

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
 Data File : VN070376.D
 Acq On : 30 Dec 2021 4:36
 Operator : JC/MD
 Sample : M5007-06
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-07RE

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: VN070376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.445	164	170	190	rVB3	85889	141561	2.75%	0.426%
2	4.596	956	972	999	rVB2	25152	79728	1.55%	0.240%
3	5.079	1129	1152	1176	rBV5	41852	159975	3.11%	0.481%
4	5.621	1327	1354	1383	rBV4	109430	397604	7.73%	1.196%
5	7.045	1867	1885	1909	rBV4	40261	115744	2.25%	0.348%
6	7.327	1972	1990	2013	rVB5	36343	103480	2.01%	0.311%
7	8.024	2228	2250	2261	rBV2	662631	1593335	30.98%	4.794%
8	8.086	2261	2273	2292	rVV	1179881	2702713	52.54%	8.132%
9	8.174	2292	2306	2332	rVB4	270590	685698	13.33%	2.063%
10	8.440	2384	2405	2430	rBV	808923	1864485	36.25%	5.610%
11	8.617	2450	2471	2494	rBV	902351	2187212	42.52%	6.581%
12	8.968	2582	2602	2633	rBV	1844302	3865180	75.14%	11.630%
13	9.424	2757	2772	2791	rBV9	25468	66247	1.29%	0.199%
14	9.593	2820	2835	2857	rBV	76209	173613	3.38%	0.522%
15	9.882	2926	2943	2966	rBV	585664	1171431	22.77%	3.525%
16	10.014	2972	2992	3022	rBV	975444	2006663	39.01%	6.038%
17	10.199	3043	3061	3076	rBV7	34903	75296	1.46%	0.227%
18	10.371	3109	3125	3135	rBV4	56256	102620	2.00%	0.309%
19	10.443	3135	3152	3184	rVV	2751708	5143720	100.00%	15.477%
20	10.861	3297	3308	3330	rVB10	38481	107522	2.09%	0.324%
21	11.744	3616	3637	3661	rBV	2405130	4372517	85.01%	13.156%
22	12.733	3988	4006	4028	rBV	1737953	3125948	60.77%	9.406%
23	13.675	4341	4357	4380	rBV	1630688	2886494	56.12%	8.685%
24	14.150	4518	4534	4548	rBV3	57299	106042	2.06%	0.319%

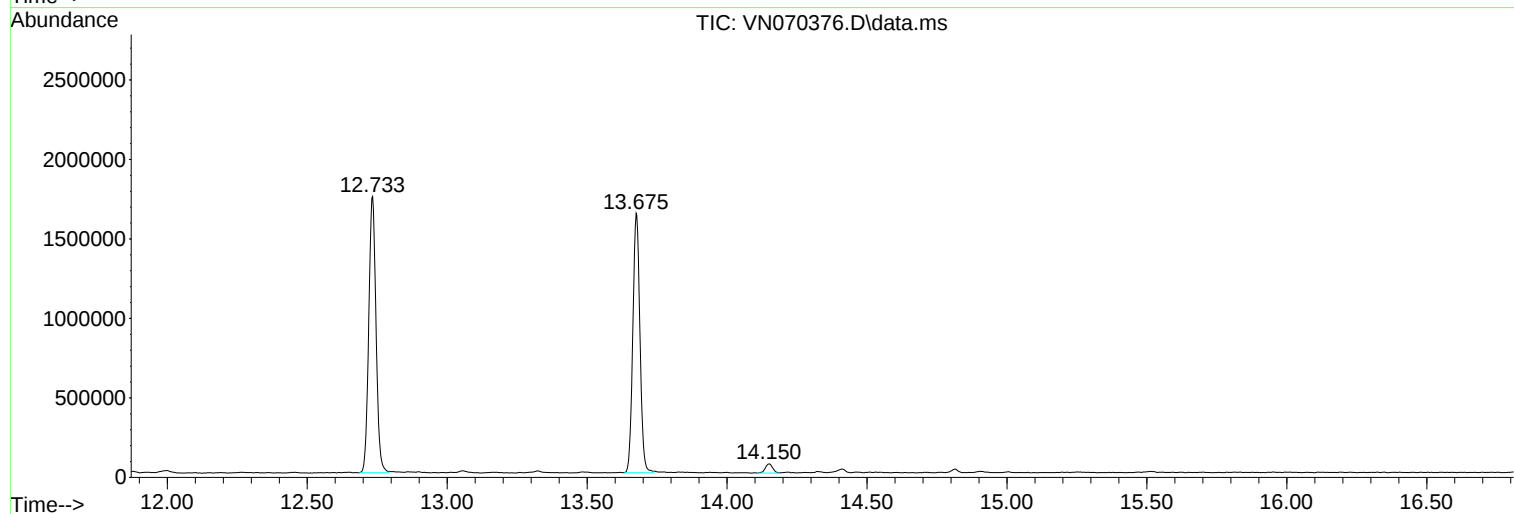
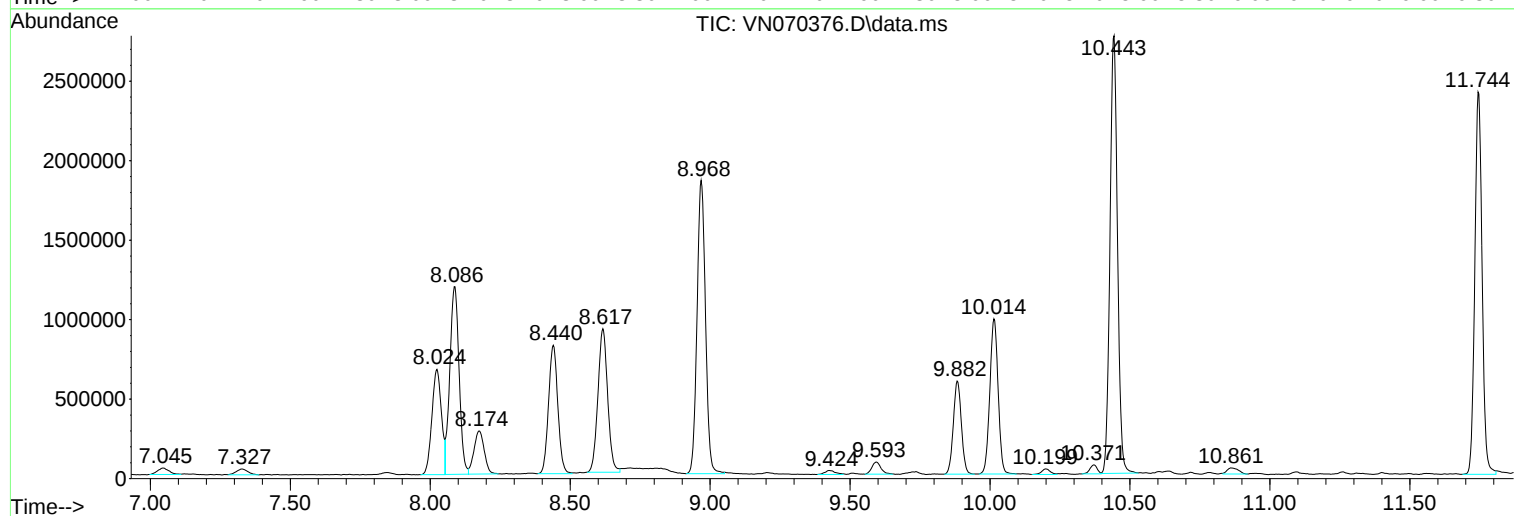
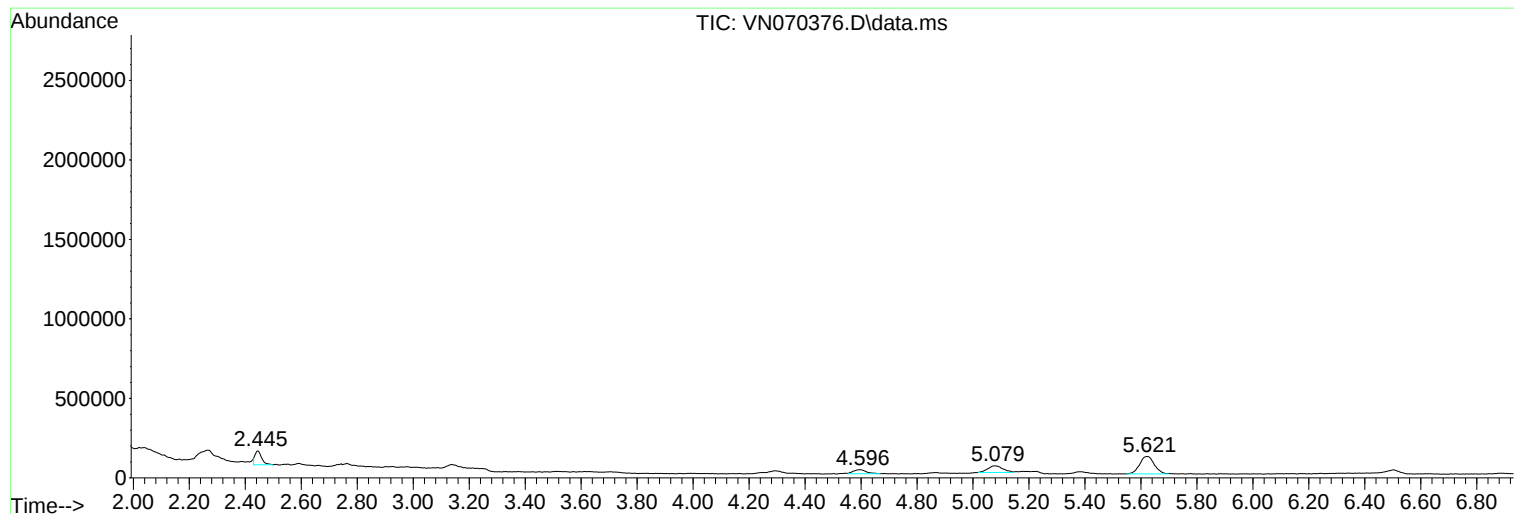
Sum of corrected areas: 33234828

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070376.D
Acq On : 30 Dec 2021 4:36
Operator : JC/MD
Sample : M5007-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-07RE

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070376.D
Acq On : 30 Dec 2021 4:36
Operator : JC/MD
Sample : M5007-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-07RE

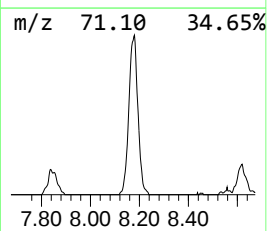
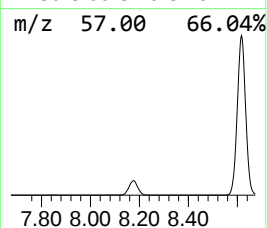
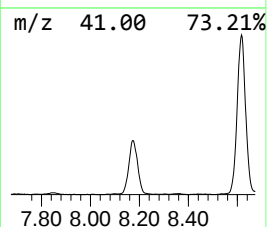
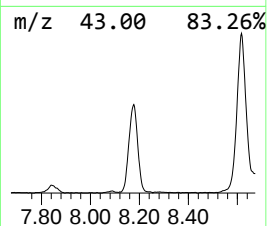
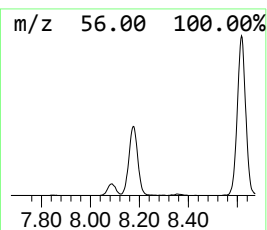
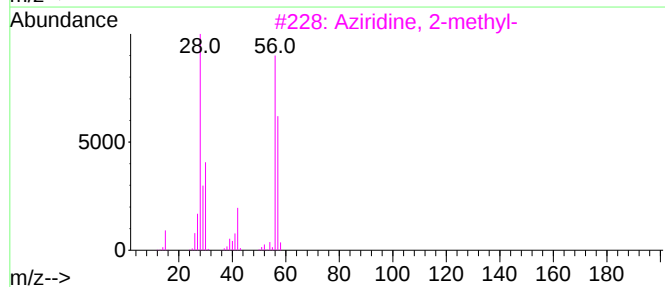
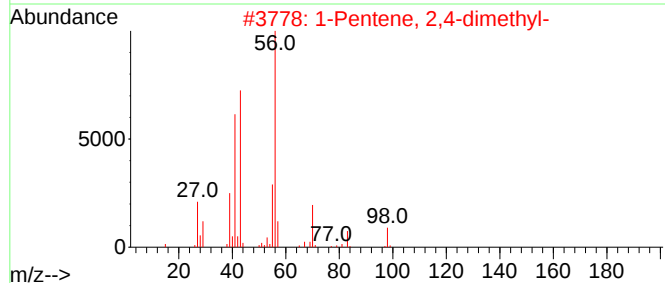
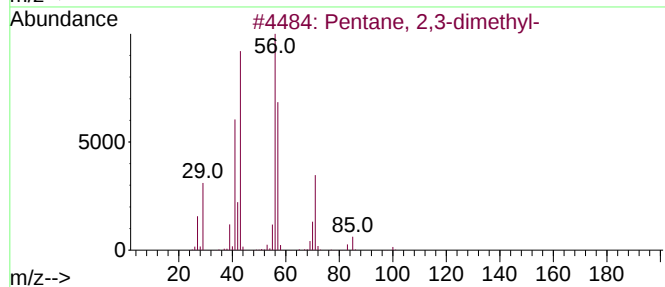
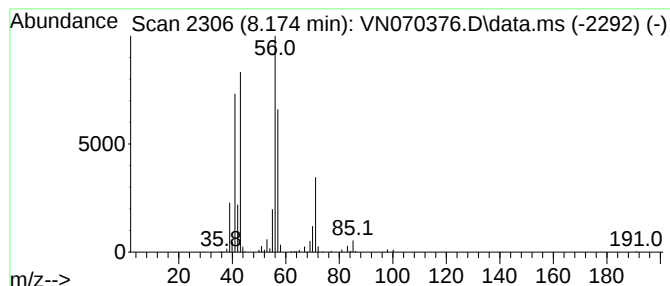
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	12.69 ug/l	685698	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	59
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
4			4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	47
5			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070376.D
Acq On : 30 Dec 2021 4:36
Operator : JC/MD
Sample : M5007-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-07RE

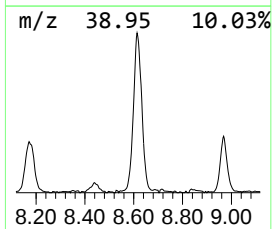
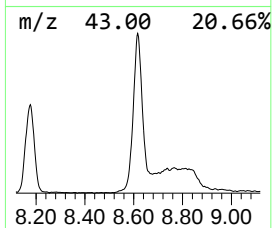
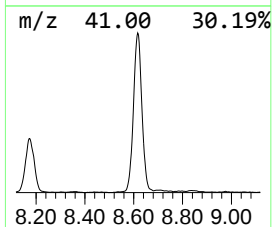
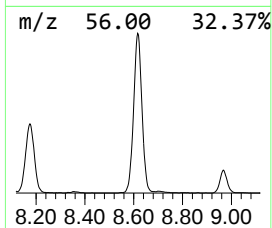
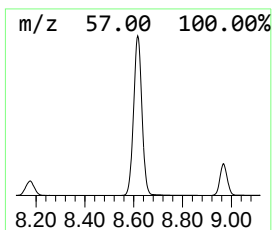
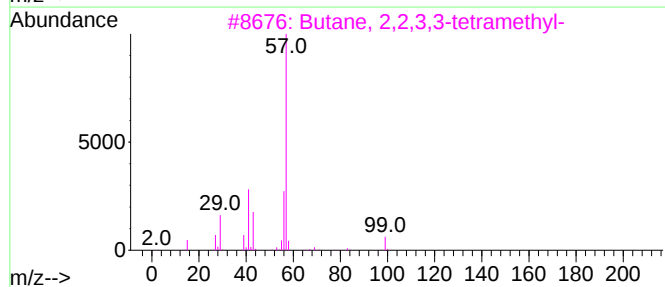
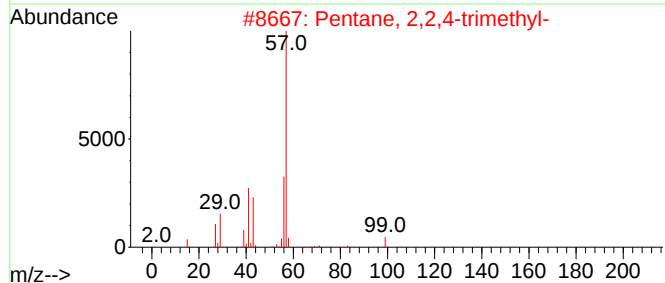
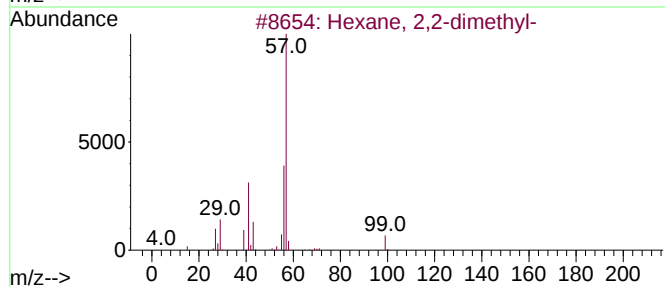
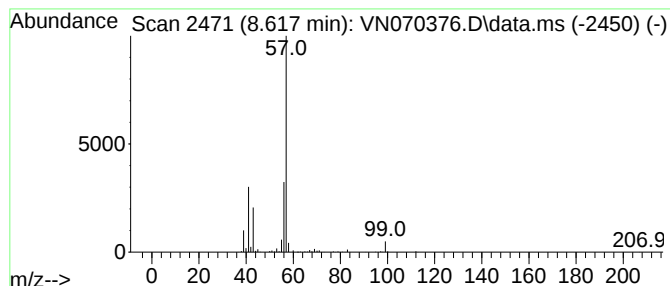
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	28.29 ug/l	2187210	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070376.D
Acq On : 30 Dec 2021 4:36
Operator : JC/MD
Sample : M5007-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-07RE

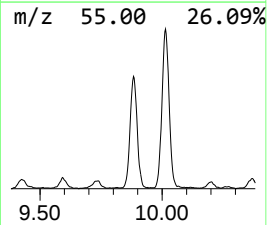
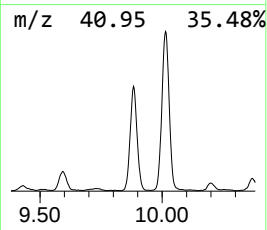
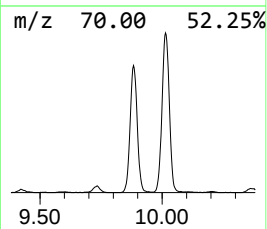
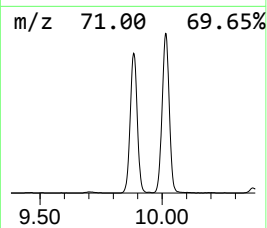
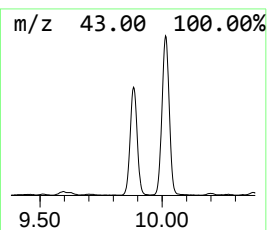
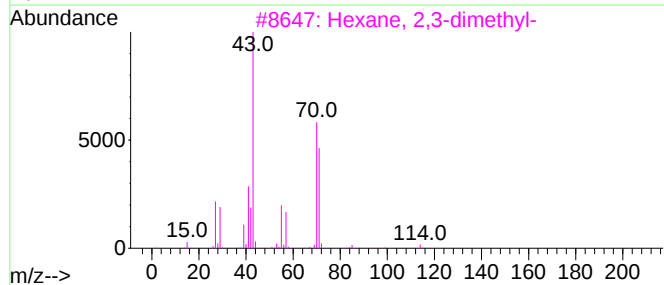
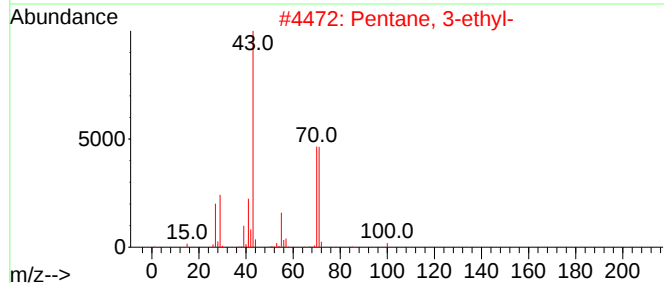
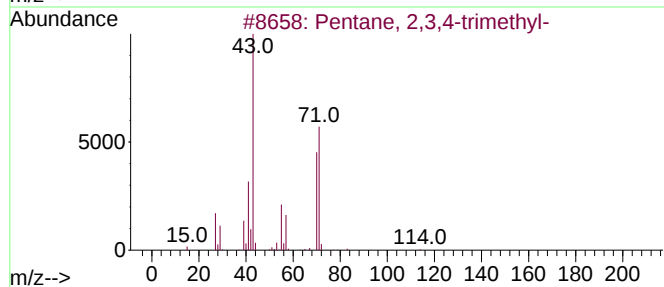
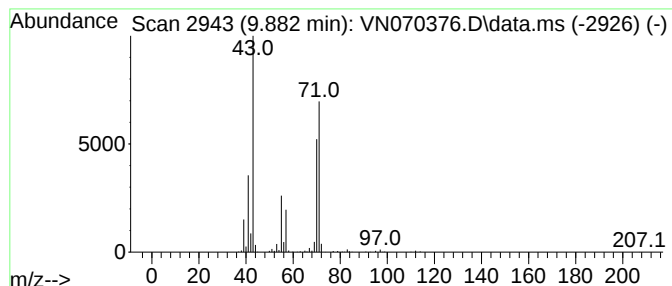
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.882	15.15 ug/l	1171430	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			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
3			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070376.D
Acq On : 30 Dec 2021 4:36
Operator : JC/MD
Sample : M5007-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-07RE

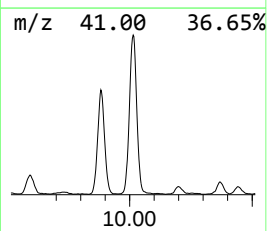
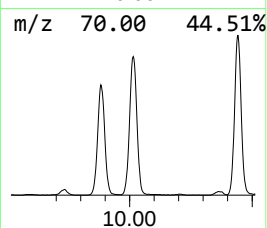
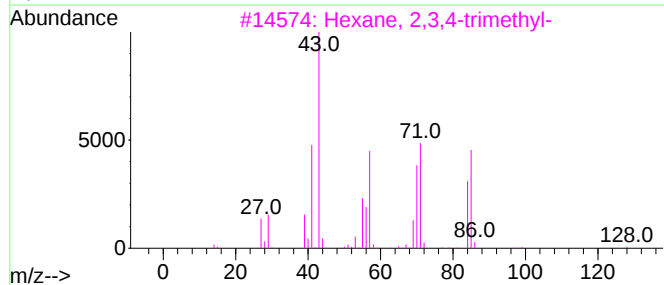
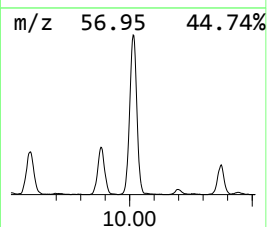
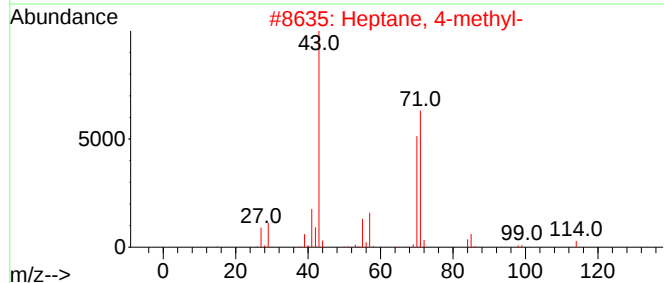
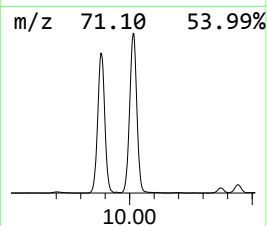
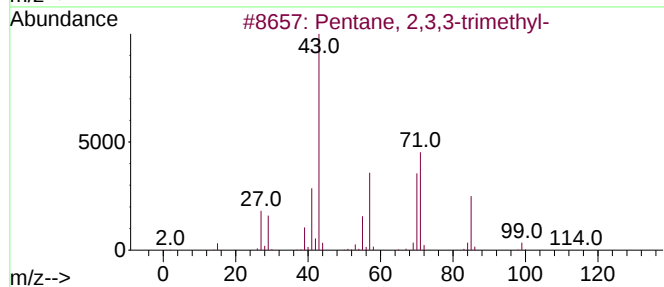
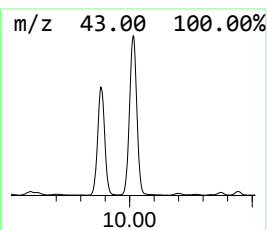
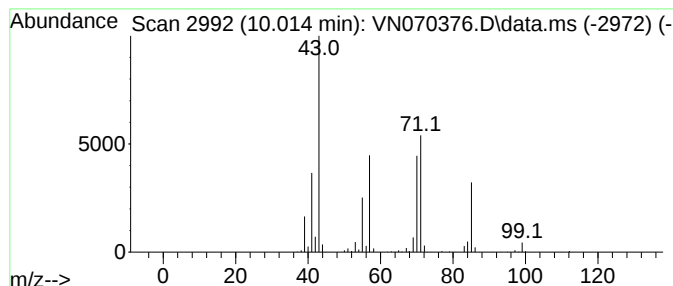
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	25.96 ug/l	2006660	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, 2,3,4-trimethyl-	128	C9H20	000921-47-1	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 : VN070376.D
Acq On : 30 Dec 2021 4:36
Operator : JC/MD
Sample : M5007-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-07RE

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.174	12.7	ug/l	685698	1	8.088	2702710	50.0
Hexane, 2,2-dim...	8.617	28.3	ug/l	2187210	2	8.968	3865180	50.0
Pentane, 2,3,4-...	9.882	15.2	ug/l	1171430	2	8.968	3865180	50.0
Pentane, 2,3,3-...	10.014	26.0	ug/l	2006660	2	8.968	3865180	50.0