl-2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.595	8.88 ug/l	663463	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
4			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	56
5			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070384.D
Acq On : 30 Dec 2021 8:00
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

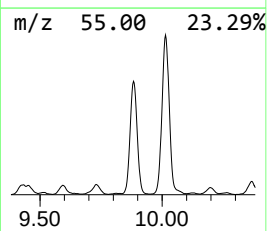
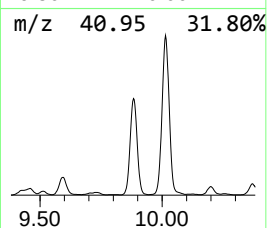
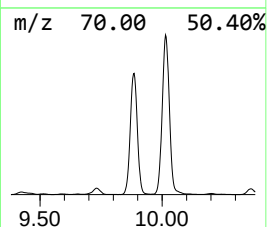
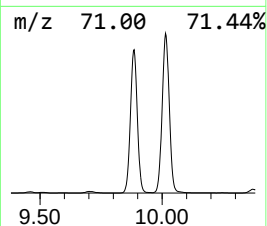
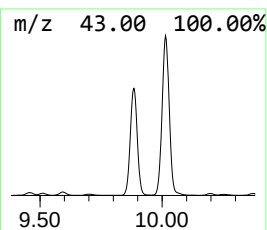
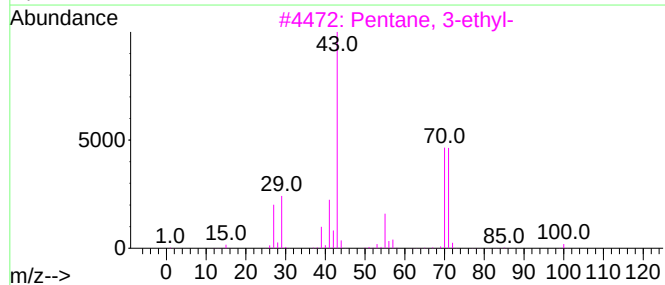
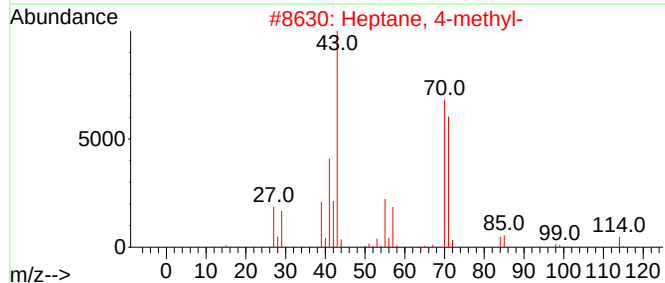
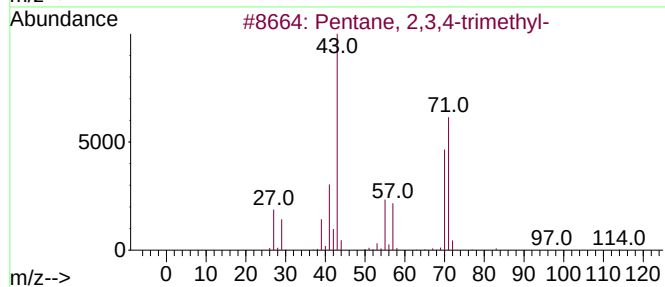
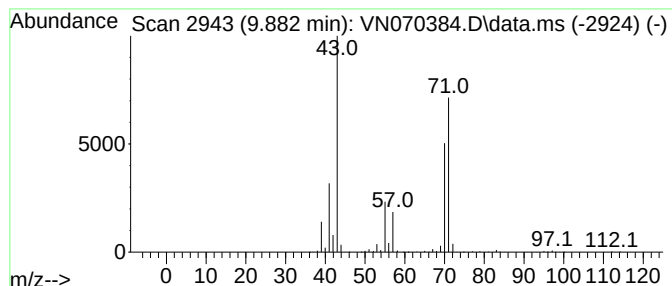
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.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.
9.882	67.63 ug/l	5050820	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	74
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070384.D
Acq On : 30 Dec 2021 8:00
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

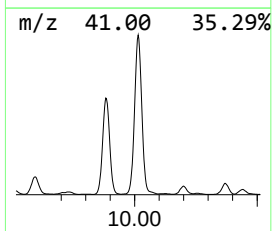
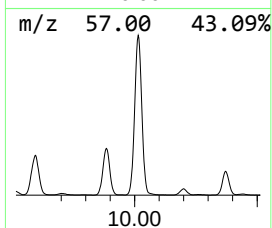
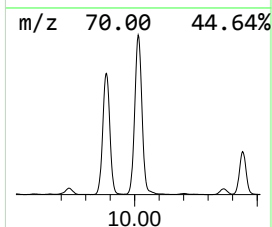
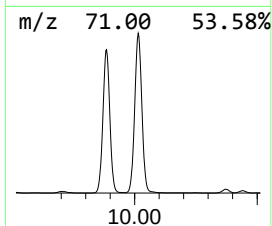
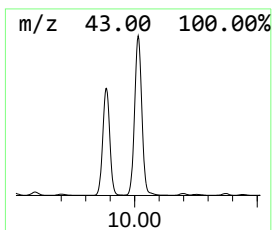
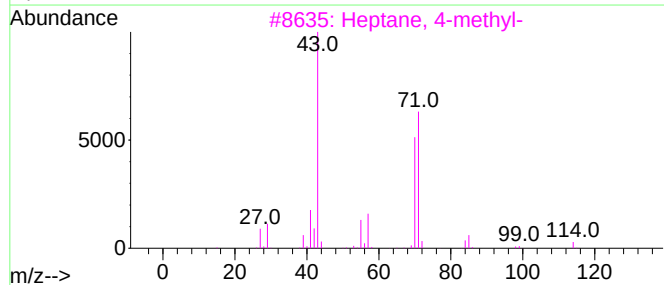
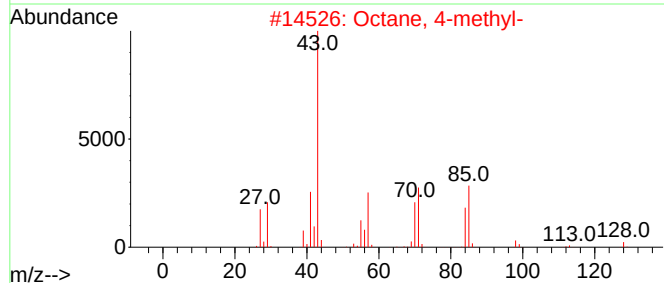
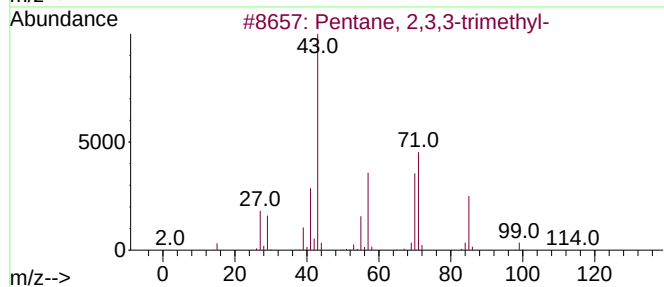
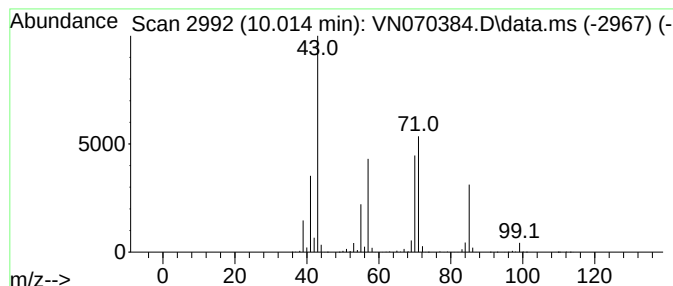
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	117.60 ug/l	8783040	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			Octane, 4-methyl-	128	C9H20	002216-34-4	78
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070384.D
Acq On : 30 Dec 2021 8:00
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 50 Sample Multiplier: 1

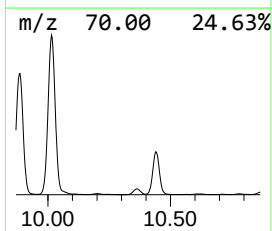
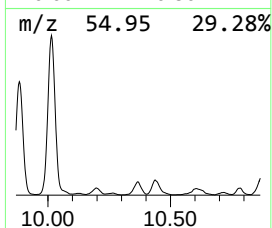
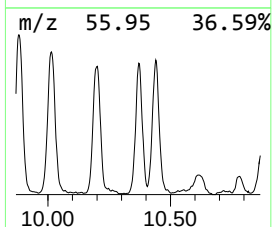
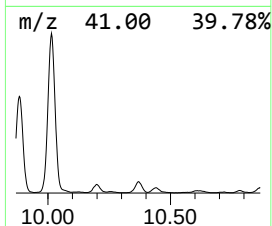
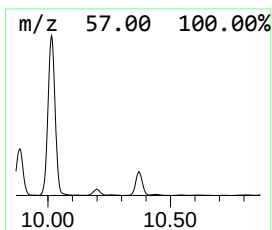
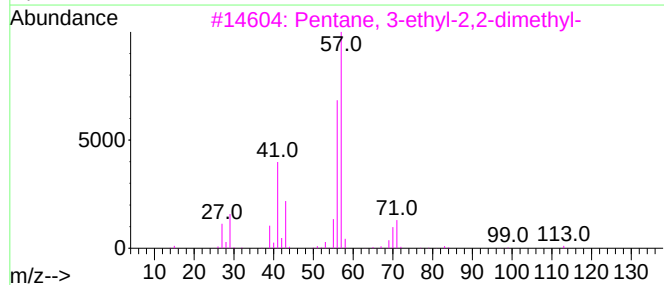
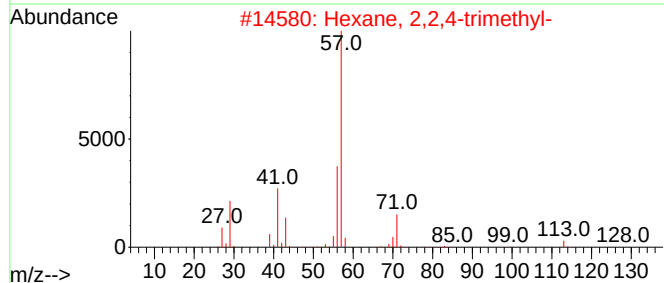
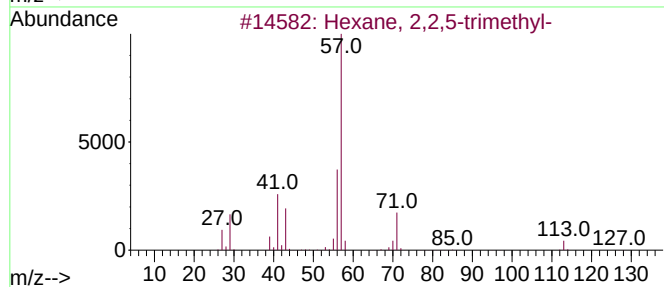
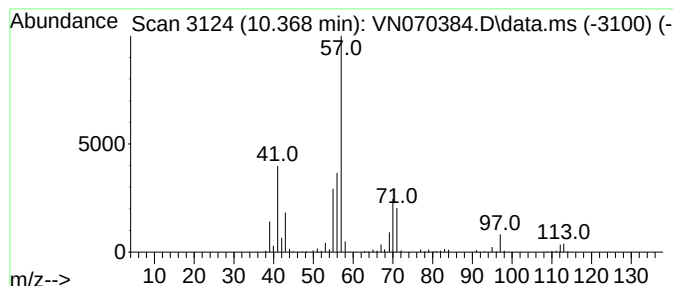
Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

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

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

Peak Number 9 Hexane, 2,2,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.368	5.67 ug/l	483868	Chlorobenzene-d5		11.746	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexane, 2,2,5-trimethyl-		128	C9H20	003522-94-9	50
2	Hexane, 2,2,4-trimethyl-		128	C9H20	016747-26-5	50
3	Pentane, 3-ethyl-2,2-dimethyl-		128	C9H20	016747-32-3	43
4	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	40
5	1-Hexene, 5,5-dimethyl-		112	C8H16	007116-86-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070384.D
Acq On : 30 Dec 2021 8:00
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

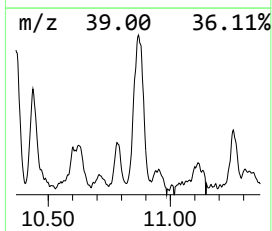
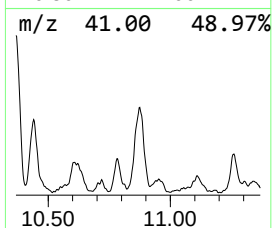
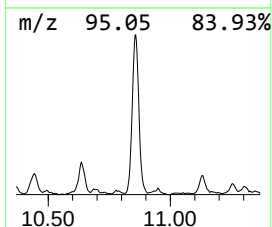
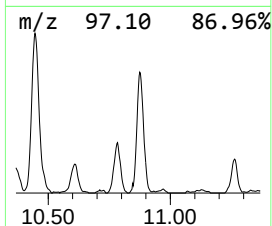
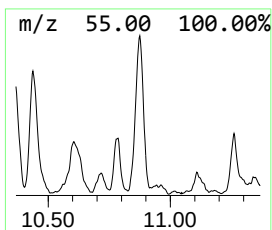
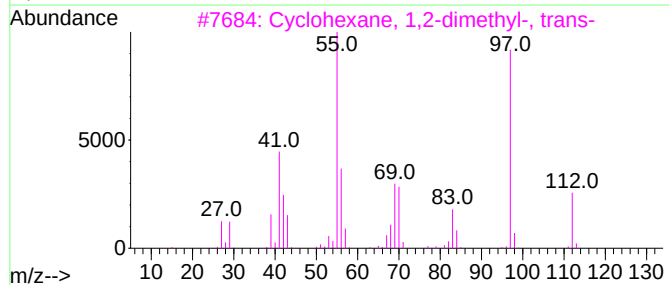
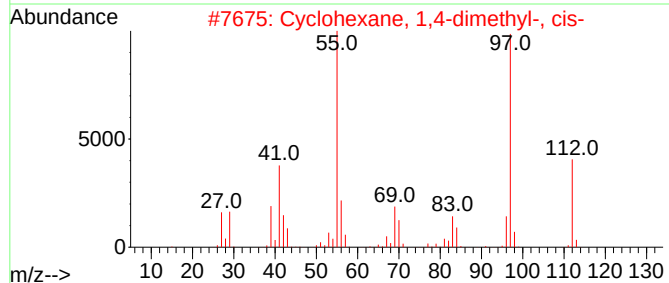
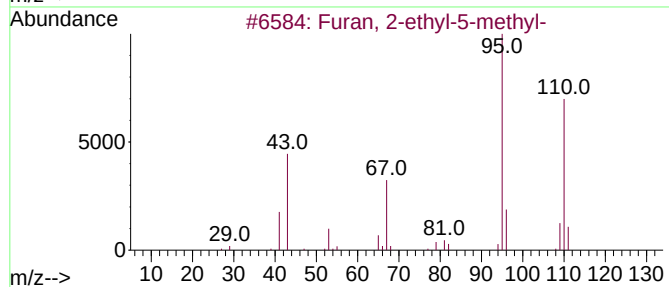
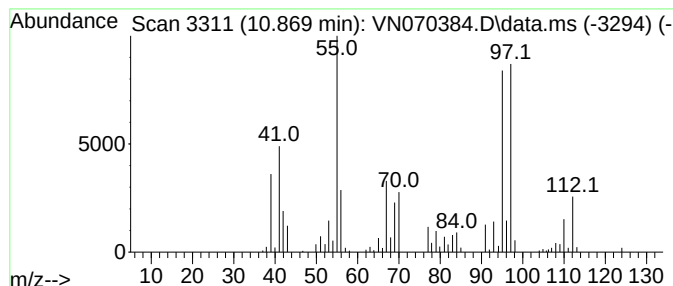
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 10 Furan, 2-ethyl-5-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	6.14 ug/l	524516	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	80
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	60
3			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	60
4			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	55
5			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070384.D
Acq On : 30 Dec 2021 8:00
Operator : JC/MD
Sample : M5007-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-09RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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-	3.140	12.6	ug/l	661353	1	8.088	2619280	50.0
Butane, 2,3-dim...	5.076	9.2	ug/l	481194	1	8.088	2619280	50.0
Pentane, 2,4-di...	7.045	30.2	ug/l	1580840	1	8.088	2619280	50.0
Pentane, 2,3-di...	8.174	115.7	ug/l	6061790	1	8.088	2619280	50.0
Butane, 2,2,3,3...	8.617	112.1	ug/l	8370890	2	8.968	3734160	50.0
Pentane, 3-ethy...	9.595	8.9	ug/l	663463	2	8.968	3734160	50.0
Pentane, 2,3,4-...	9.882	67.6	ug/l	5050820	2	8.968	3734160	50.0
Pentane, 2,3,3-...	10.014	117.6	ug/l	8783040	2	8.968	3734160	50.0
Hexane, 2,2,5-t...	10.368	5.7	ug/l	483868	3	11.746	4269500	50.0
Furan, 2-ethyl-...	10.869	6.1	ug/l	524516	3	11.746	4269500	50.0