

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
 Data File : VN065482.D
 Acq On : 11 Jan 2021 21:02
 Operator : JC/MD
 Sample : M1058-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB-2021-WW-000-05

Integration Parameters: RTEINT.P

Integrator: RTE

Smoother: 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\82N122220W.M

Title : SW846 8260

Signal : TIC: VN065482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.544	830	872	904	rBV2	163408	584338	3.43%	1.752%
2	5.003	988	1015	1049	rBV	317796	1172596	6.88%	3.517%
3	5.521	1150	1176	1228	rBV	1268611	4072194	23.88%	12.213%
4	6.019	1312	1331	1379	rBV2	110695	368017	2.16%	1.104%
5	6.582	1465	1506	1545	rBV	1141188	3659917	21.46%	10.976%
6	7.556	1791	1809	1819	rBV2	135944	342241	2.01%	1.026%
7	7.627	1819	1831	1863	rVB	245409	612065	3.59%	1.836%
8	7.994	1928	1945	1973	rBV	137710	332333	1.95%	0.997%
9	8.553	2104	2119	2145	rVB	369986	768506	4.51%	2.305%
10	8.804	2181	2197	2220	rBV	203695	418618	2.45%	1.255%
11	10.061	2573	2588	2616	rBV	601522	1099785	6.45%	3.298%
12	10.605	2740	2757	2789	rBV	9460095	17052097	100.00%	51.141%
13	11.379	2982	2998	3023	rBV	598105	1062341	6.23%	3.186%
14	12.376	3294	3308	3332	rBV	506386	864850	5.07%	2.594%
15	13.318	3588	3601	3621	rBV	542298	933707	5.48%	2.800%

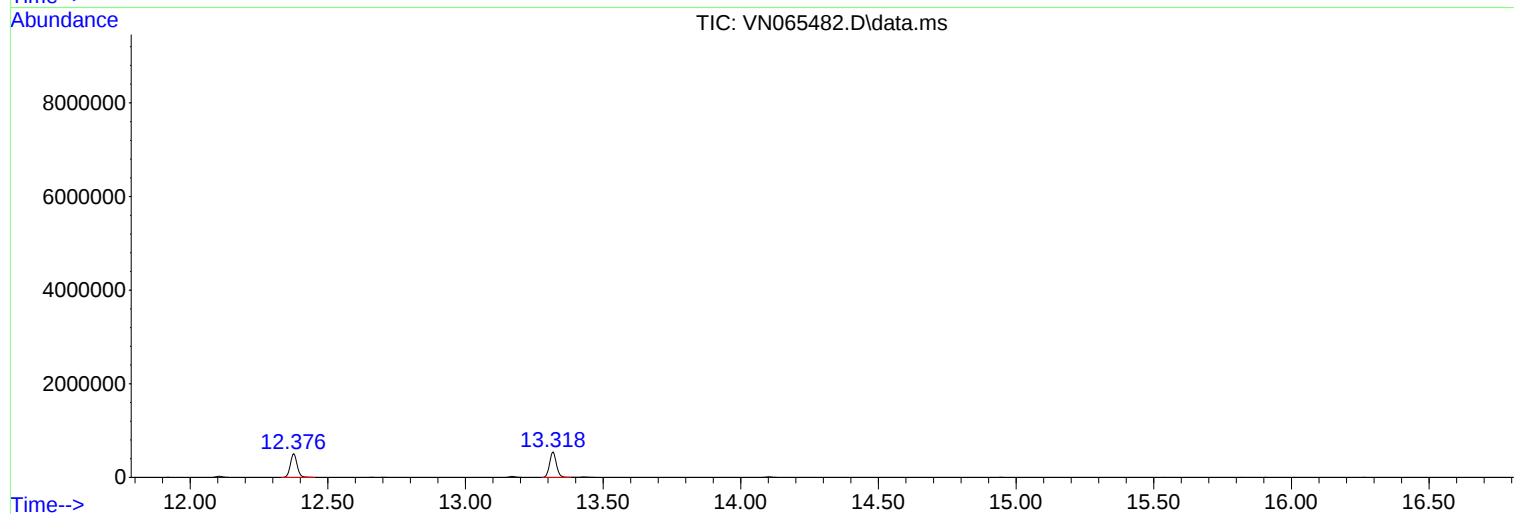
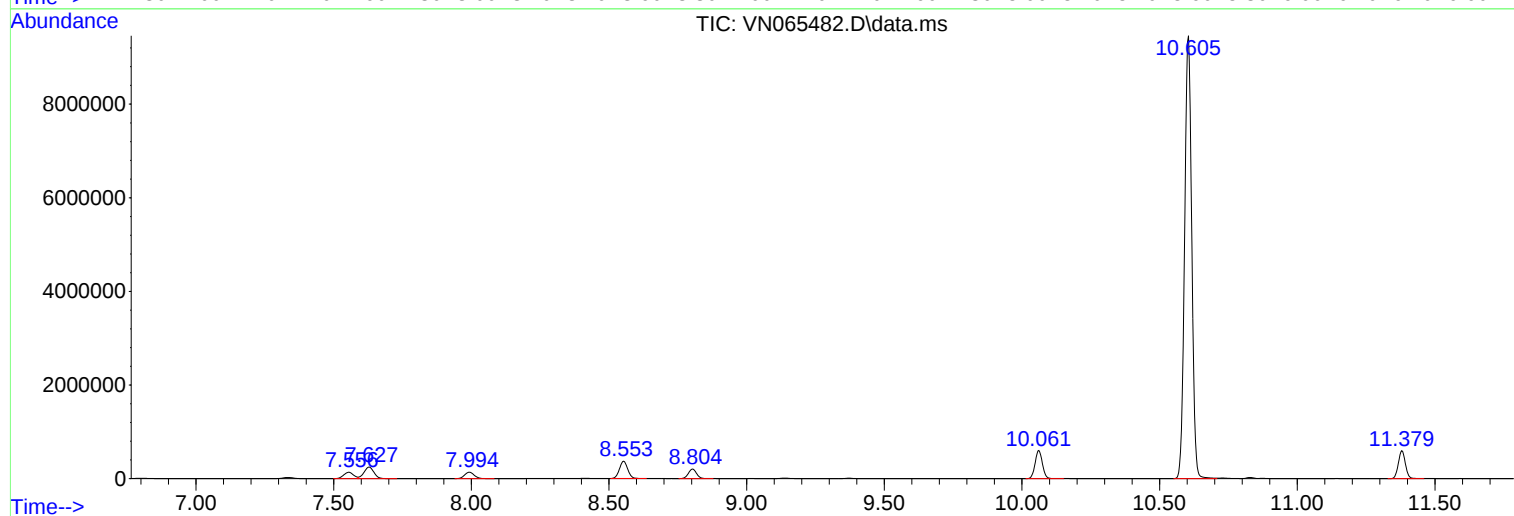
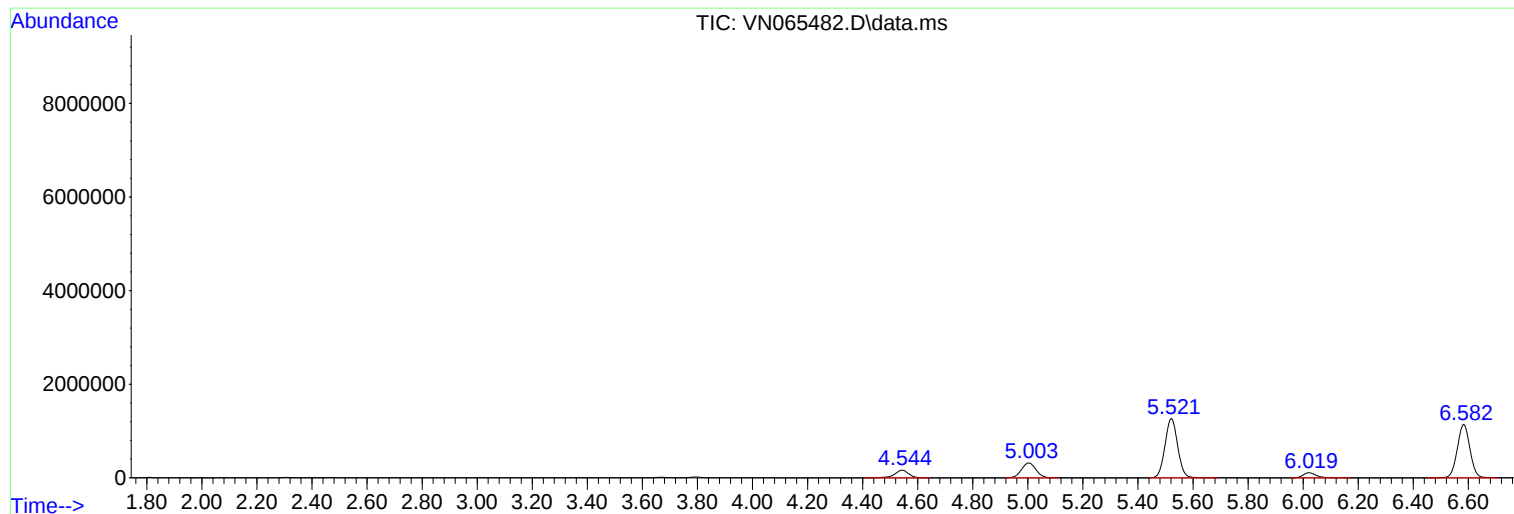
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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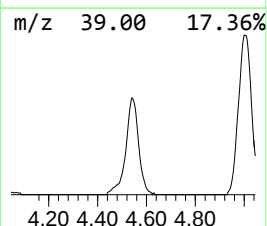
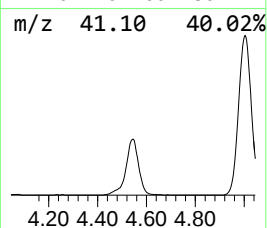
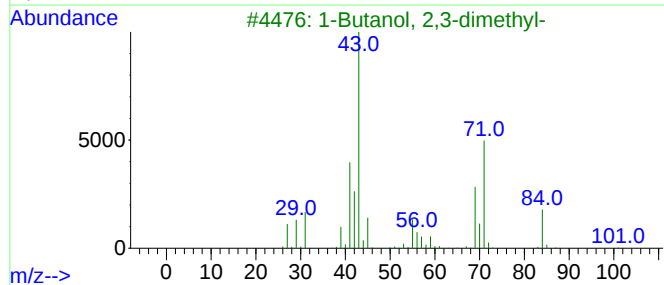
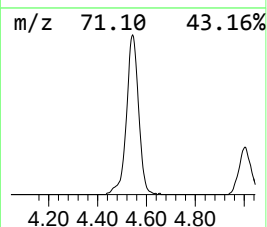
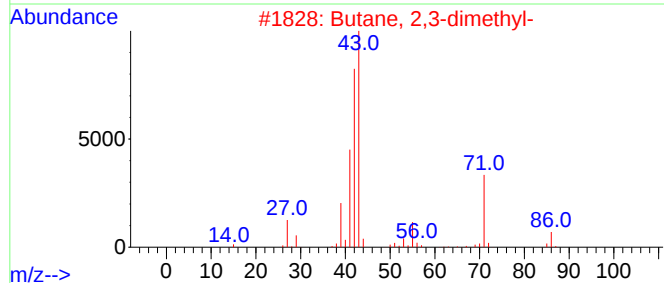
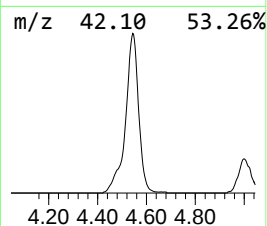
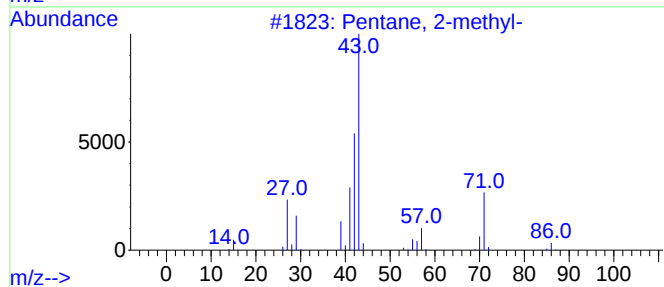
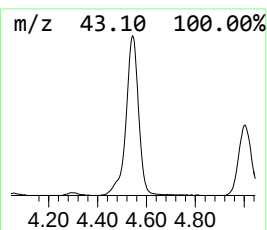
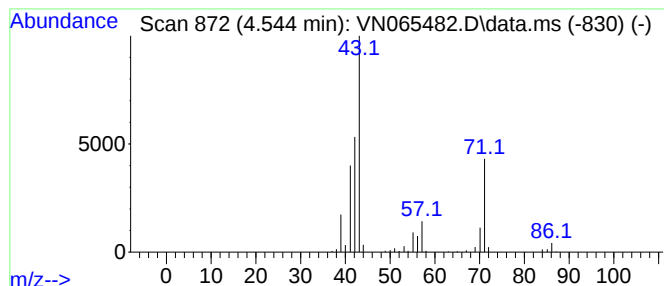
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.544	47.73 ug/l	584338	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	49
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4			Pentane	72	C5H12	000109-66-0	43
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	42



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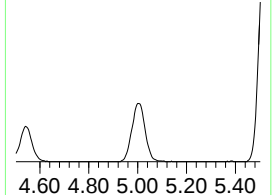
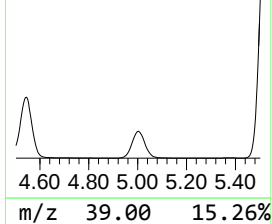
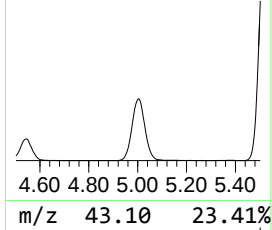
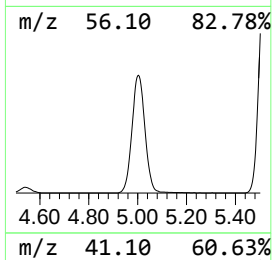
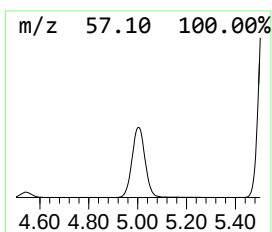
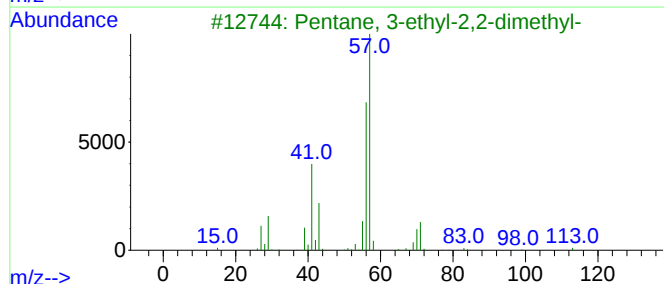
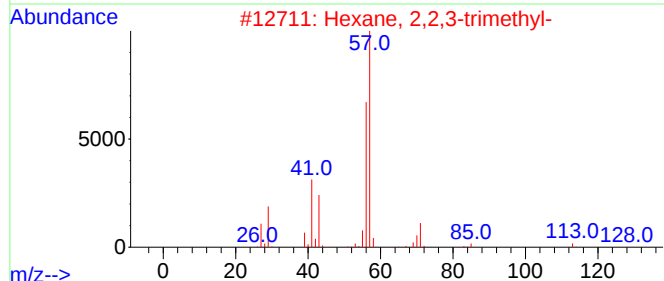
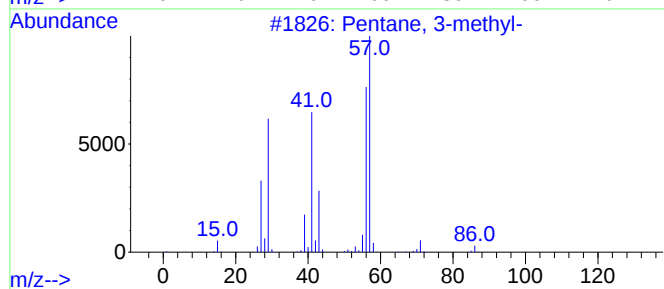
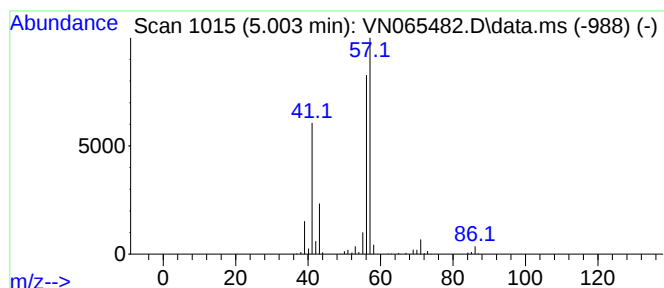
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.003	95.79 ug/l	1172600	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	56
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50



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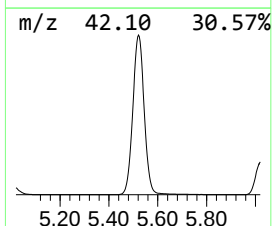
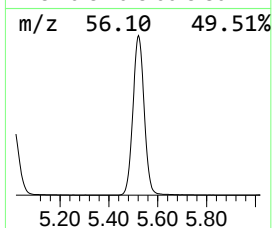
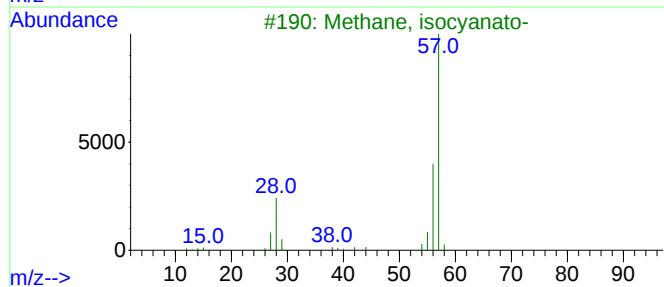
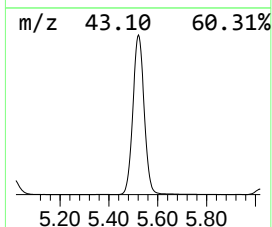
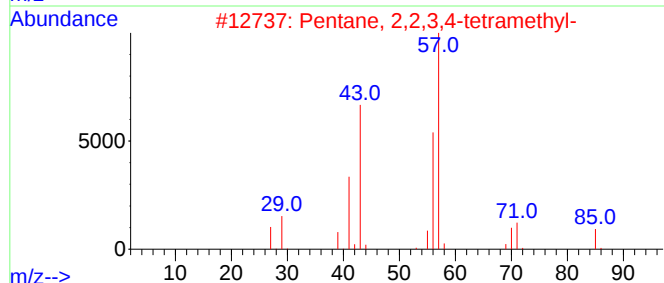
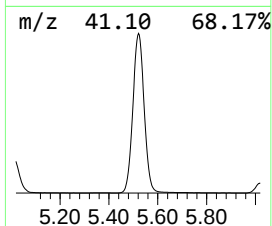
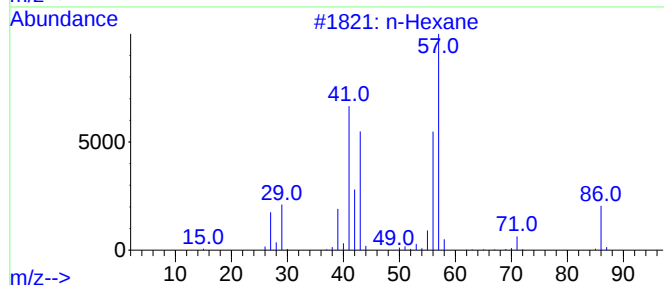
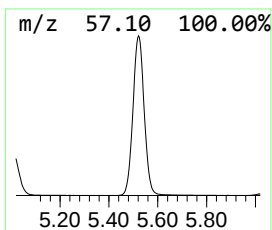
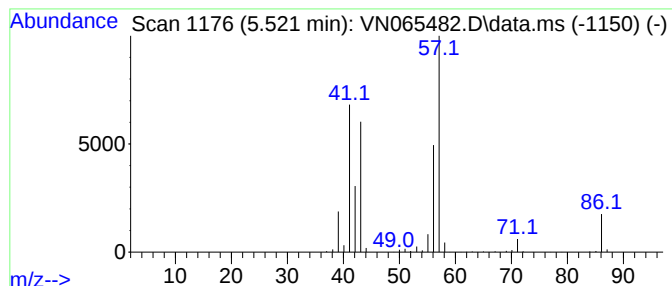
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.521	332.66 ug/l	4072190	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	94
2			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
3			Methane, isocyanato-	57	C2H3NO	000624-83-9	37
4			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35
5			Butanal, 2-methyl-	86	C5H10O	000096-17-3	35



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
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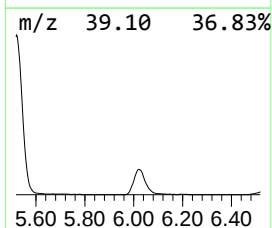
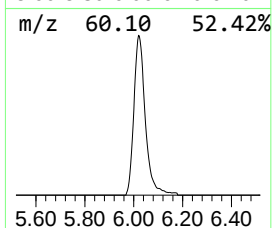
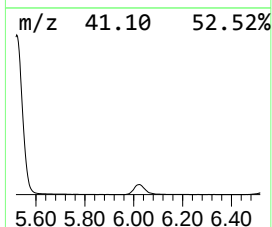
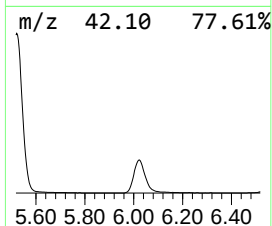
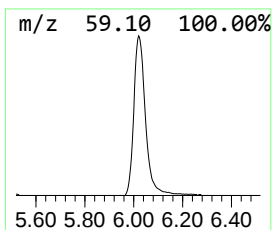
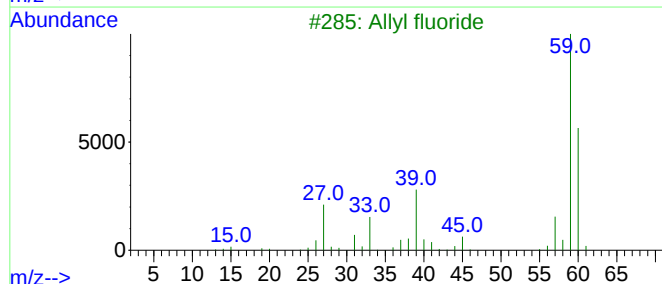
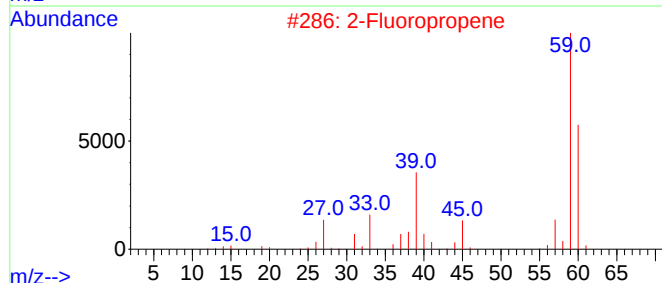
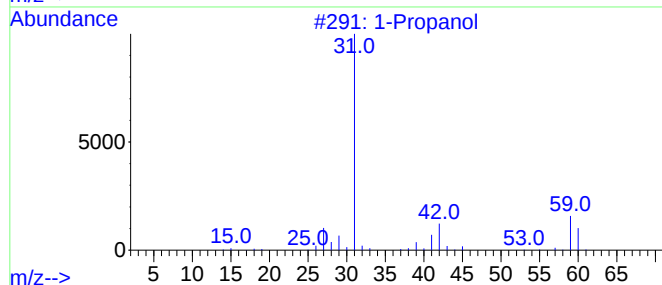
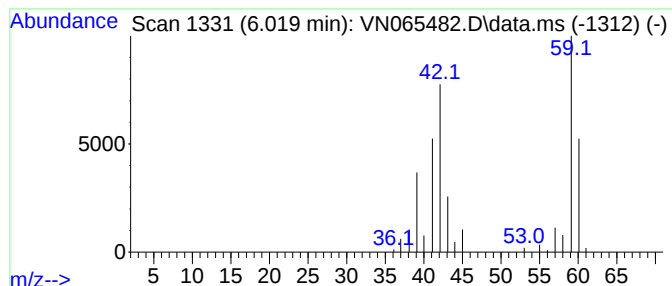
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.019	30.06 ug/l	368017	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	78
2			2-Fluoropropene	60	C3H5F	001184-60-7	49
3			Allyl fluoride	60	C3H5F	000818-92-8	47
4			Cyclopropane	42	C3H6	000075-19-4	12
5			Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9



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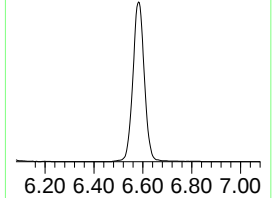
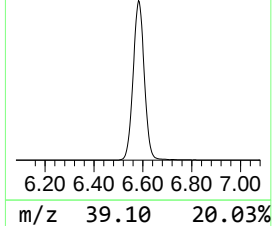
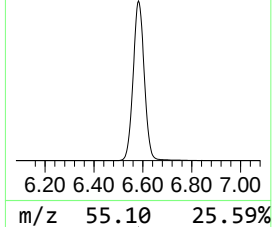
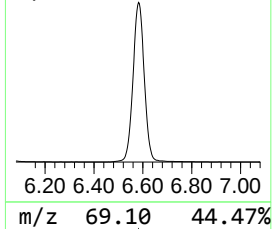
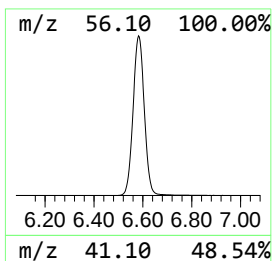
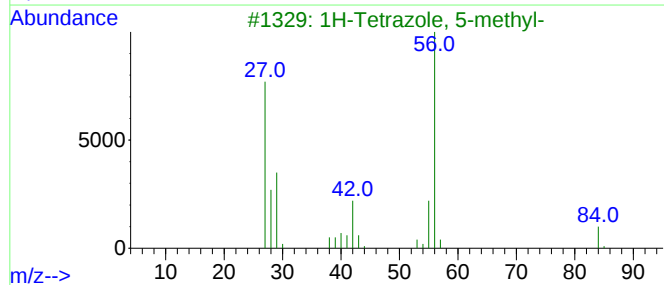
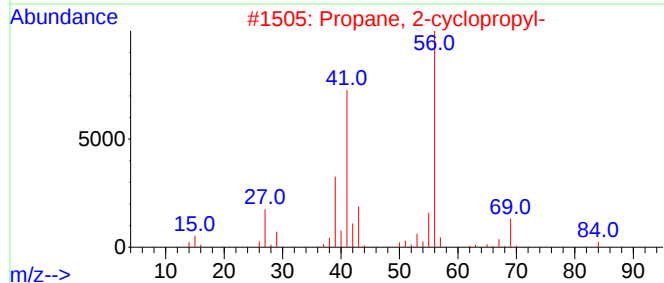
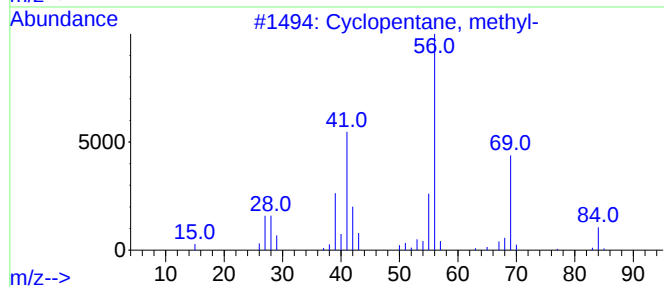
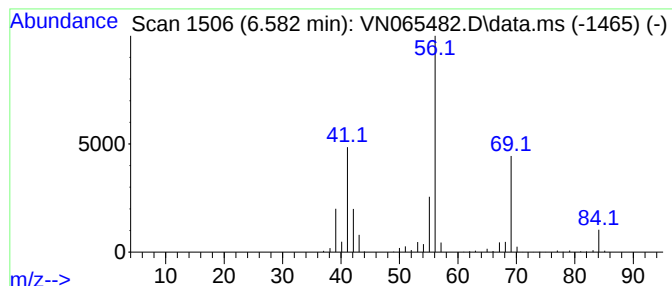
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.582	298.98 ug/l	3659920	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2-methyl-	4.544	47.7	ug/l	584338	1	7.630	612065	50.0
Pentane, 3-methyl-	5.003	95.8	ug/l	1172600	1	7.630	612065	50.0
n-Hexane	5.521	332.7	ug/l	4072190	1	7.630	612065	50.0
1-Propanol	6.019	30.1	ug/l	368017	1	7.630	612065	50.0
Cyclopentane, m...	6.582	299.0	ug/l	3659920	1	7.630	612065	50.0