

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
 Data File : VN080849.D
 Acq On : 31 Jan 2024 18:43
 Operator : JC\MD
 Sample : P1284-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1247

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\82N012924W.M
 Title : SW846 8260

Signal : TIC: VN080849.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	18	22	27	rVB3	9920	14577	1.09%	0.238%
2	4.436	413	422	431	rBV3	8530	25914	1.94%	0.423%
3	7.224	887	896	906	rBV2	27015	73579	5.52%	1.202%
4	8.171	1045	1057	1061	rBV2	79499	189211	14.19%	3.090%
5	8.224	1061	1066	1074	rVB2	131531	293319	21.99%	4.791%
6	8.529	1112	1118	1119	rBV2	9877	14527	1.09%	0.237%
7	8.576	1119	1126	1141	rVB	108235	255747	19.17%	4.177%
8	9.106	1207	1216	1225	rVB	286718	586929	44.01%	9.586%
9	9.271	1236	1244	1252	rBV3	23764	55399	4.15%	0.905%
10	9.653	1299	1309	1315	rBV6	6678	17809	1.34%	0.291%
11	10.570	1455	1465	1474	rBV	340230	650682	48.79%	10.627%
12	11.865	1672	1685	1694	rBV	416641	779613	58.45%	12.733%
13	12.423	1768	1780	1788	rBV2	54460	96685	7.25%	1.579%
14	12.853	1843	1853	1864	rBV	263805	486033	36.44%	7.938%
15	12.941	1864	1868	1874	rVB3	17013	28724	2.15%	0.469%
16	13.082	1887	1892	1896	rBV3	8522	15740	1.18%	0.257%
17	13.241	1913	1919	1922	rBV3	24862	41015	3.08%	0.670%
18	13.270	1922	1924	1929	rVV2	20702	31537	2.36%	0.515%
19	13.341	1929	1936	1945	rVB	908541	1333754	100.00%	21.784%
20	13.688	1989	1995	2003	rVB2	51101	88955	6.67%	1.453%
21	13.794	2006	2013	2021	rBV	379520	640644	48.03%	10.463%
22	13.876	2021	2027	2037	rVV	148293	247186	18.53%	4.037%
23	14.253	2087	2091	2098	rVB5	12088	16654	1.25%	0.272%
24	15.347	2273	2277	2281	rBV4	11334	18226	1.37%	0.298%
25	15.394	2281	2285	2291	rVB2	37674	61082	4.58%	0.998%
26	15.823	2353	2358	2367	rVB3	11151	20904	1.57%	0.341%
27	15.935	2372	2377	2385	rVB6	10413	20993	1.57%	0.343%
28	16.123	2400	2409	2414	rBV6	9234	17239	1.29%	0.282%

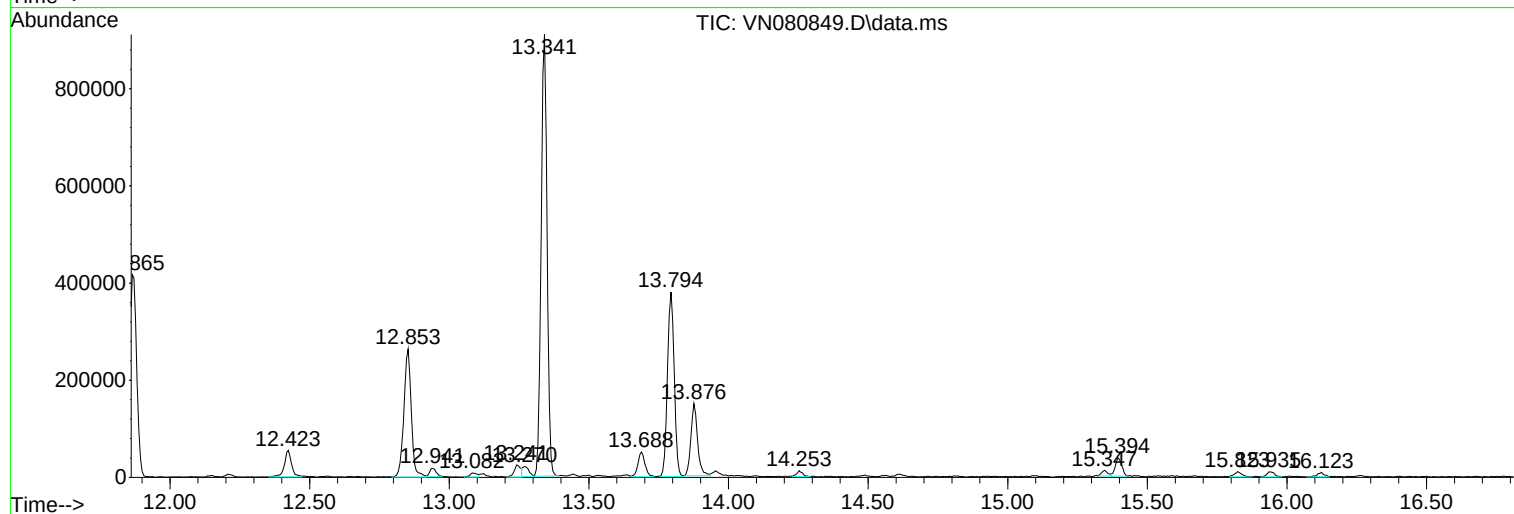
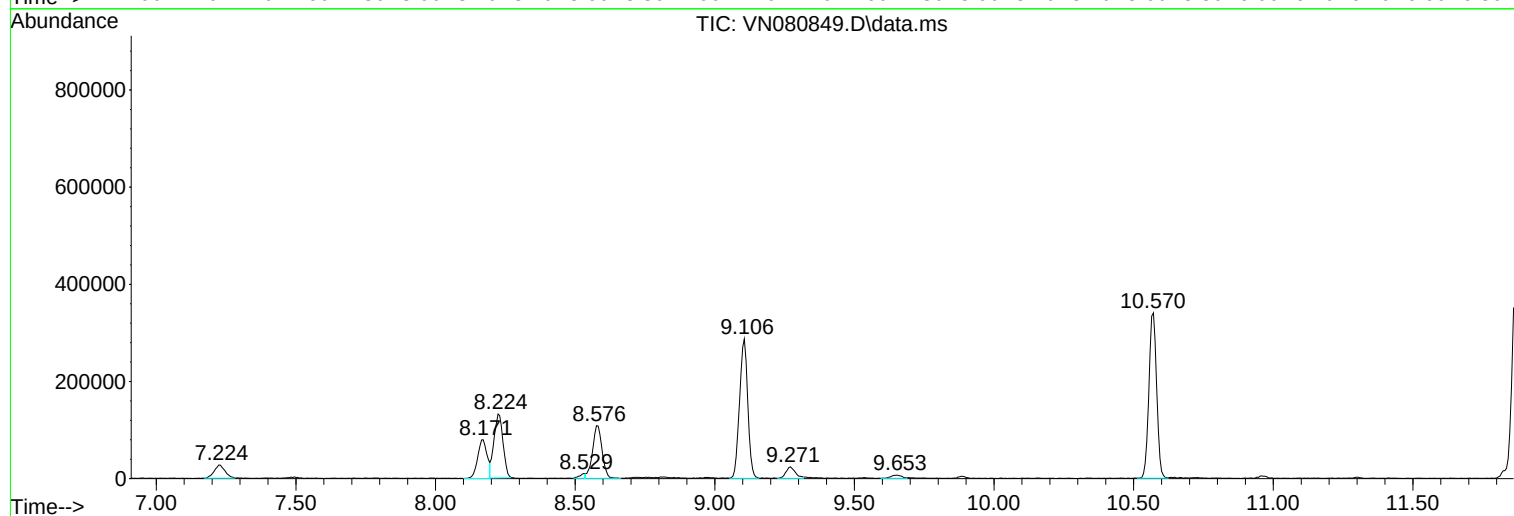
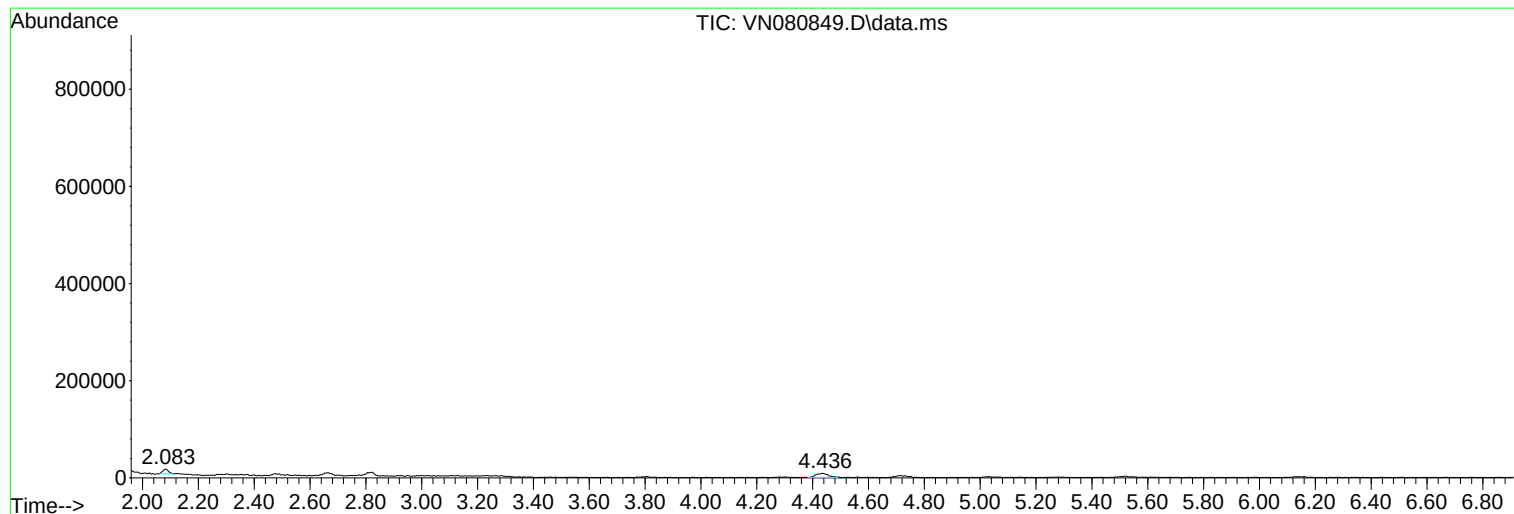
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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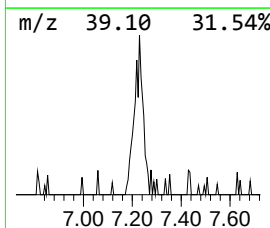
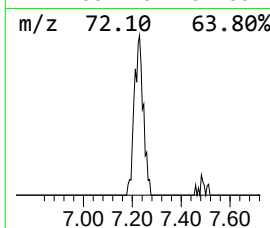
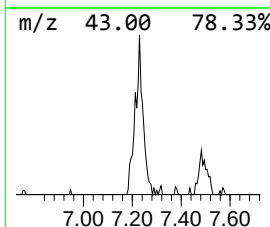
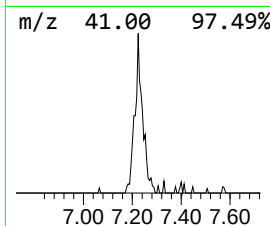
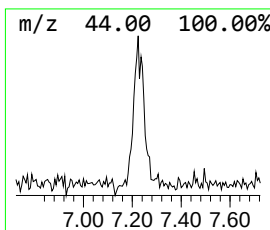
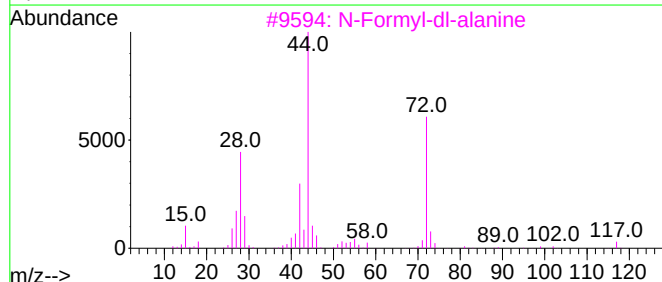
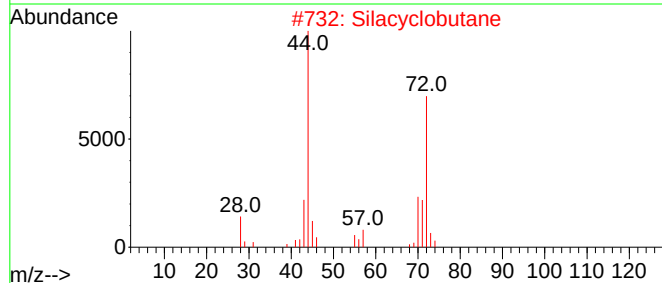
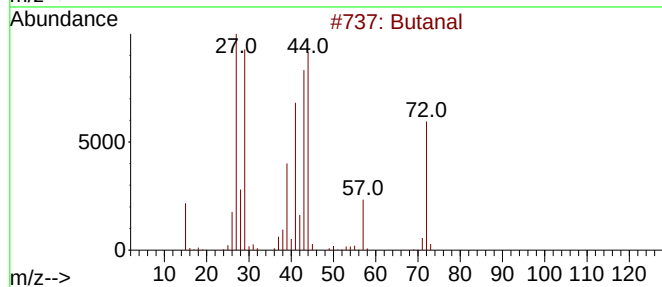
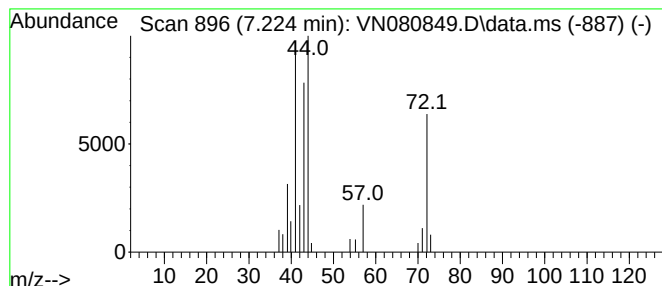
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	12.54 ug/l	73579	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	80
2			Silacyclobutane	72	C3H8Si	1000434-34-1	43
3			N-Formyl-dl-alanine	117	C4H7NO3	005893-10-7	28
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	22
5			Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	22



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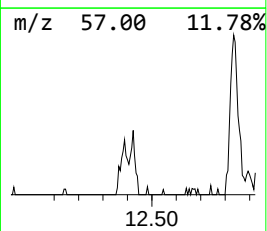
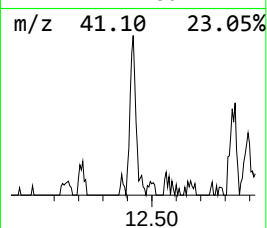
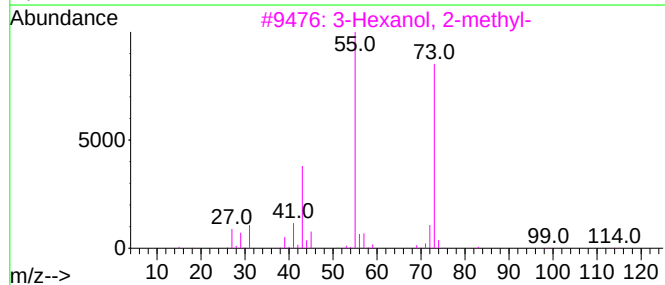
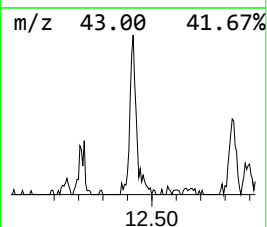
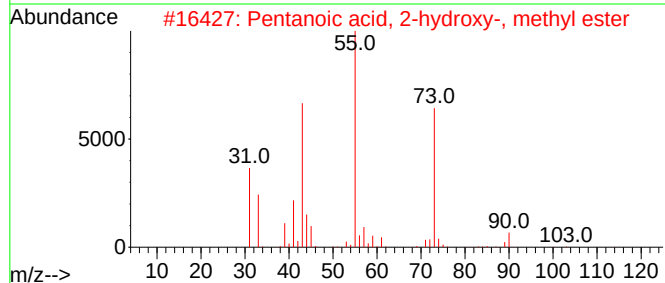
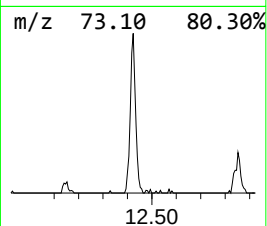
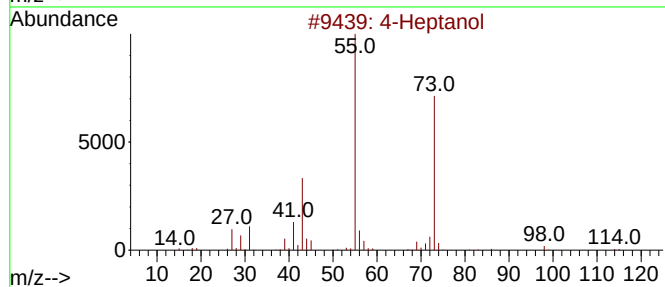
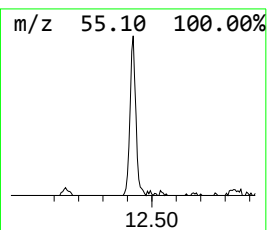
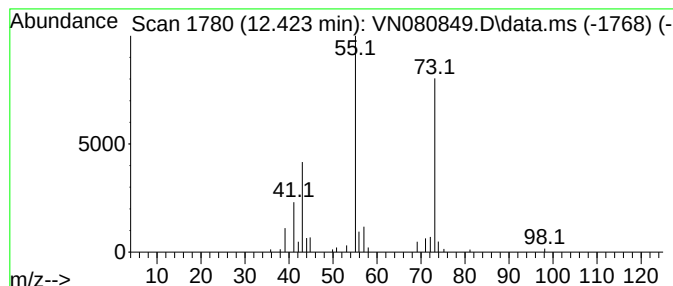
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TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Heptanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.423	6.20 ug/l	96685	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	83
2			Pentanoic acid, 2-hydroxy-, meth...	132	C6H12O3	007445-76-3	72
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	56
4			DL-4,5-Octanediol	146	C8H18O2	1000099-07-1	38
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	28



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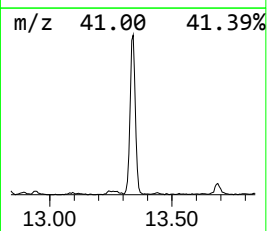
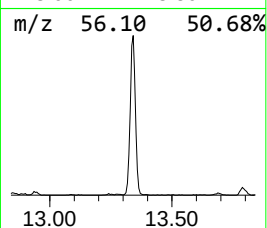
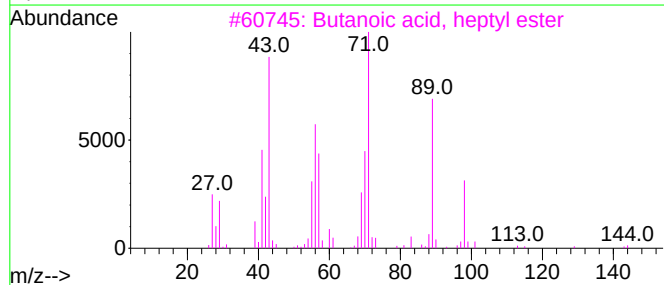
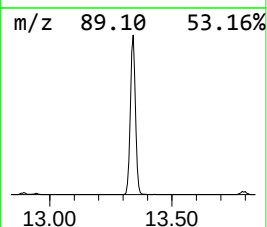
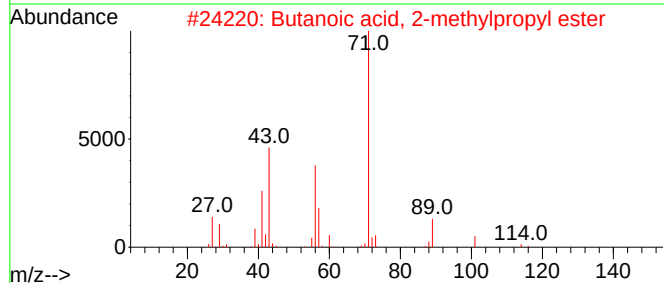
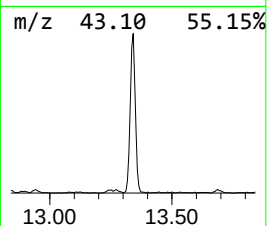
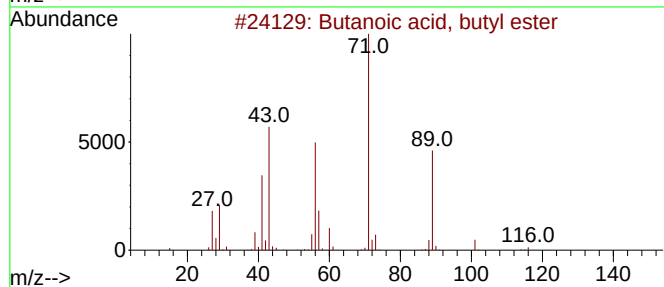
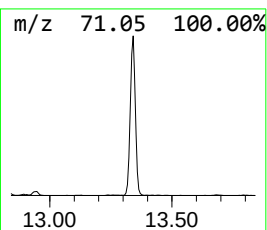
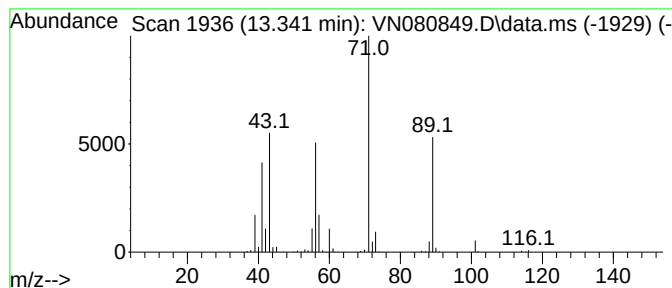
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Quant Title : SW846 8260

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

Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	104.10 ug/l	1333750	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	59



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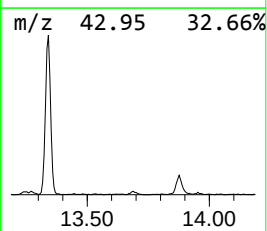
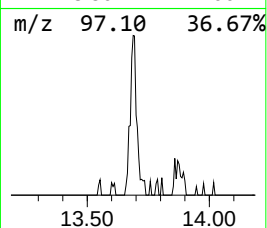
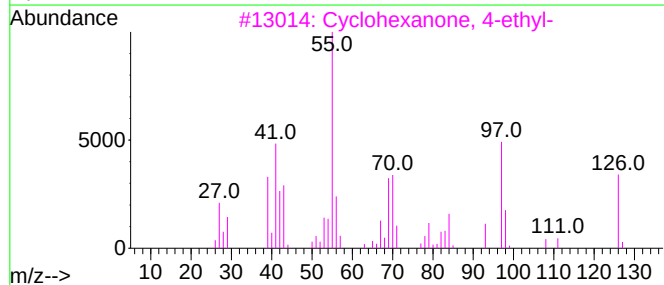
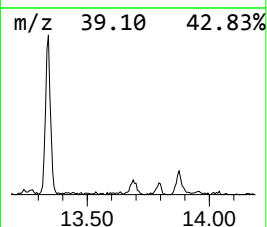
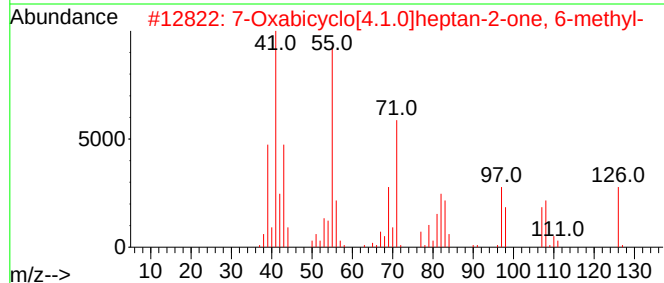
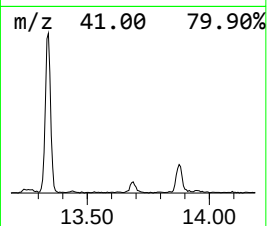
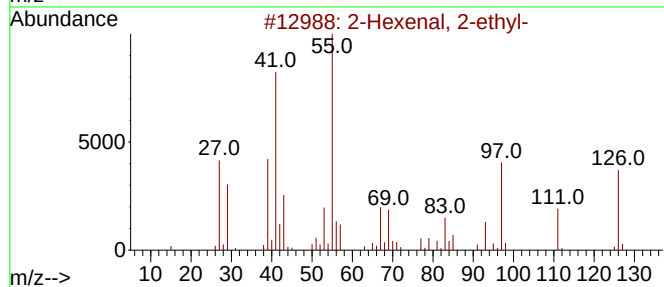
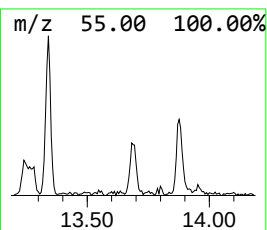
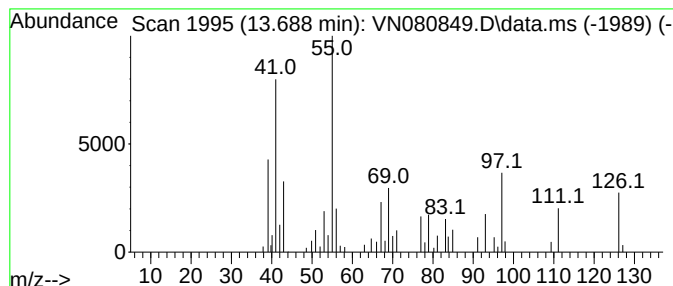
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	6.94 ug/l	88955	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	83
2			7-Oxabicyclo[4.1.0]heptan-2-one,...	126	C7H10O2	021889-89-4	50
3			Cyclohexanone, 4-ethyl-	126	C8H14O	005441-51-0	43
4			1-Nonylcycloheptane	224	C16H32	1000371-47-7	38
5			3-Nonene, (E)-	126	C9H18	020063-92-7	37



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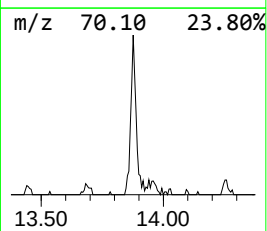
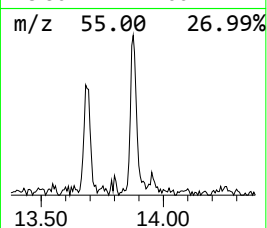
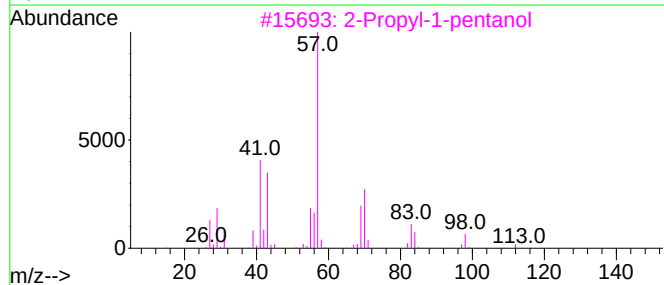
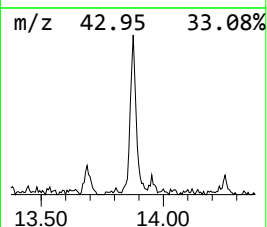
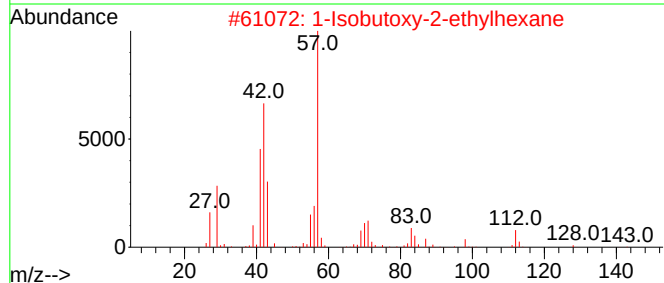
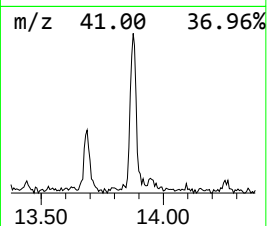
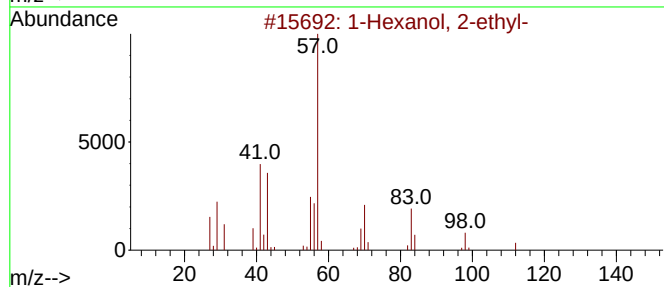
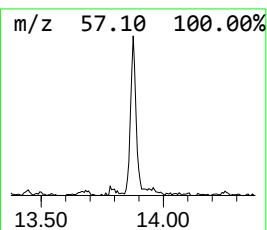
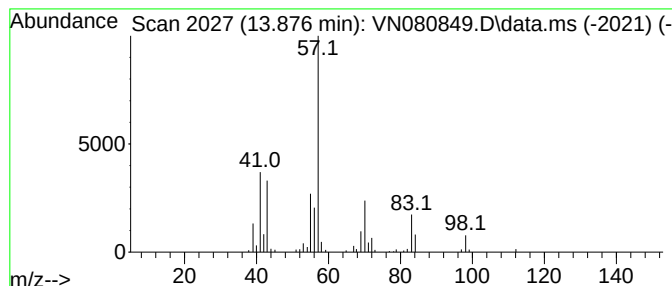
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	19.29 ug/l	247186	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	86
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	12.5	ug/l	73579	1	8.229	293319	50.0
4-Heptanol	12.423	6.2	ug/l	96685	3	11.865	779613	50.0
Butanoic acid, ...	13.341	104.1	ug/l	1333750	4	13.794	640644	50.0
2-Hexenal, 2-et...	13.688	6.9	ug/l	88955	4	13.794	640644	50.0
1-Hexanol, 2-et...	13.876	19.3	ug/l	247186	4	13.794	640644	50.0