

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
 Data File : VN081798.D
 Acq On : 18 Apr 2024 19:30
 Operator : JC\MD
 Sample : P2121-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 4827

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\82N041524W.M
 Title : SW846 8260

Signal : TIC: VN081798.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	13	22	28	rBV	61152	94139	11.44%	1.807%
2	2.812	139	146	153	rBV3	21574	45590	5.54%	0.875%
3	4.424	412	420	425	rBV2	9035	22862	2.78%	0.439%
4	6.712	791	809	811	rBV4	59746	142103	17.28%	2.728%
5	7.230	886	897	905	rBV6	13277	36492	4.44%	0.701%
6	8.165	1045	1056	1061	rBV	180247	449818	54.68%	8.636%
7	8.224	1061	1066	1081	rVB	323423	717960	87.28%	13.784%
8	8.577	1113	1126	1140	rVB	113302	260580	31.68%	5.003%
9	9.100	1206	1215	1223	rBV	244150	534587	64.99%	10.263%
10	9.271	1237	1244	1250	rBV3	8273	19747	2.40%	0.379%
11	10.565	1457	1464	1471	rBV	287738	536489	65.22%	10.300%
12	10.630	1471	1475	1483	rVB4	4379	8988	1.09%	0.173%
13	11.865	1674	1685	1697	rVB	262307	470946	57.25%	9.041%
14	12.418	1775	1779	1784	rBV3	15036	21557	2.62%	0.414%
15	12.847	1844	1852	1863	rBV	205415	365185	44.40%	7.011%
16	12.941	1863	1868	1874	rVB4	10234	16458	2.00%	0.316%
17	13.076	1886	1891	1899	rBV6	5048	8861	1.08%	0.170%
18	13.247	1913	1920	1921	rBV3	11331	14717	1.79%	0.283%
19	13.265	1921	1923	1929	rVV5	8589	14156	1.72%	0.272%
20	13.335	1929	1935	1948	rVV	547140	822563	100.00%	15.792%
21	13.794	2002	2013	2020	rBV	258216	425710	51.75%	8.173%
22	13.871	2020	2026	2037	rVB	65040	111944	13.61%	2.149%
23	14.253	2086	2091	2096	rBV4	6802	11289	1.37%	0.217%
24	15.400	2280	2286	2291	rBV3	17695	32433	3.94%	0.623%
25	15.829	2352	2359	2365	rVB5	6340	13245	1.61%	0.254%
26	16.117	2403	2408	2416	rVB4	5362	10411	1.27%	0.200%

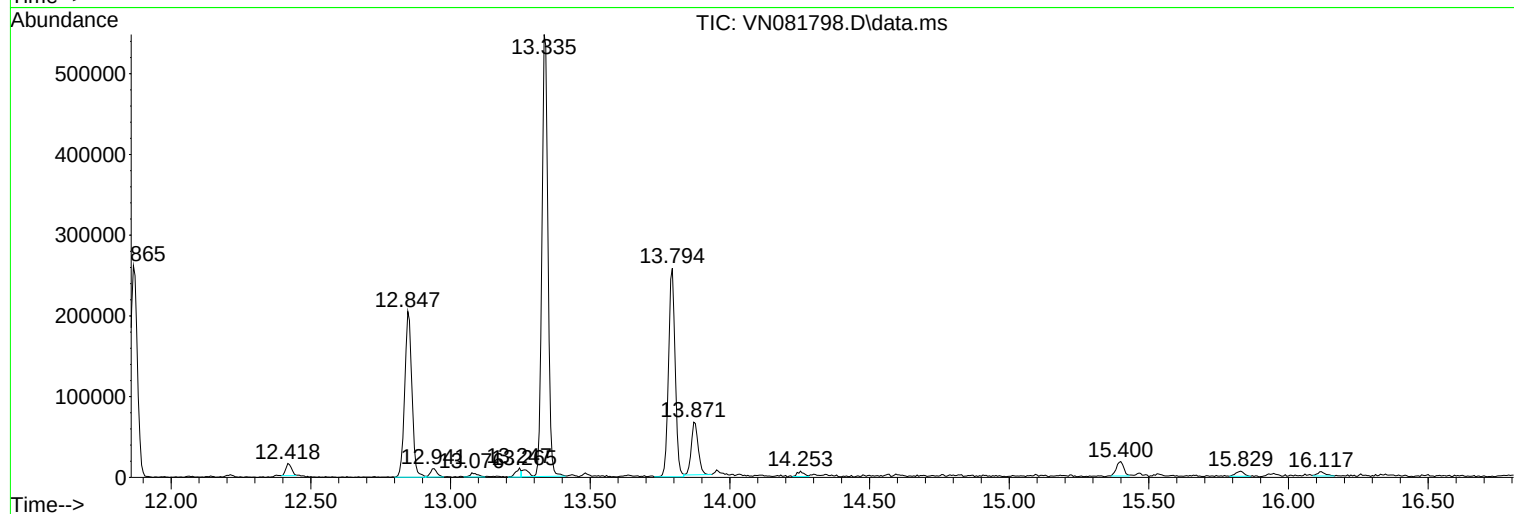
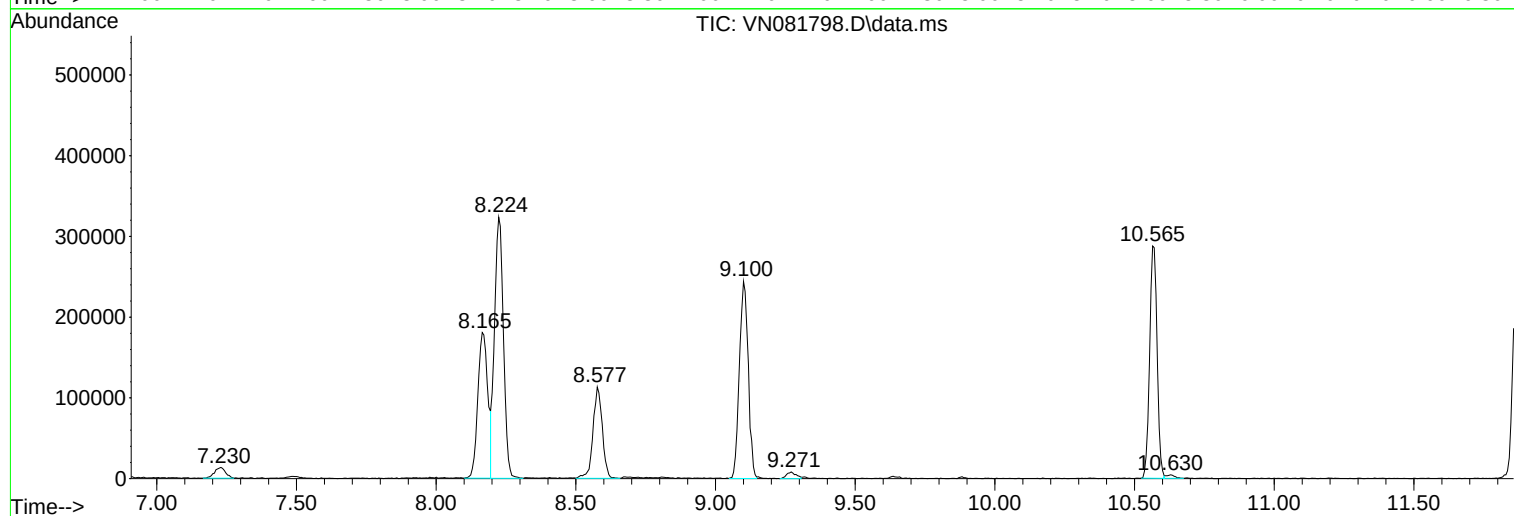
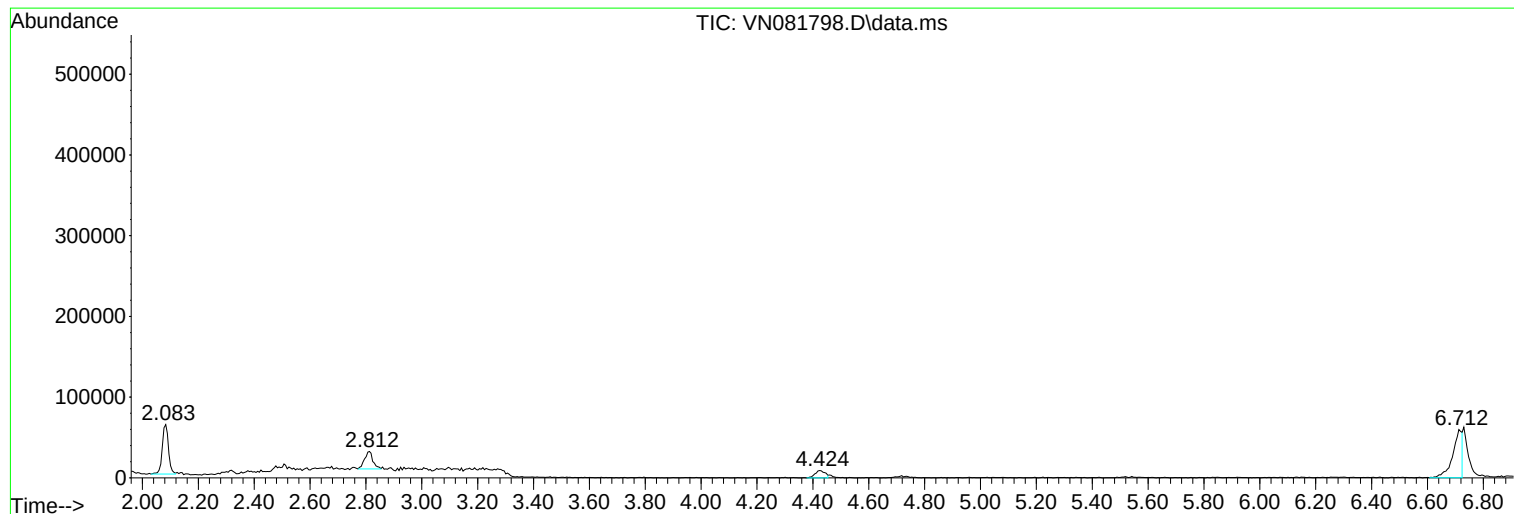
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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



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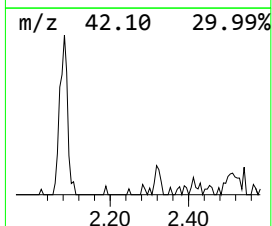
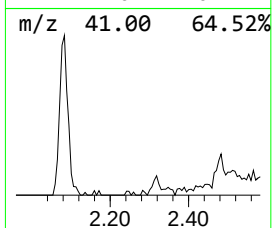
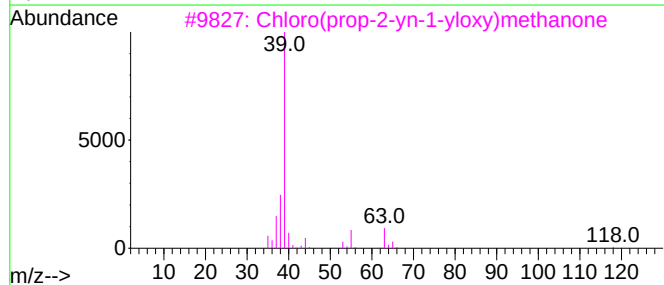
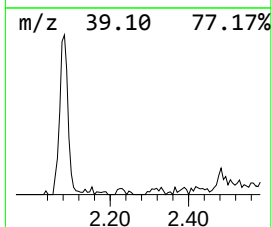
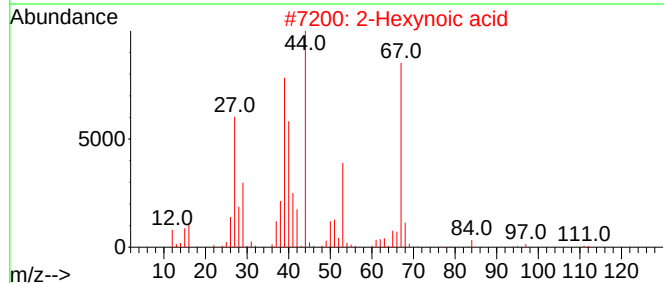
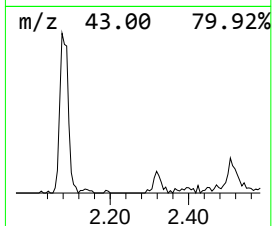
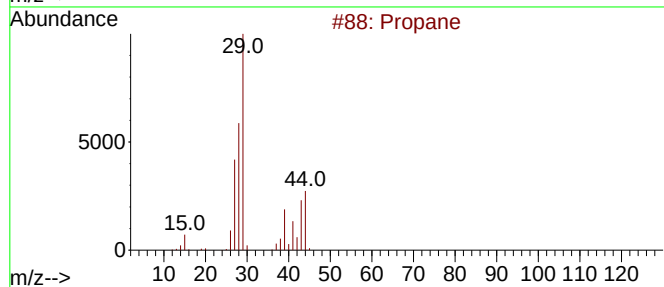
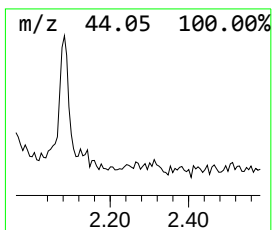
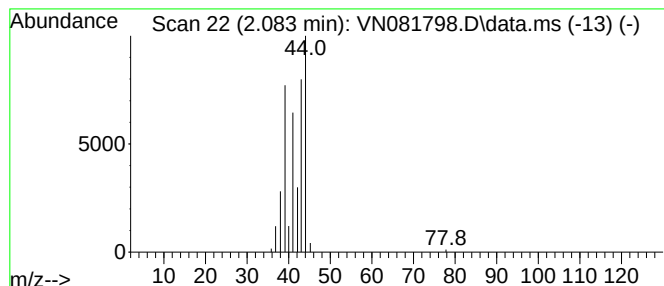
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	6.56 ug/l	94139	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	72
2			2-Hexynoic acid	112	C6H8O2	000764-33-0	43
3			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	9
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Acetaldehyde	44	C2H4O	000075-07-0	5



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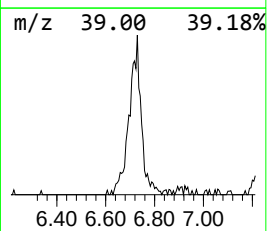
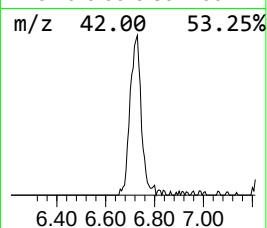
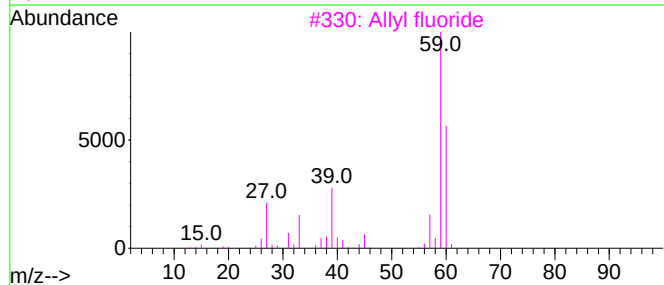
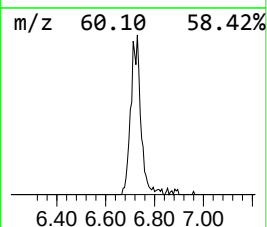
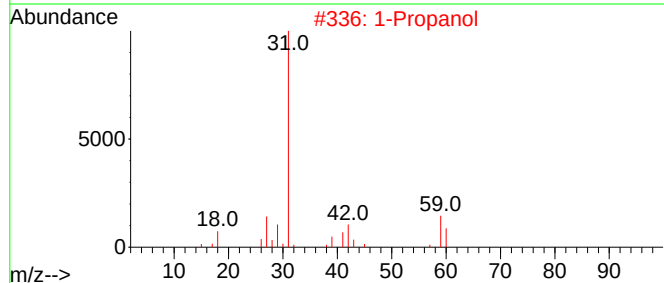
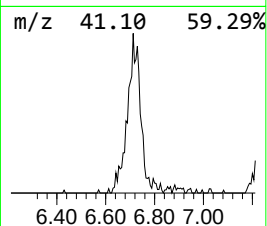
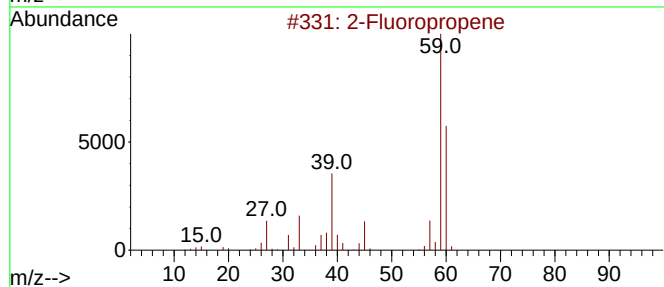
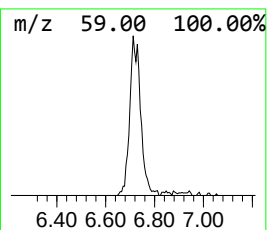
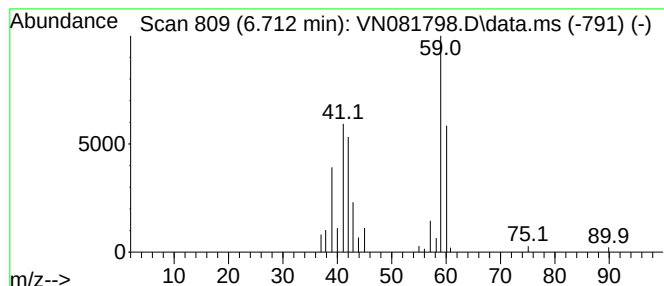
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Fluoropropene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.712	9.90 ug/l	142103	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluoropropene			60	C3H5F	001184-60-7	72
2	1-Propanol			60	C3H8O	000071-23-8	64
3	Allyl fluoride			60	C3H5F	000818-92-8	49
4	Cyclopropane			42	C3H6	000075-19-4	27
5	Cyclopropanecarboxaldehyde			70	C4H6O	001489-69-6	16



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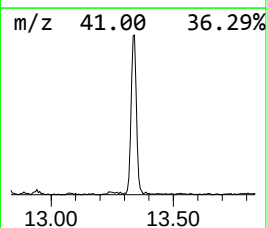
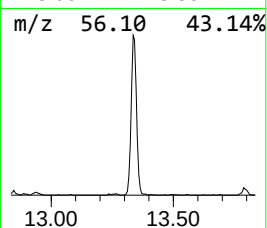
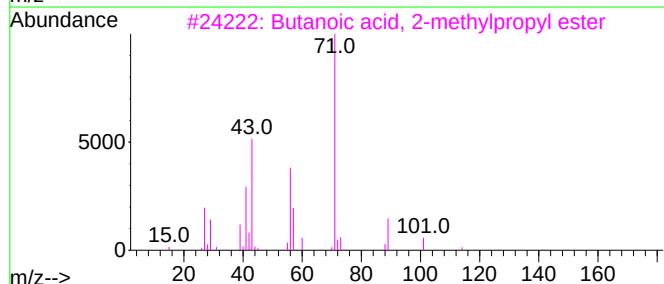
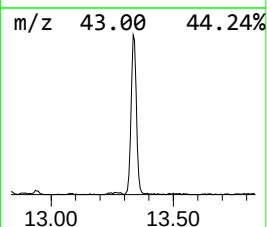
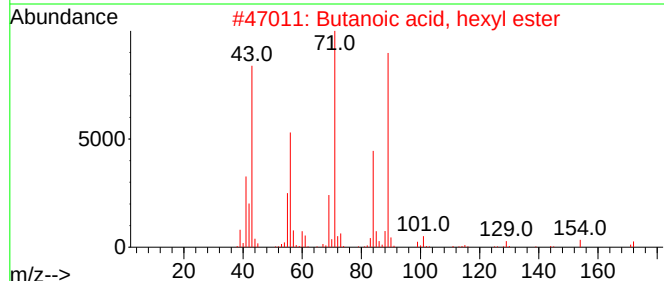
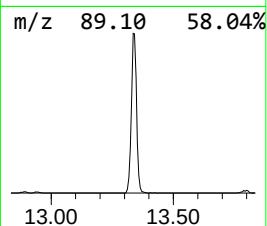
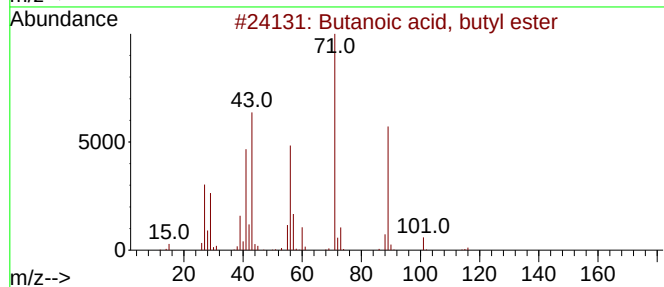
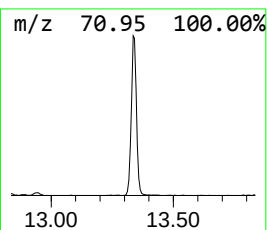
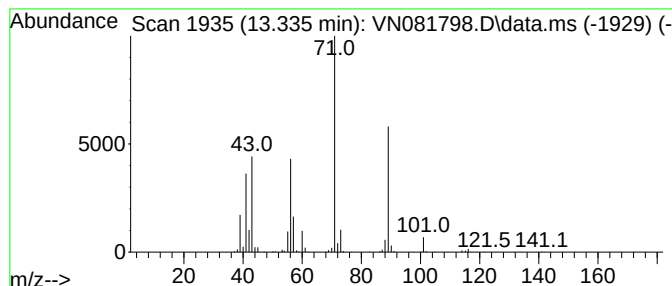
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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	96.61 ug/l	822563	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	72
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



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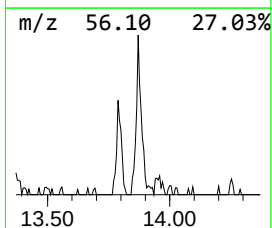
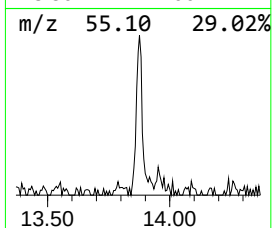
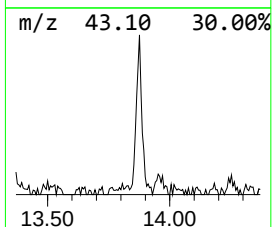
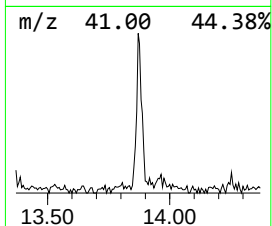
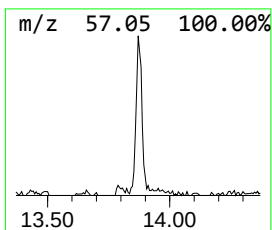
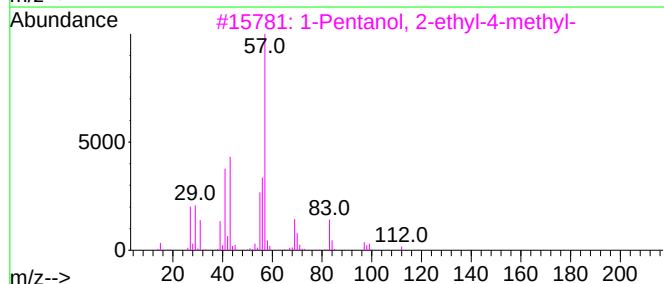
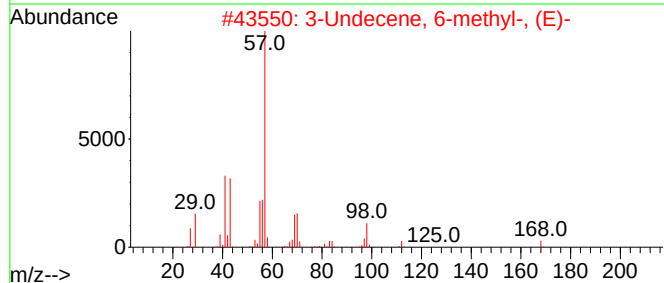
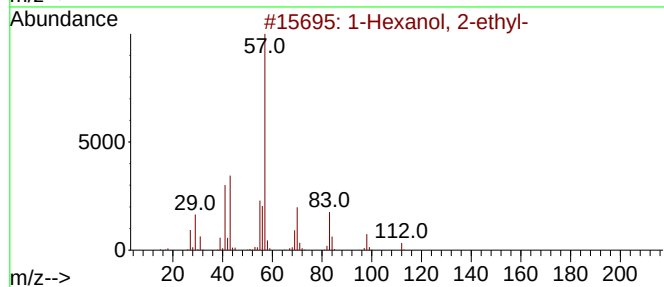
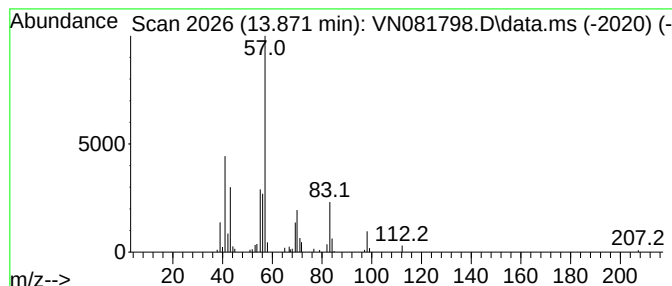
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	13.15 ug/l	111944	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			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	2.083	6.6	ug/l	94139	1	8.230	717960	50.0
2-Fluoropropene	6.712	9.9	ug/l	142103	1	8.230	717960	50.0
Butanoic acid, ...	13.335	96.6	ug/l	822563	4	13.794	425710	50.0
1-Hexanol, 2-et...	13.871	13.2	ug/l	111944	4	13.794	425710	50.0