

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
 Data File : VN081469.D
 Acq On : 19 Mar 2024 14:34
 Operator : JC\MD
 Sample : P1772-10
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1352

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\82N031824W.M
 Title : SW846 8260

Signal : TIC: VN081469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	27	rBV2	21706	35178	1.18%	0.176%
2	7.224	884	896	907	rBV3	59302	169081	5.66%	0.846%
3	8.165	1046	1056	1061	rBV	348961	853253	28.58%	4.269%
4	8.224	1061	1066	1079	rVB	673677	1439515	48.22%	7.203%
5	8.576	1109	1126	1139	rBV	366674	853042	28.58%	4.268%
6	9.100	1205	1215	1227	rBV	905105	1855990	62.18%	9.287%
7	9.265	1236	1243	1259	rBV2	53715	148514	4.98%	0.743%
8	9.647	1298	1308	1314	rBV5	12313	33163	1.11%	0.166%
9	10.565	1455	1464	1473	rBV	1363974	2510955	84.12%	12.564%
10	11.864	1672	1685	1696	rBV	1215201	2188215	73.31%	10.949%
11	12.212	1737	1744	1749	rBV2	17501	30828	1.03%	0.154%
12	12.423	1774	1780	1785	rBV	91777	140370	4.70%	0.702%
13	12.847	1842	1852	1863	rBV	913668	1673659	56.07%	8.375%
14	12.941	1863	1868	1874	rVV2	31529	50083	1.68%	0.251%
15	13.082	1886	1892	1897	rBV4	34371	68589	2.30%	0.343%
16	13.259	1912	1922	1929	rBV	721163	1224904	41.03%	6.129%
17	13.335	1929	1935	1943	rVB	1942320	2985080	100.00%	14.937%
18	13.500	1957	1963	1967	rBV6	15805	30332	1.02%	0.152%
19	13.688	1986	1995	2006	rVV2	318352	574471	19.24%	2.875%
20	13.794	2006	2013	2020	rVV	1169129	1935247	64.83%	9.683%
21	13.876	2020	2027	2036	rVV	471834	798247	26.74%	3.994%
22	13.953	2036	2040	2047	rVB5	28087	52166	1.75%	0.261%
23	14.253	2085	2091	2095	rBV4	22410	38058	1.27%	0.190%
24	14.482	2122	2130	2136	rBV9	15240	33998	1.14%	0.170%
25	14.611	2146	2152	2160	rBV5	27211	40473	1.36%	0.203%
26	15.347	2270	2277	2281	rBV3	59636	108346	3.63%	0.542%
27	15.394	2281	2285	2291	rVV2	66963	113289	3.80%	0.567%

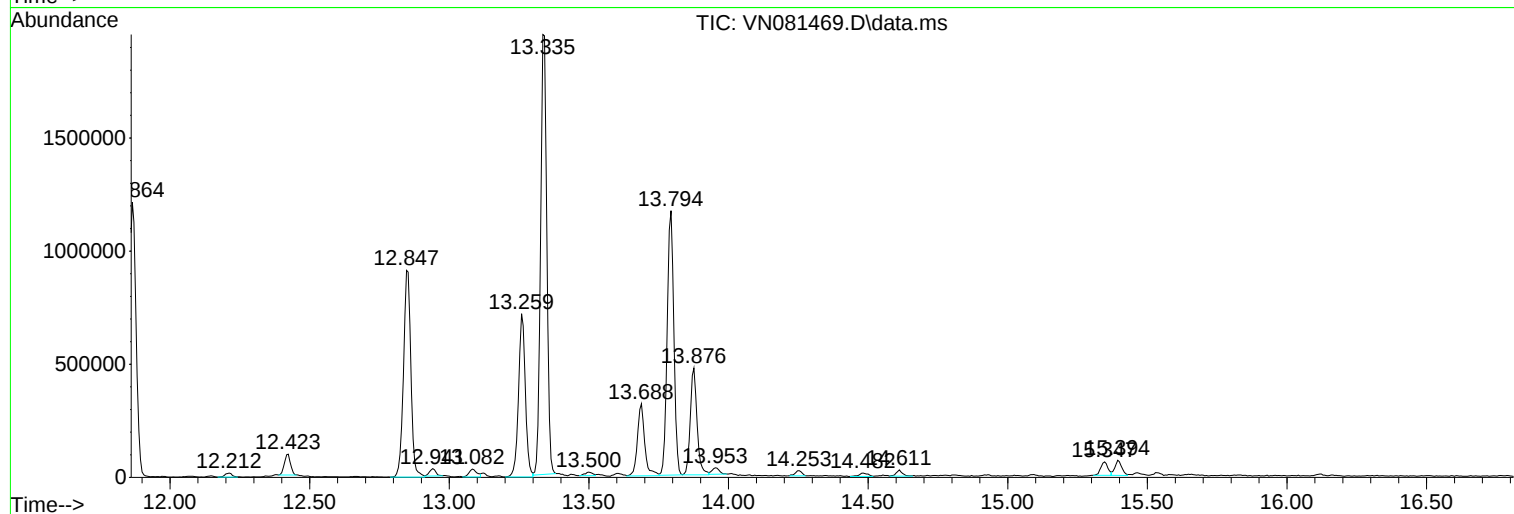
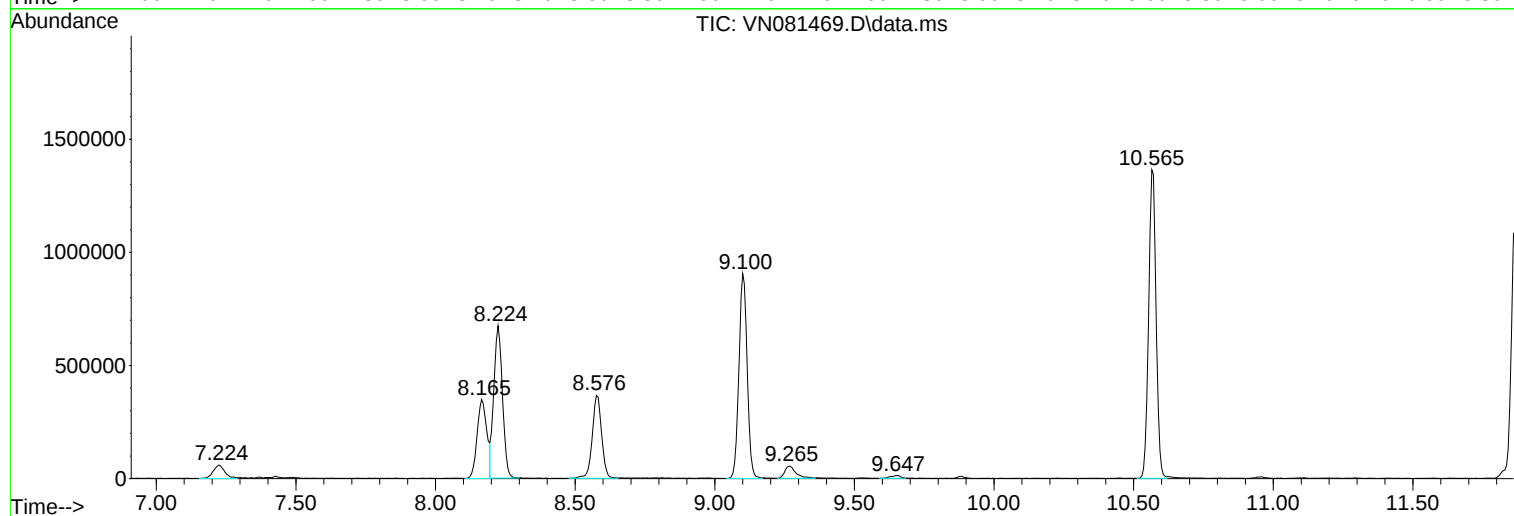
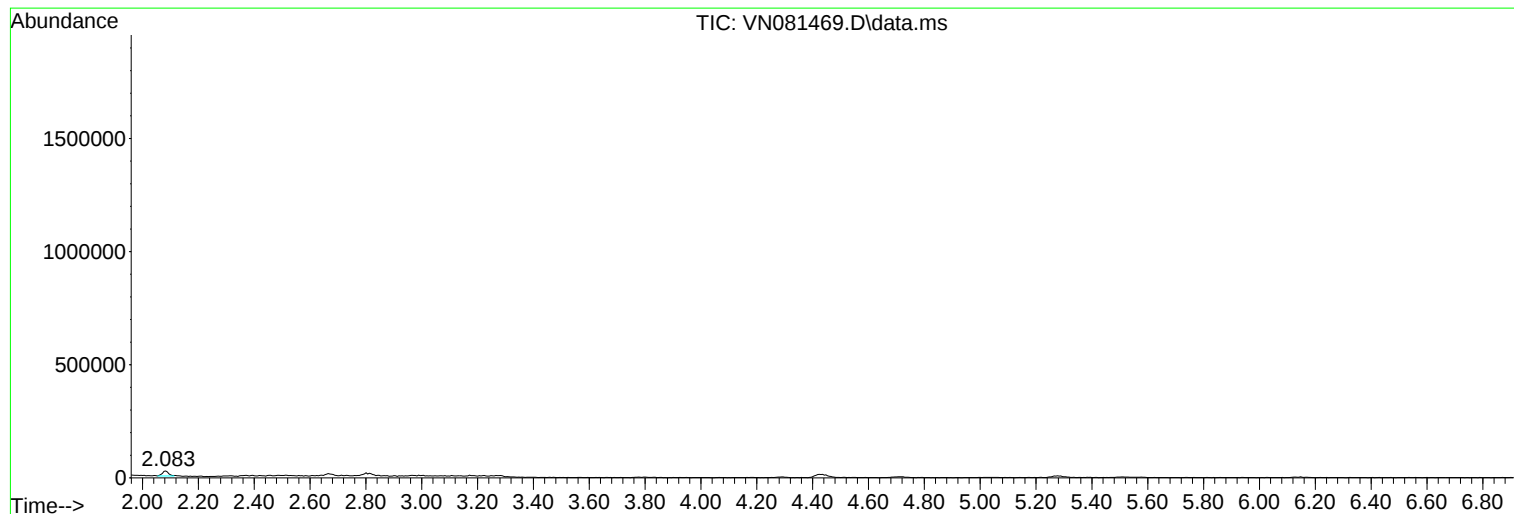
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Instrument :
MSVOA_N
ClientSampleId :
1352

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



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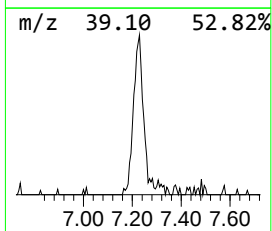
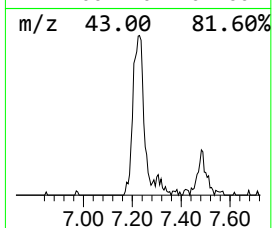
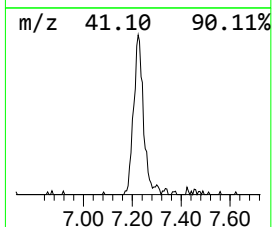
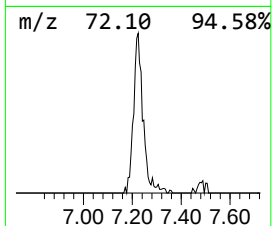
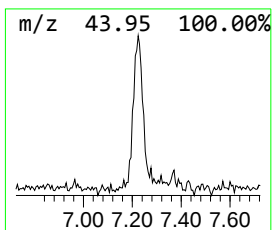
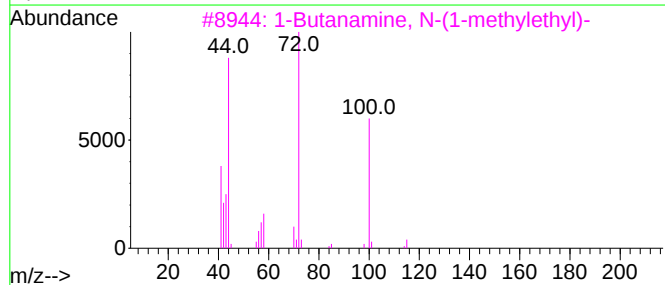
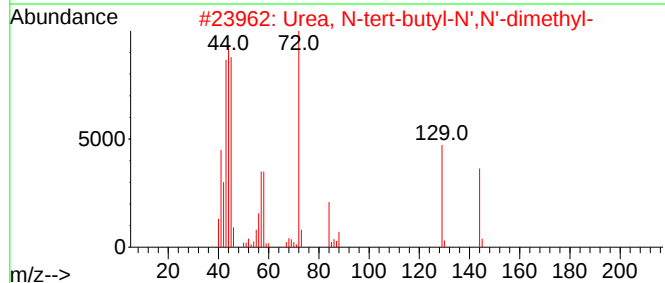
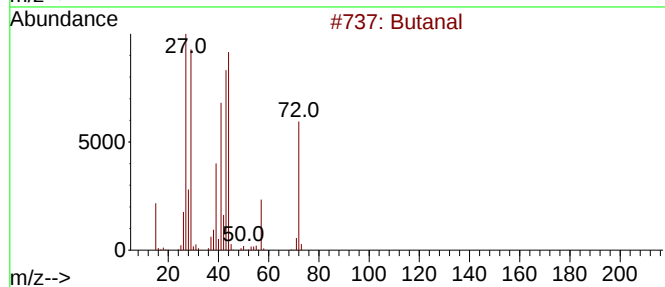
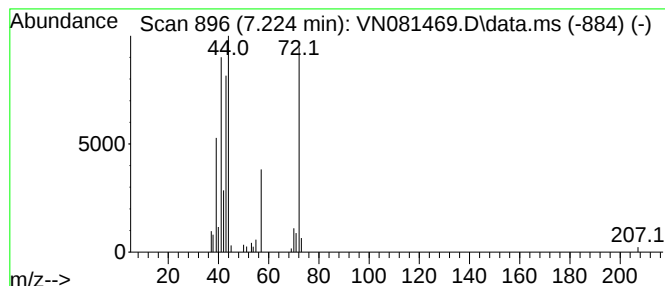
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	5.87 ug/l	169081	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	80
2			Urea, N-tert-butyl-N',N'-dimethyl-	144	C7H16N2O	1000360-40-1	50
3			1-Butanamine, N-(1-methylethyl)-	115	C7H17N	039099-23-5	50
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			Propane	44	C3H8	000074-98-6	38



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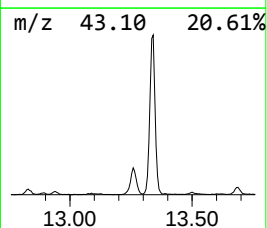
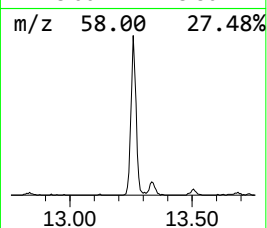
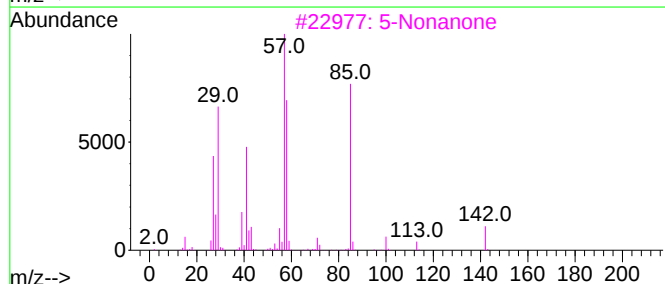
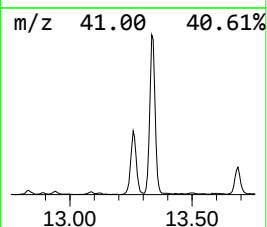
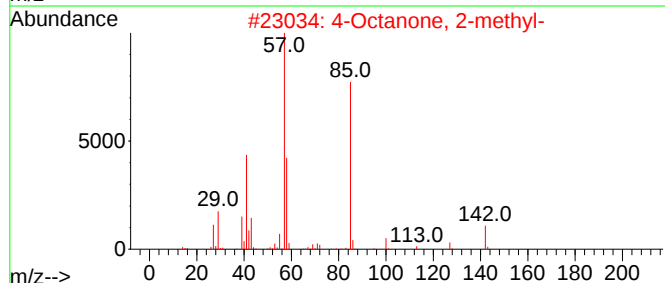
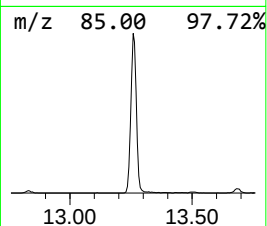
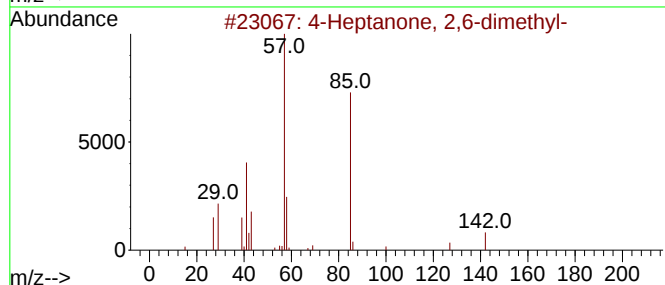
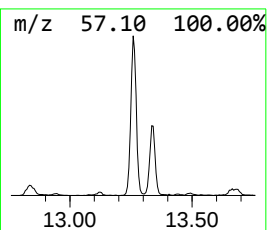
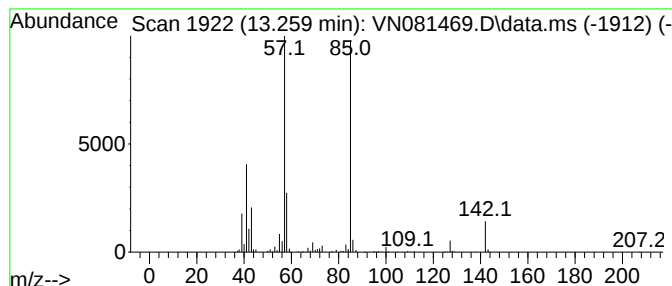
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TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	31.65 ug/l	1224900	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	53
5			2,4-Heptanedione, 6-methyl-	142	C8H14O2	003002-23-1	53



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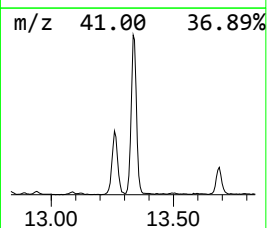
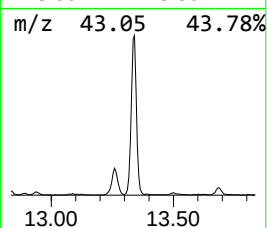
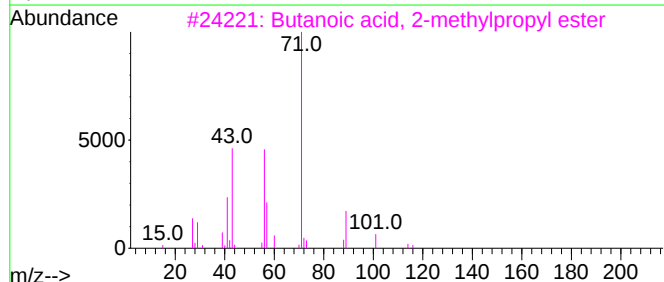
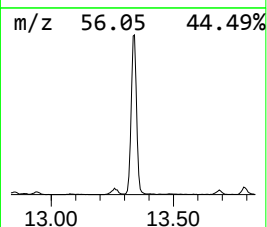
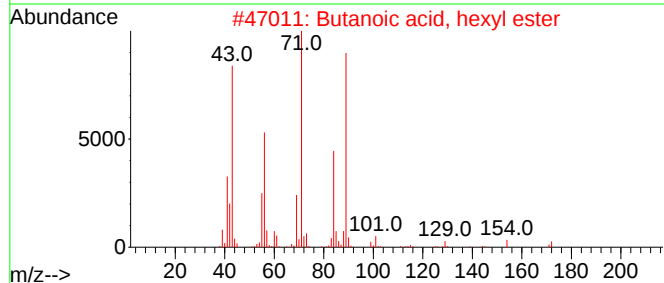
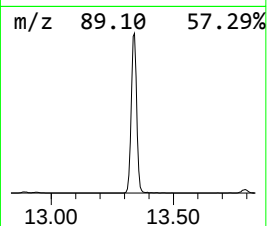
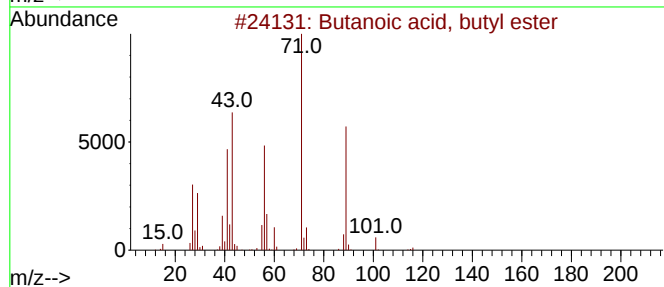
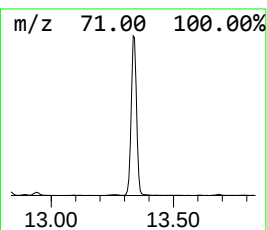
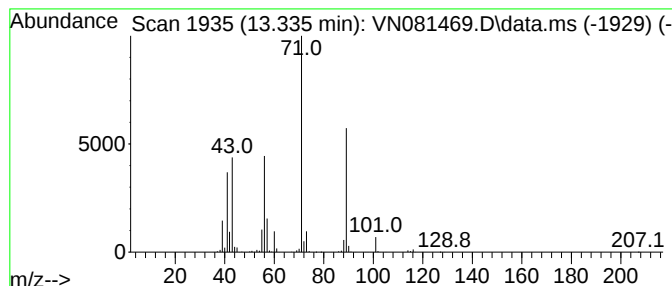
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	77.12 ug/l	2985080	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



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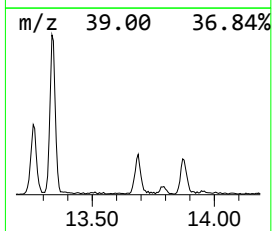
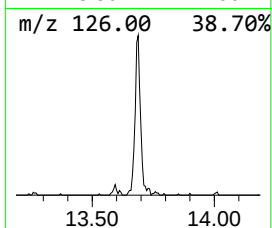
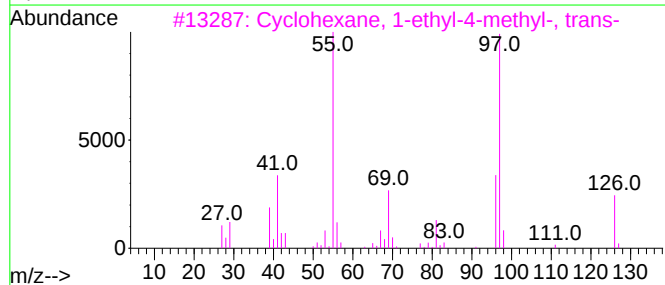
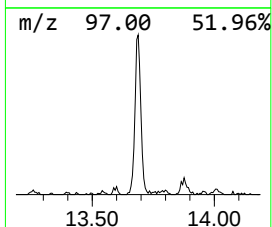
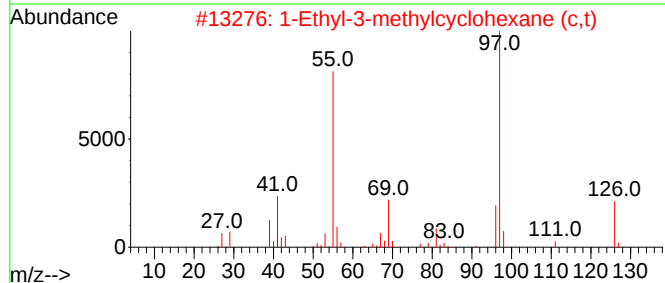
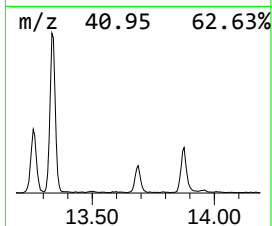
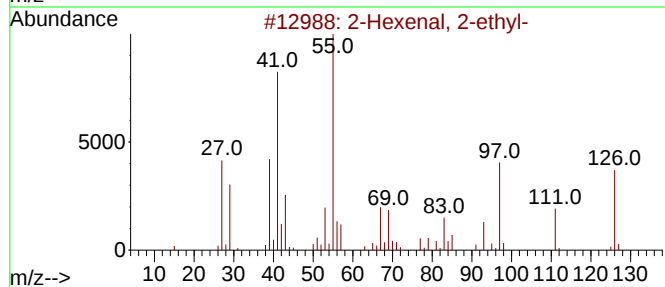
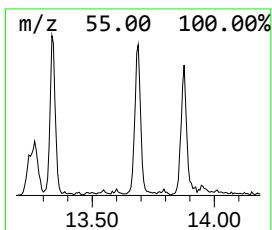
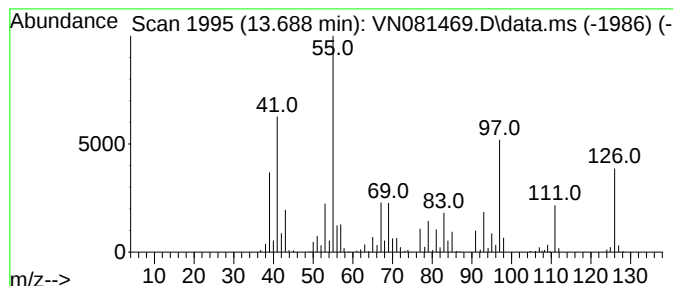
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Peak Number 4 2-Hexenal, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	14.84 ug/l	574471	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	96
2			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	47
3			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	47
4			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	47
5			1-Nonylcycloheptane	224	C16H32	1000371-47-7	38



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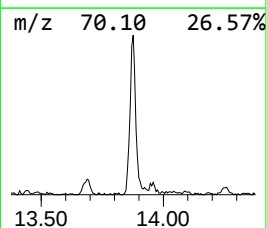
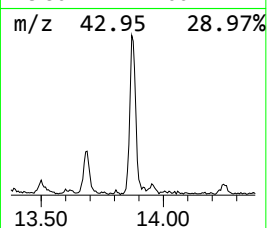
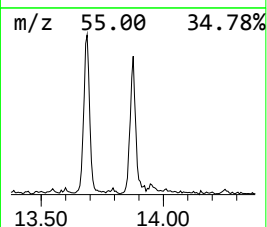
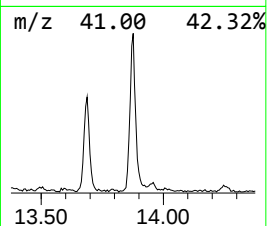
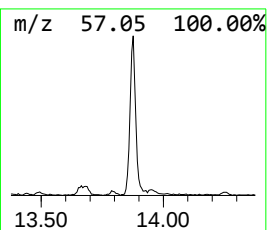
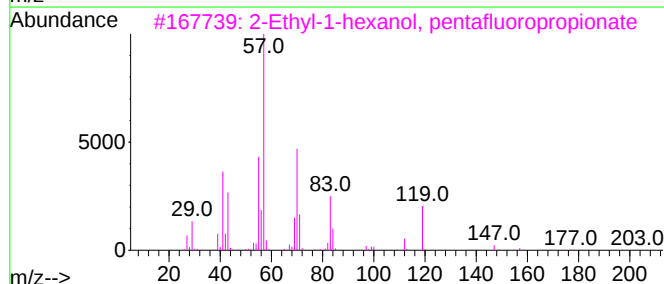
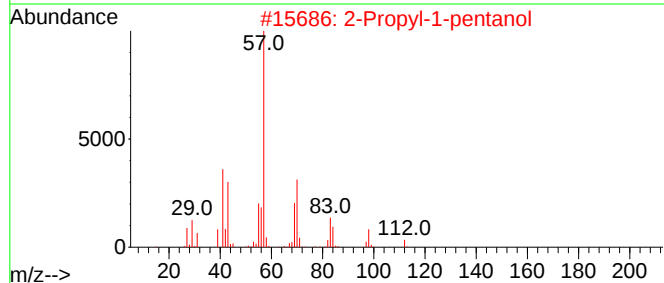
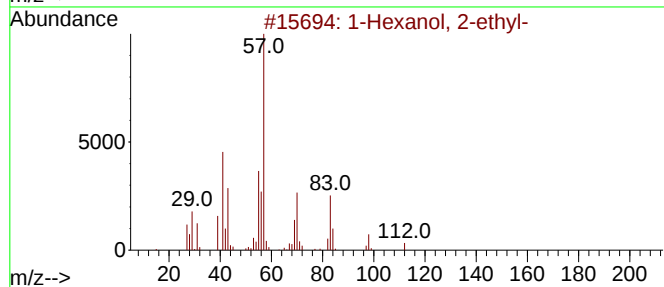
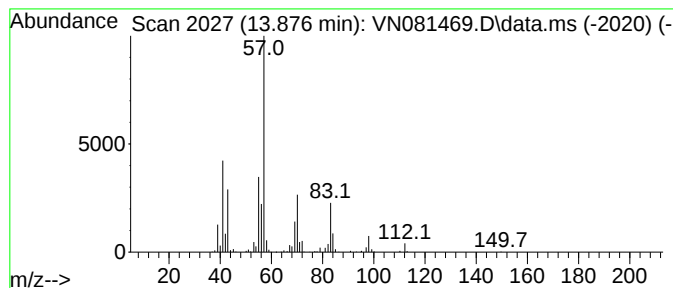
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	20.62 ug/l	798247	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	5.9	ug/l	169081	1	8.224	1439520	50.0
4-Heptanone, 2,...	13.259	31.6	ug/l	1224900	4	13.794	1935250	50.0
Butanoic acid, ...	13.335	77.1	ug/l	2985080	4	13.794	1935250	50.0
2-Hexenal, 2-et...	13.688	14.8	ug/l	574471	4	13.794	1935250	50.0
1-Hexanol, 2-et...	13.876	20.6	ug/l	798247	4	13.794	1935250	50.0