

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070049.D
 Acq On : 13 Dec 2021 23:42
 Operator : JC/MD
 Sample : M5007-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 29 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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.271	98	105	137	rVB4	178464	423409	5.46%	0.902%
2	2.445	160	170	188	rVB3	216165	368162	4.75%	0.784%
3	5.618	1326	1353	1383	rBV4	100396	364573	4.70%	0.776%
4	7.045	1867	1885	1908	rBV4	58029	167539	2.16%	0.357%
5	7.327	1967	1990	2019	rBV3	153537	431139	5.56%	0.918%
6	8.021	2226	2249	2261	rBV	858953	2065277	26.62%	4.398%
7	8.085	2261	2273	2291	rVV	1407635	3232780	41.67%	6.883%
8	8.174	2292	2306	2328	rVB3	337813	850314	10.96%	1.811%
9	8.440	2385	2405	2431	rBV2	958922	2265099	29.20%	4.823%
10	8.617	2452	2471	2493	rVB	519759	1244586	16.04%	2.650%
11	8.968	2581	2602	2629	rBV	2389178	5033515	64.89%	10.718%
12	9.512	2796	2805	2820	rVB7	40440	80917	1.04%	0.172%
13	9.593	2822	2835	2851	rVV2	52044	106252	1.37%	0.226%
14	9.882	2925	2943	2965	rBV	495485	998487	12.87%	2.126%
15	10.014	2973	2992	3012	rBV	722578	1488911	19.19%	3.170%
16	10.371	3112	3125	3135	rBV2	92851	167265	2.16%	0.356%
17	10.440	3135	3151	3181	rVV	3955519	7378440	95.12%	15.711%
18	10.641	3217	3226	3239	rVB5	62716	119841	1.54%	0.255%
19	10.717	3242	3254	3267	rVB3	54495	96890	1.25%	0.206%
20	11.744	3617	3637	3681	rBV	4256422	7757361	100.00%	16.517%
21	12.731	3988	4005	4034	rBV	3328201	5904663	76.12%	12.573%
22	13.675	4340	4357	4392	rBV	3703758	6419310	82.75%	13.668%

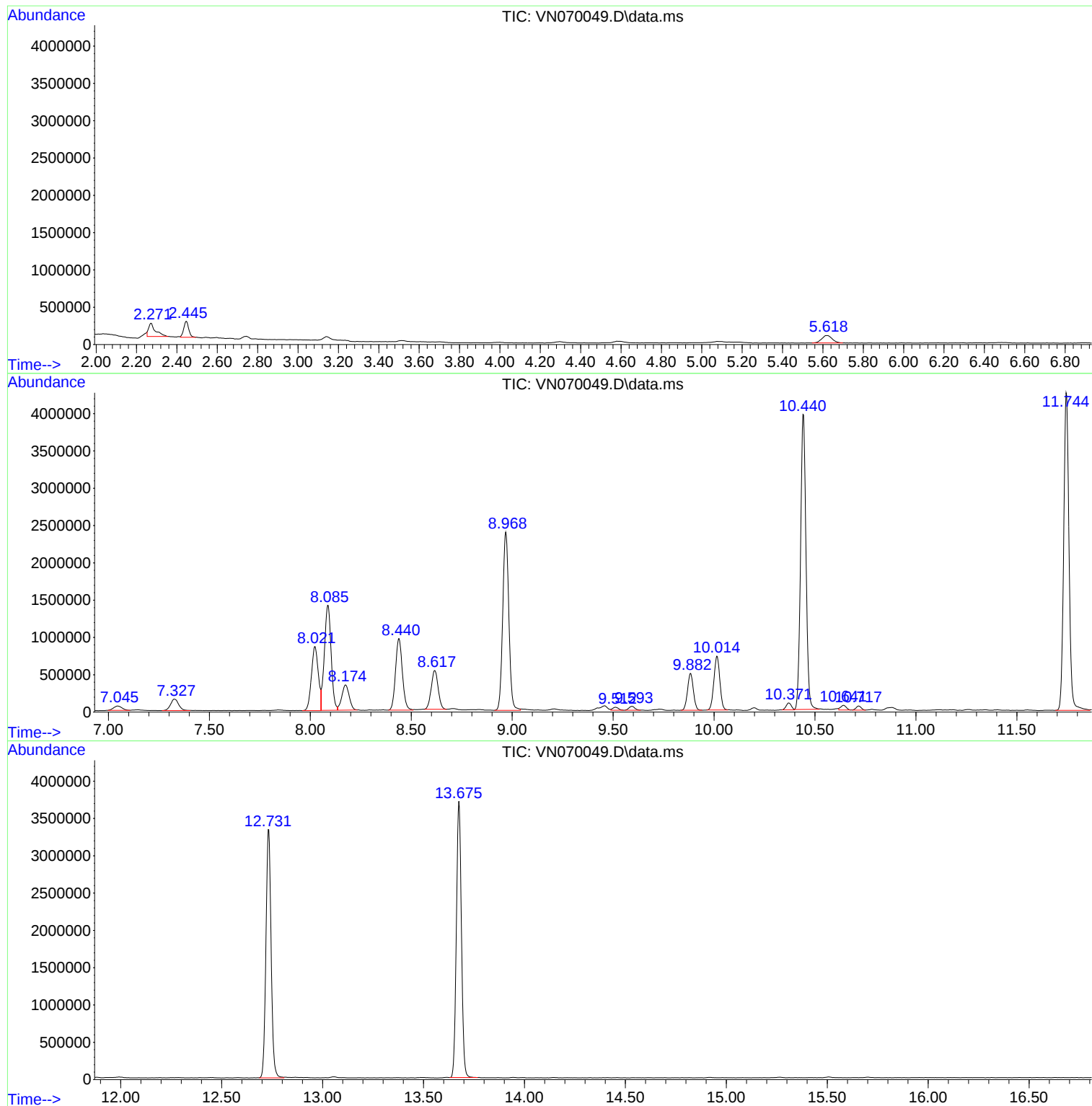
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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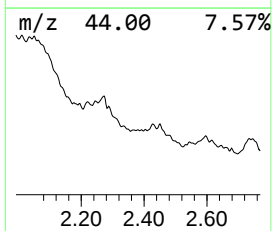
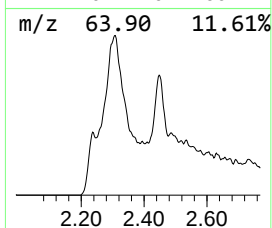
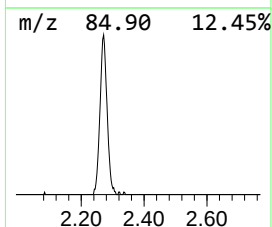
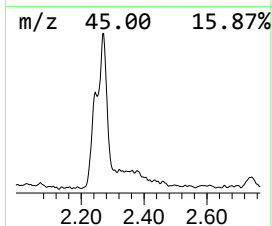
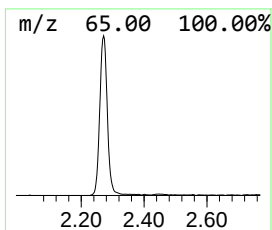
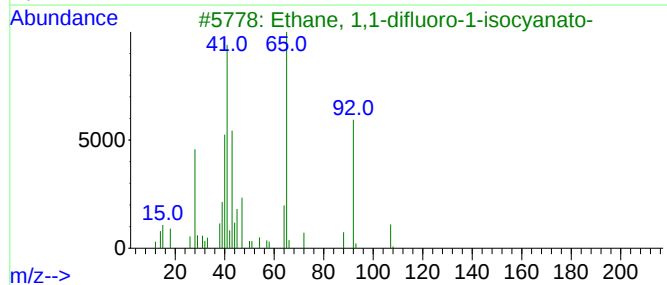
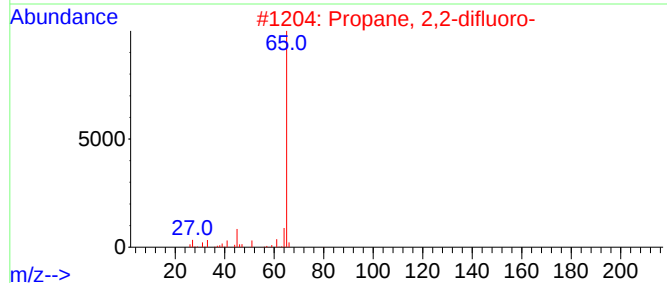
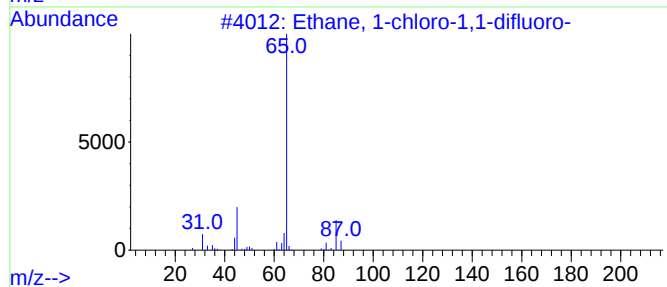
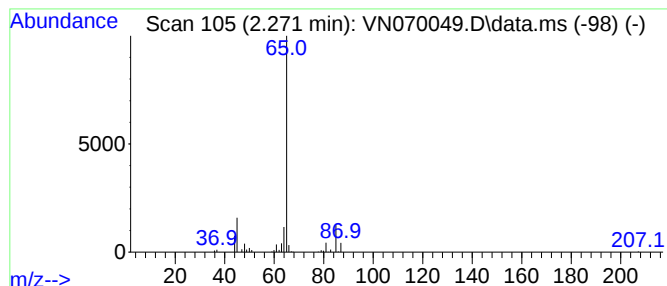
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.271	6.55 ug/l	423409	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	83
2			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	64
3			Ethane, 1,1-difluoro-1-isocyanato-	107	C3H3F2NO	001645-88-1	4
4			Dichloroacetic acid, pent-2-en-4...	192	C7H6Cl2O2	1000299-43-1	4
5			2,2-Difluoropropionic acid	110	C3H4F2O2	000373-96-6	4



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TOLL-MW-04

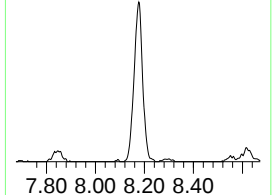
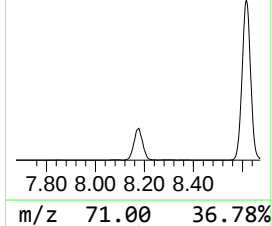
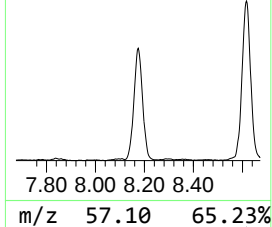
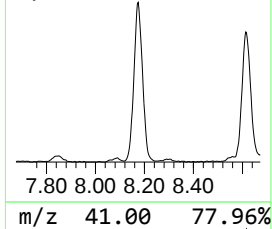
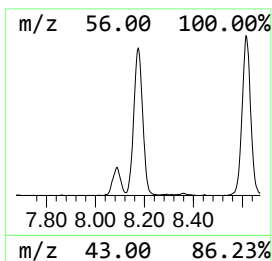
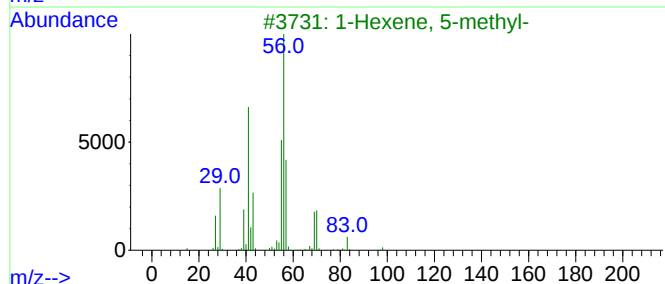
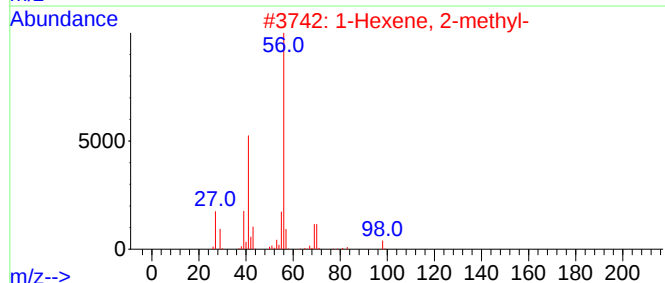
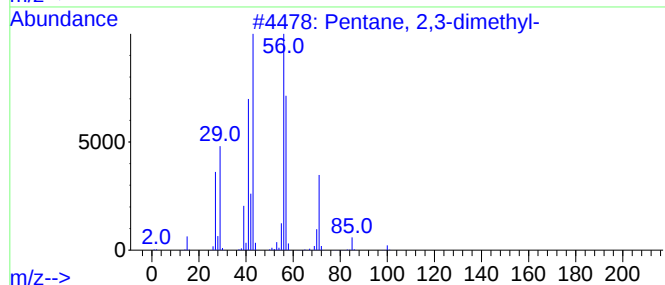
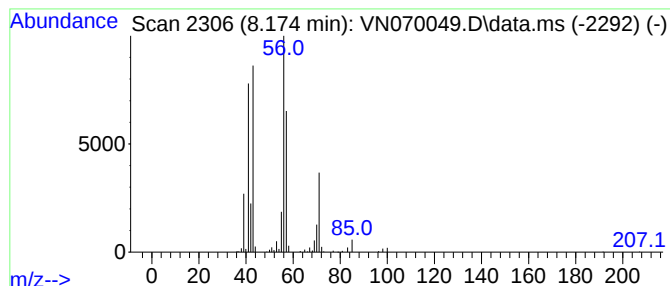
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	13.15 ug/l	850314	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	50
3			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	50
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
5			Pentane, 1-bromo-3,4-dimethyl-	178	C7H15Br	006570-92-9	42



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TOLL-MW-04

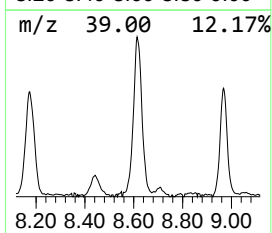
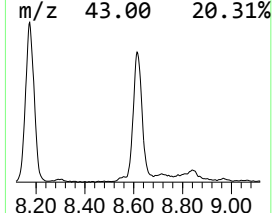
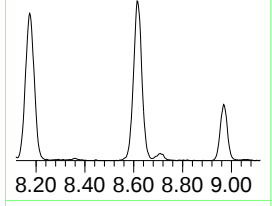
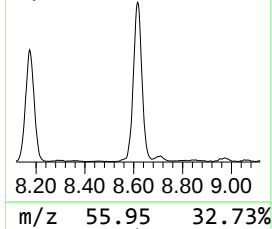
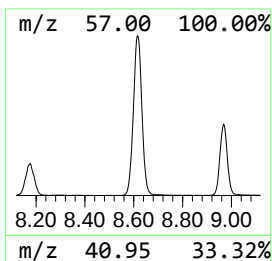
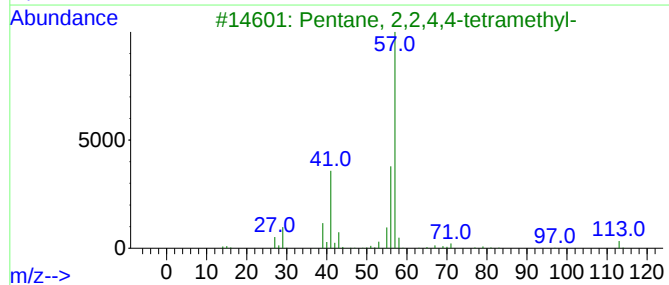
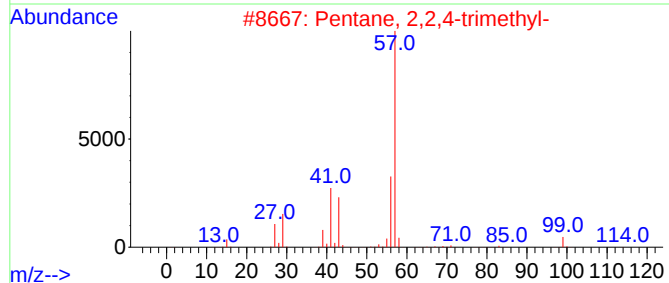
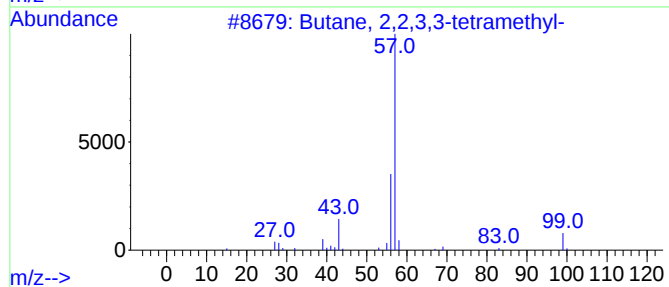
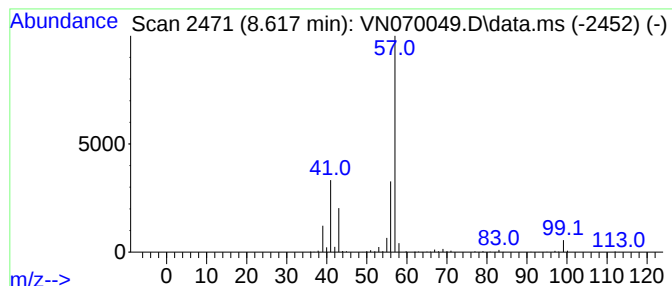
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	12.36 ug/l	1244590	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	78
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59



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Instrument :
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ClientSampleId :
TOLL-MW-04

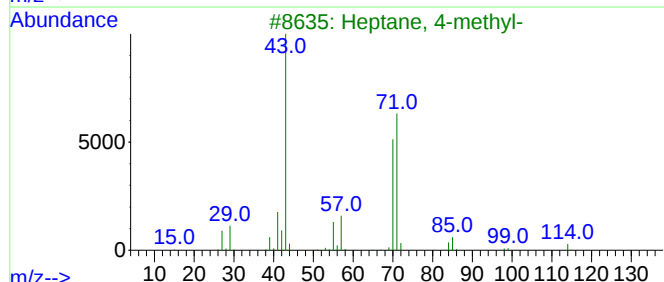
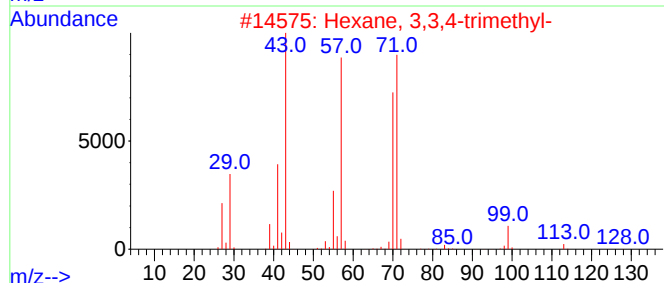
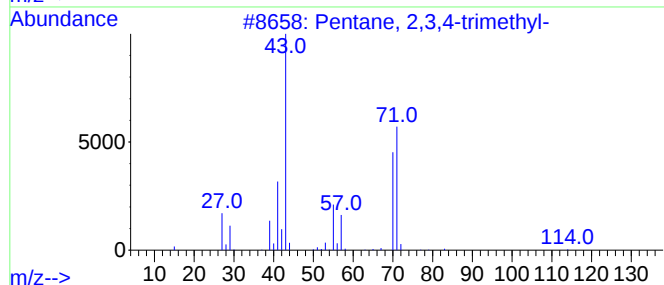
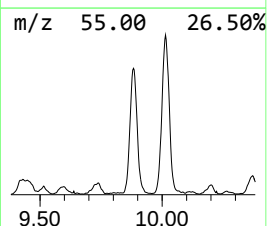
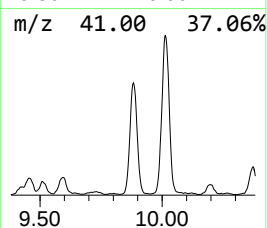
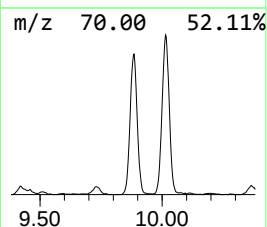
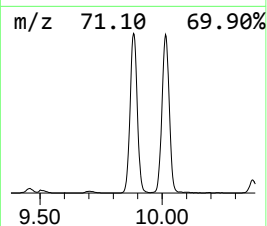
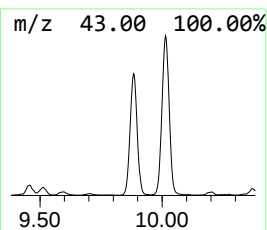
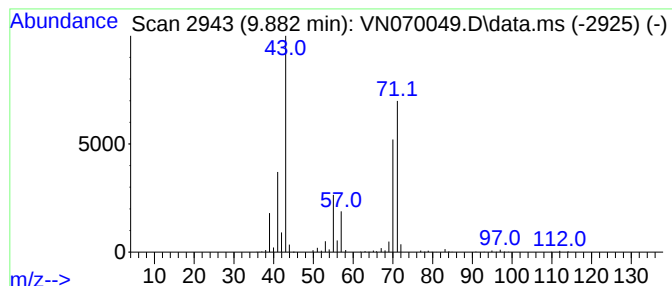
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.882	9.92 ug/l	998487	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			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	64
5			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64



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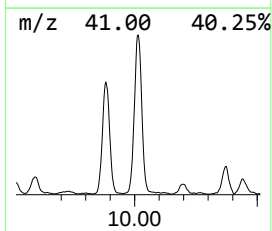
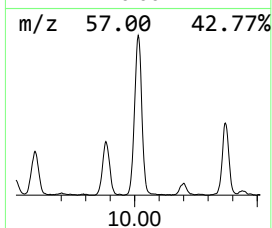
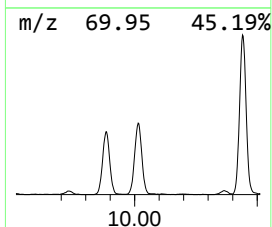
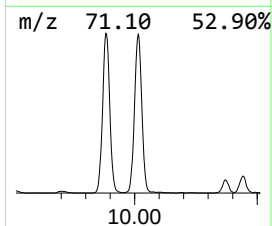
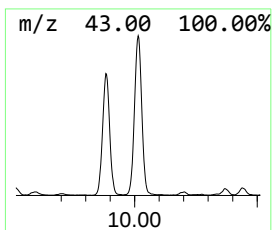
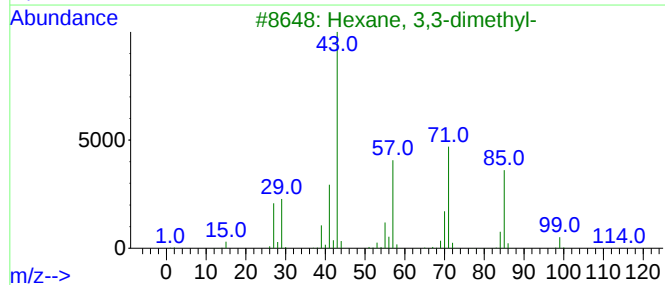
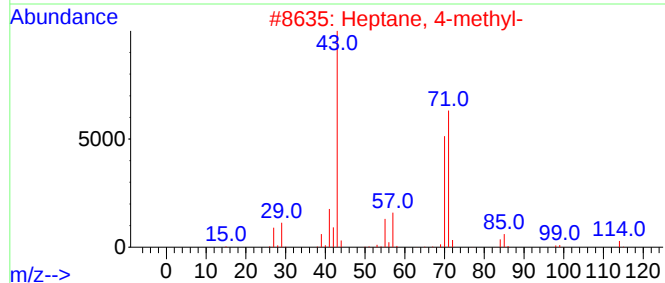
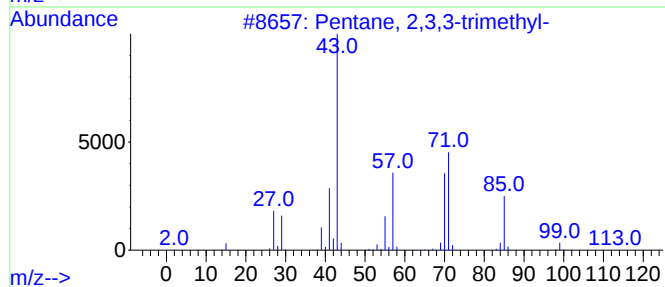
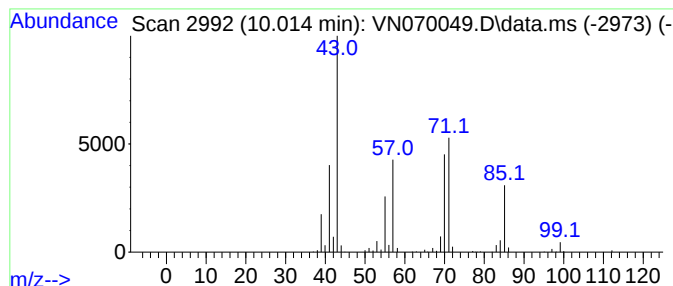
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	14.79 ug/l	1488910	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	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	59



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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
Ethane, 1-chlor...	2.271	6.5	ug/l	423409	1	8.088	3232780	50.0
Pentane, 2,3-di...	8.174	13.2	ug/l	850314	1	8.088	3232780	50.0
Butane, 2,2,3,3...	8.617	12.4	ug/l	1244590	2	8.968	5033520	50.0
Pentane, 2,3,4-...	9.882	9.9	ug/l	998487	2	8.968	5033520	50.0
Pentane, 2,3,3-...	10.014	14.8	ug/l	1488910	2	8.968	5033520	50.0