

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087581.D
Acq On : 15 Aug 2025 14:57
Operator : JC\MD
Sample : Q2840-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
0804-E

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\82N071625W.M

Title : SW846 8260

Signal : TIC: VN087581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.801	299	314	339	rBV	1948094	6678674	3.15%	2.495%
2	6.789	799	822	846	rBV	10074272	40194454	18.98%	15.017%
3	13.771	1997	2009	2016	rBV2	1323468	2681033	1.27%	1.002%
4	14.229	2079	2087	2089	rBV2	139361022	211803843	100.00%	79.131%
5	14.476	2124	2129	2149	rVB	1863153	3798778	1.79%	1.419%
6	14.782	2170	2181	2200	rBV3	525392	2504859	1.18%	0.936%

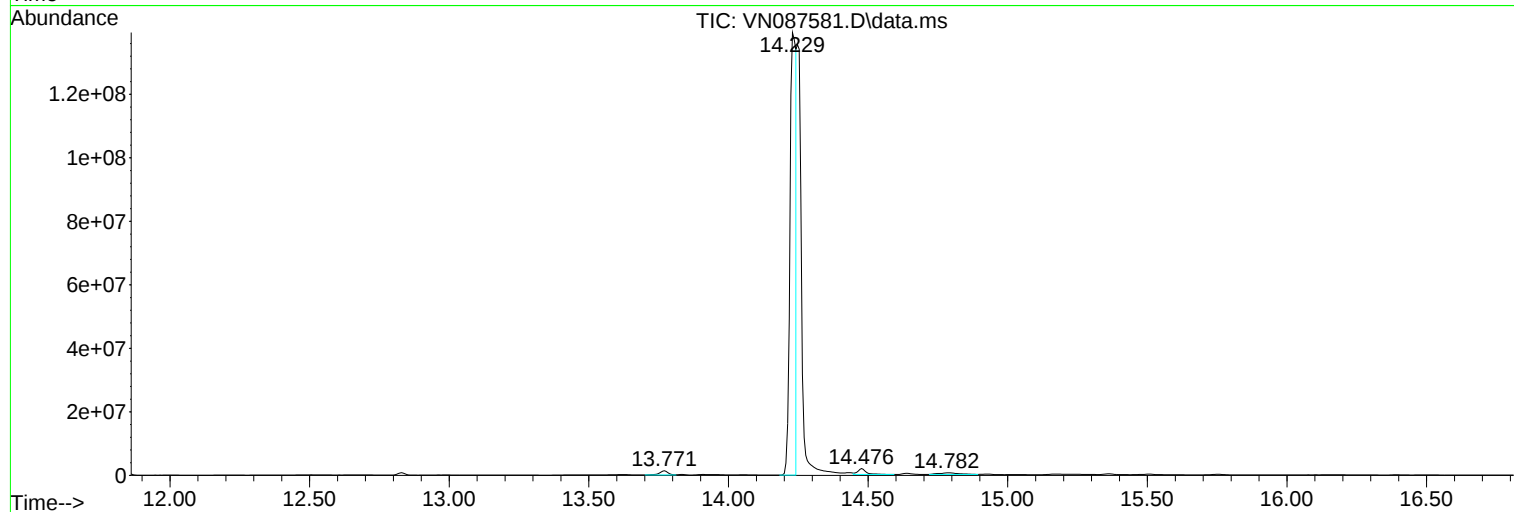
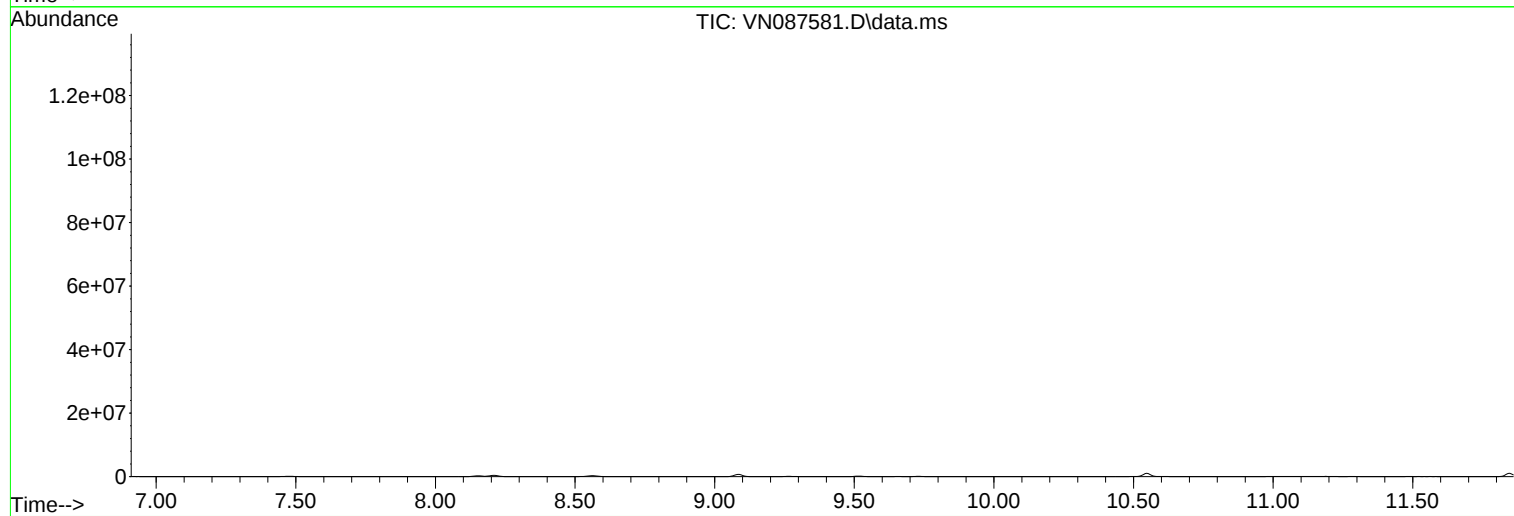
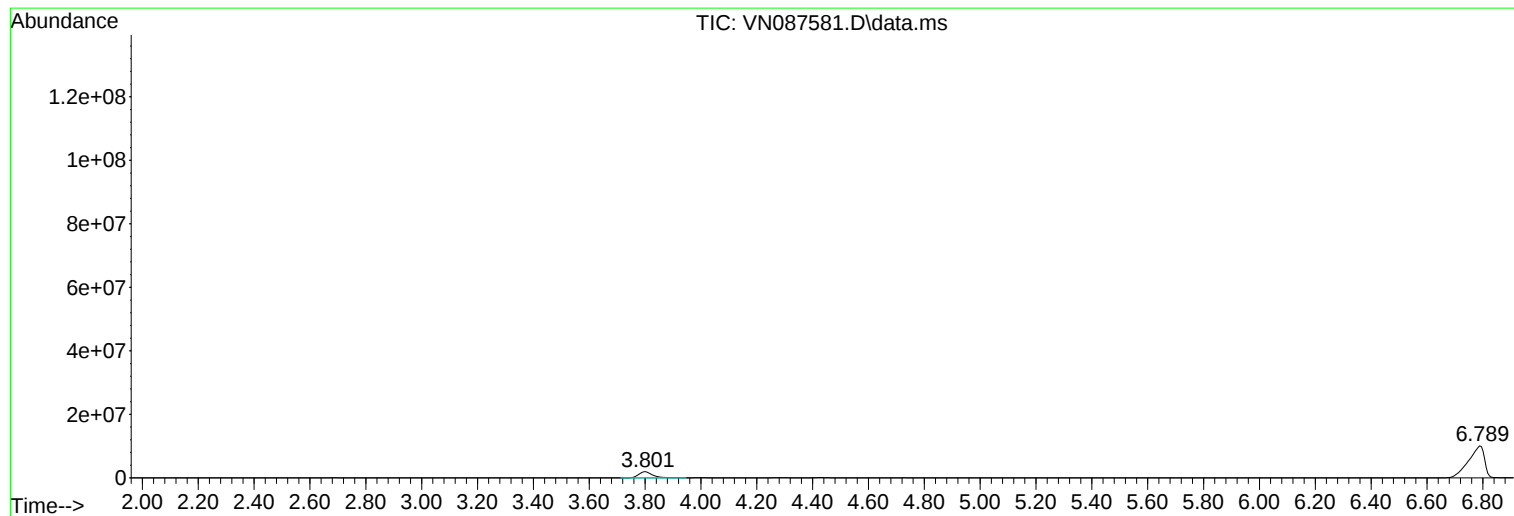
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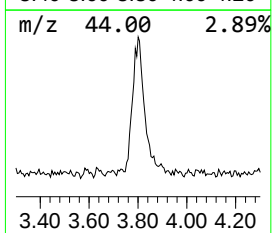
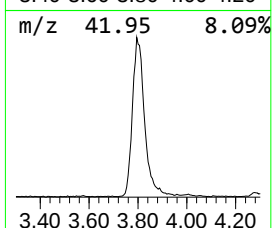
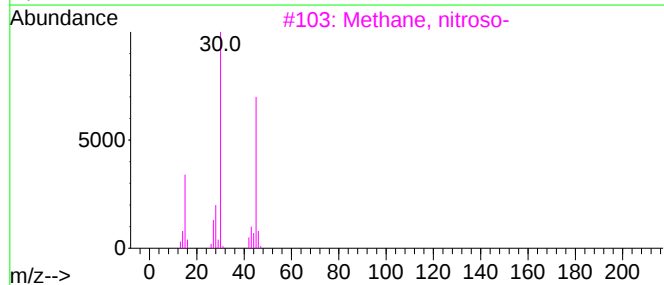
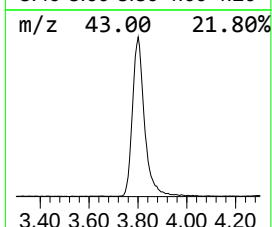
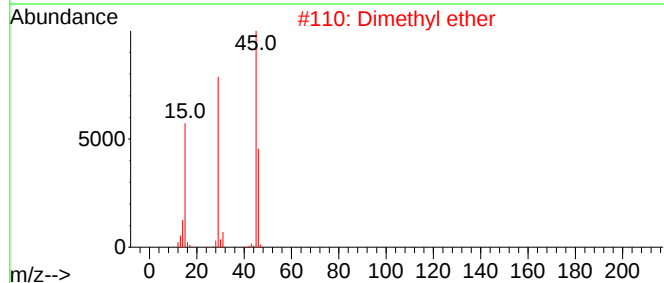
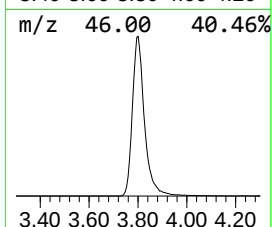
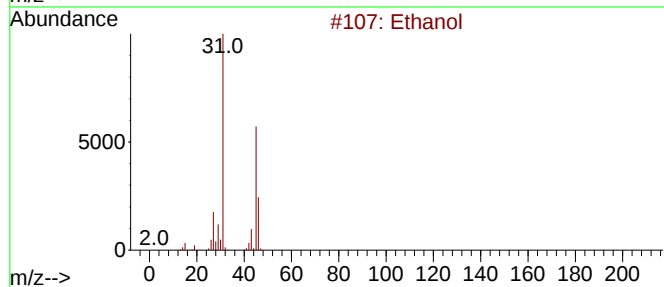
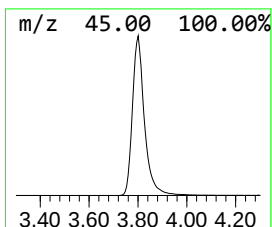
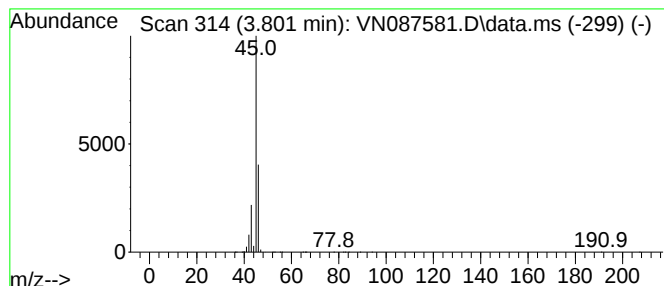
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.801	8.31 ug/l	6678670	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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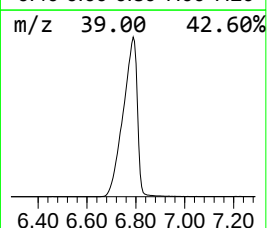
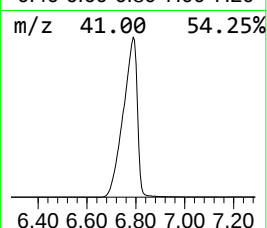
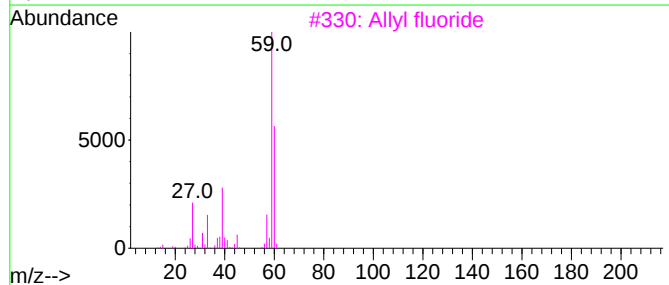
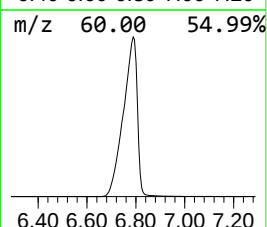
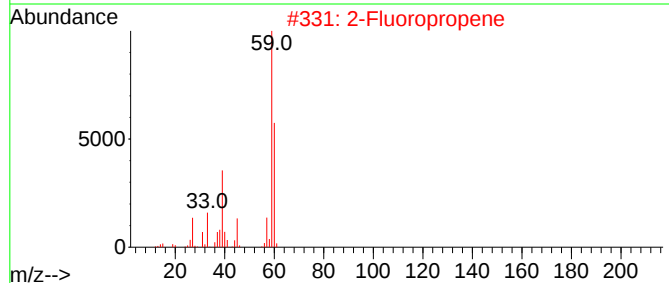
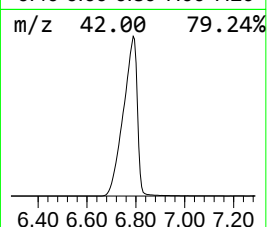
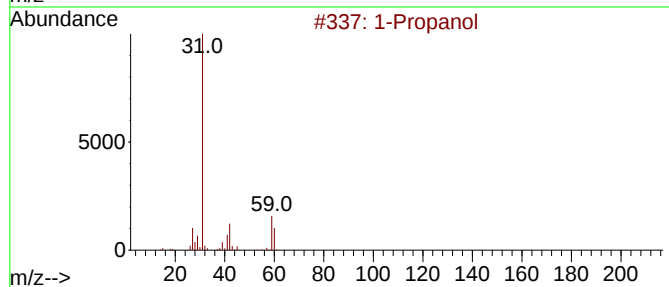
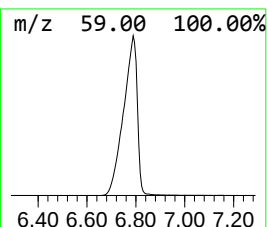
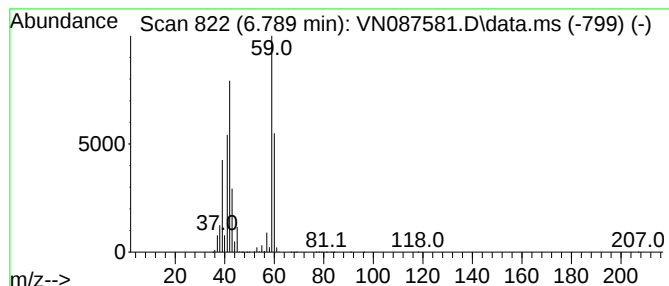
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Peak Number 2 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.789	50.00 ug/l	40194500	Pentafluorobenzene	8.206

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	64
2		2-Fluoropropene	60	C3H5F	001184-60-7	38
3		Allyl fluoride	60	C3H5F	000818-92-8	32
4		Cyclopropane	42	C3H6	000075-19-4	32
5		Propene	42	C3H6	000115-07-1	32



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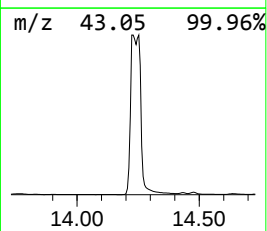
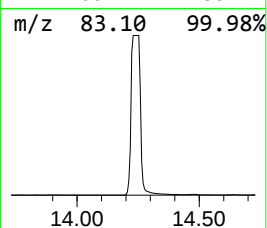
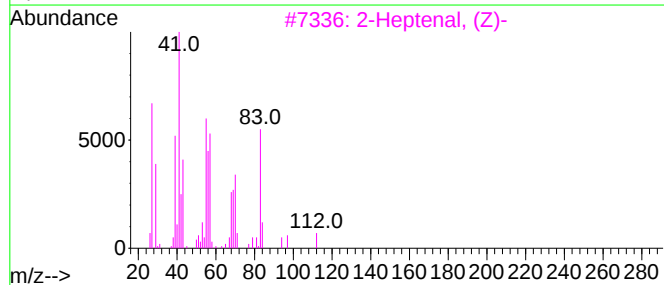
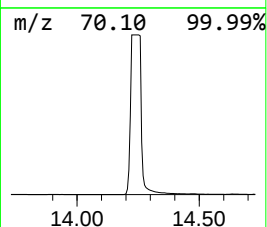
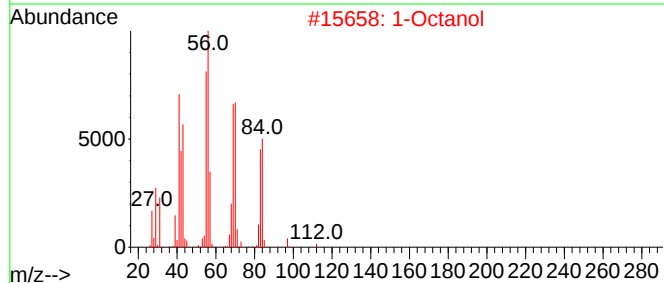
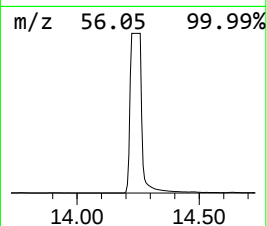
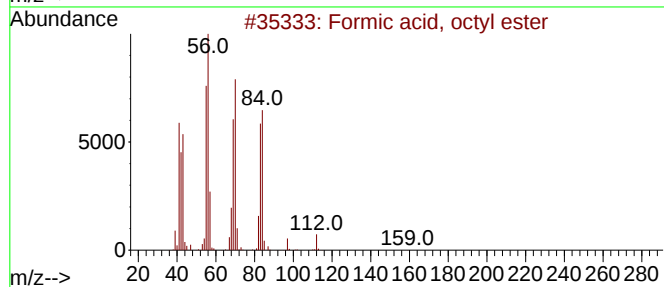
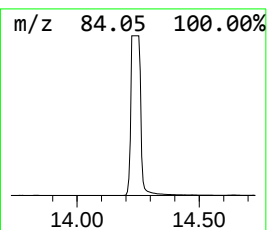
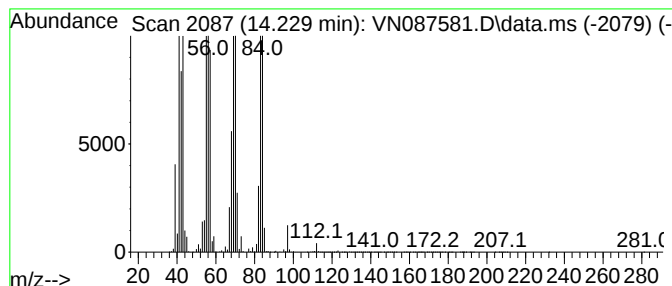
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Peak Number 3 Formic acid, octyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.229	3950.04 ug/l	211804000	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, octyl ester	158	C9H18O2	000112-32-3	64
2			1-Octanol	130	C8H18O	000111-87-5	64
3			2-Heptenal, (Z)-	112	C7H12O	057266-86-1	50
4			1-Silacyclo-3-pentene	84	C4H8Si	007049-25-4	43
5			Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	43



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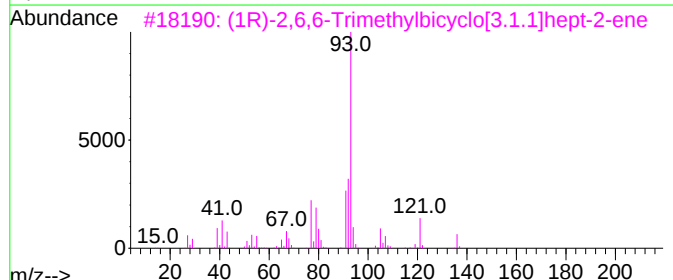
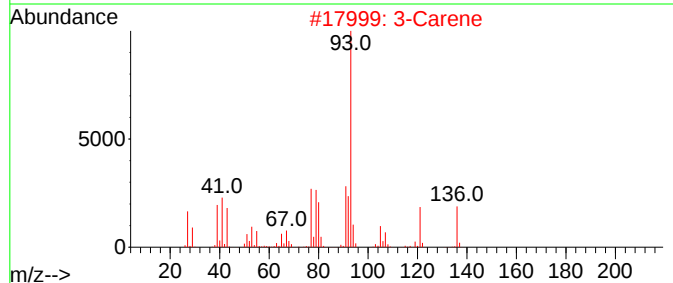
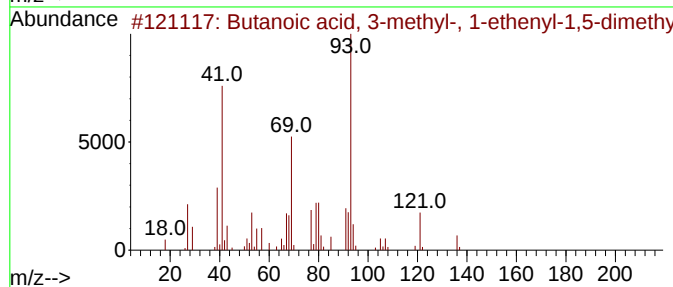
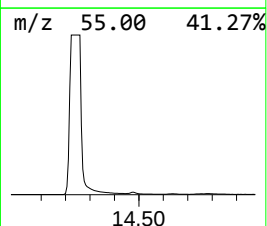
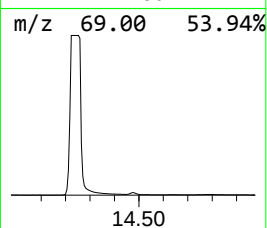
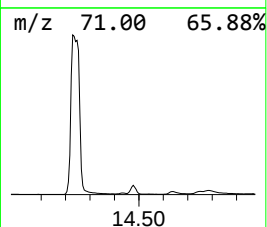
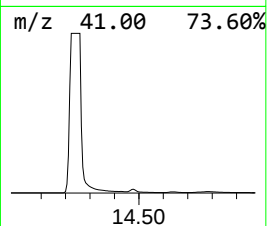
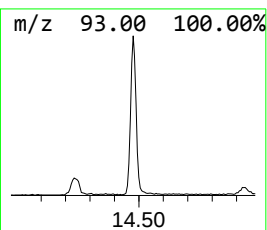
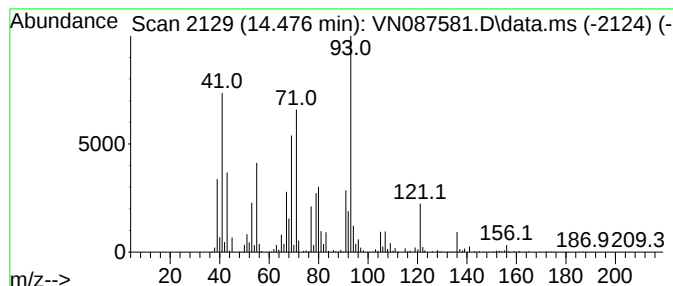
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Peak Number 4 Butanoic acid, 3-methyl-, 1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.476	70.85 ug/l	3798780	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-, 1-ethe...	238	C15H26O2	001118-27-0	74
2			3-Carene	136	C10H16	013466-78-9	70
3			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	60
4			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	60
5			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	58



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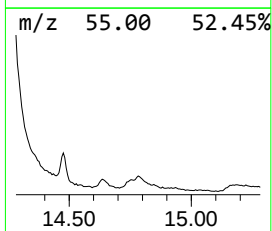
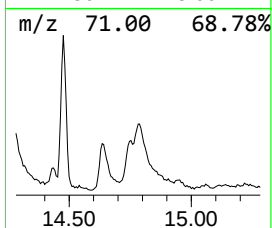
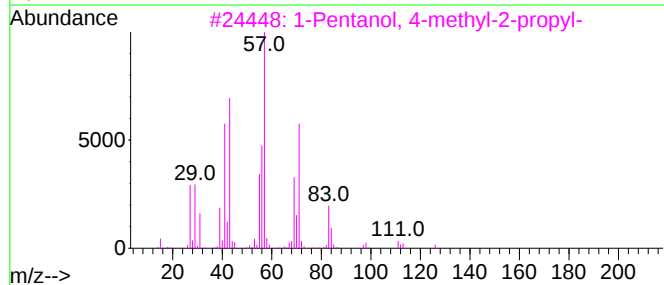
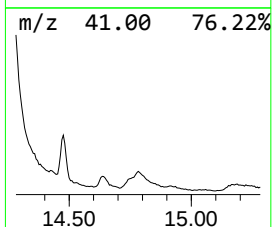
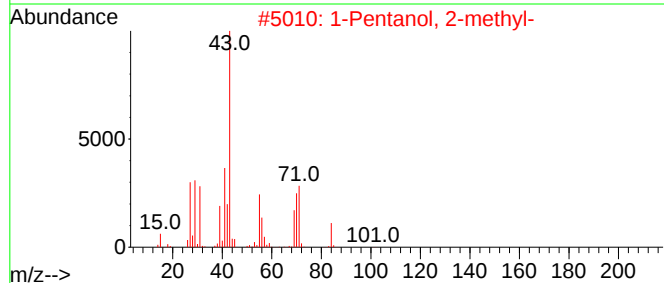
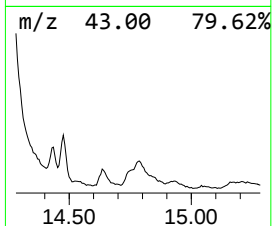
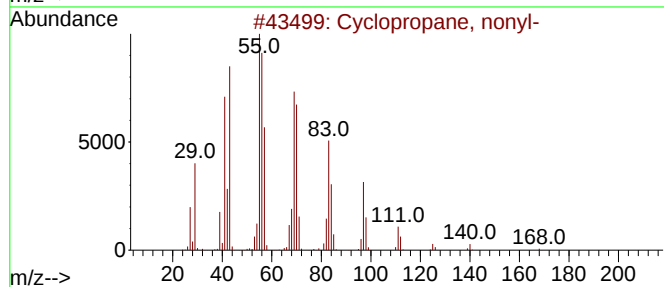
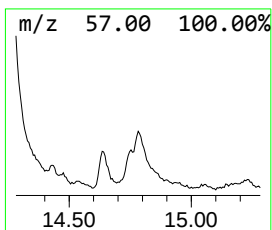
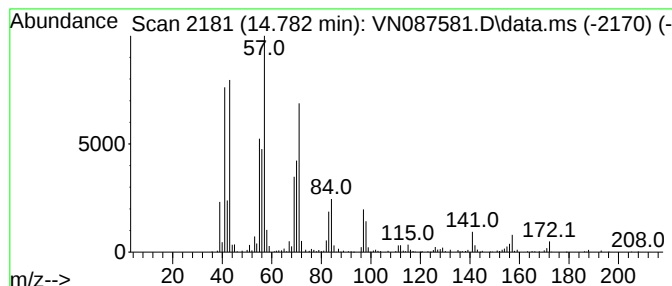
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Peak Number 5 unknown14.782 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.782	46.71 ug/l	2504860	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, nonyl-	168	C12H24	074663-85-7	43
2			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	43
3			1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	43
4			Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	38
5			2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.801	8.3	ug/l	6678670	1	8.206	40194500	50.0
1-Propanol	6.789	50.0	ug/l	40194500	1	8.206	40194500	50.0
Formic acid, oc...	14.229	3950.0	ug/l	211804000	4	13.771	2681030	50.0
Butanoic acid, ...	14.476	70.8	ug/l	3798780	4	13.771	2681030	50.0
unknown14.782	14.782	46.7	ug/l	2504860	4	13.771	2681030	50.0