

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
 Data File : VN081794.D
 Acq On : 18 Apr 2024 17:54
 Operator : JC\MD
 Sample : P2121-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 4825

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: VN081794.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.812	138	146	153	rBV6	14764	34639	2.75%	0.377%
2	3.283	224	226	234	rVB2	8269	13167	1.05%	0.143%
3	4.430	413	421	433	rBV	10658	28487	2.26%	0.310%
4	7.224	888	896	906	rBV4	26936	72351	5.75%	0.787%
5	8.171	1047	1057	1061	rBV	172341	419342	33.32%	4.563%
6	8.224	1061	1066	1078	rVB	306185	666122	52.94%	7.248%
7	8.583	1112	1127	1141	rBV	185469	434513	34.53%	4.728%
8	9.106	1205	1216	1229	rBV2	413984	877936	69.77%	9.552%
9	9.271	1236	1244	1260	rBV3	21790	56455	4.49%	0.614%
10	9.641	1302	1307	1317	rVB5	6263	13270	1.05%	0.144%
11	10.571	1457	1465	1476	rBV	662640	1219452	96.91%	13.268%
12	11.865	1670	1685	1697	rBV	581703	1072632	85.24%	11.670%
13	12.212	1738	1744	1751	rVB3	17847	29178	2.32%	0.317%
14	12.376	1767	1772	1775	rBV	18288	28529	2.27%	0.310%
15	12.423	1775	1780	1784	rVV	55875	96997	7.71%	1.055%
16	12.465	1784	1787	1796	rVB4	13380	22704	1.80%	0.247%
17	12.853	1840	1853	1860	rBV	468283	852195	67.72%	9.272%
18	12.935	1863	1867	1873	rBV2	18489	28813	2.29%	0.313%
19	13.265	1913	1923	1929	rBV2	198286	374245	29.74%	4.072%
20	13.335	1929	1935	1947	rVB	817286	1258360	100.00%	13.691%
21	13.794	2006	2013	2020	rBV	555989	948725	75.39%	10.322%
22	13.876	2020	2027	2036	rVV	229584	407932	32.42%	4.438%
23	13.953	2036	2040	2046	rVB6	15501	30423	2.42%	0.331%
24	15.394	2280	2285	2293	rVB	49457	83954	6.67%	0.913%
25	15.829	2350	2359	2371	rVB10	23276	67613	5.37%	0.736%
26	15.941	2371	2378	2384	rBV7	12489	30206	2.40%	0.329%
27	16.123	2401	2409	2414	rBV9	11156	22771	1.81%	0.248%

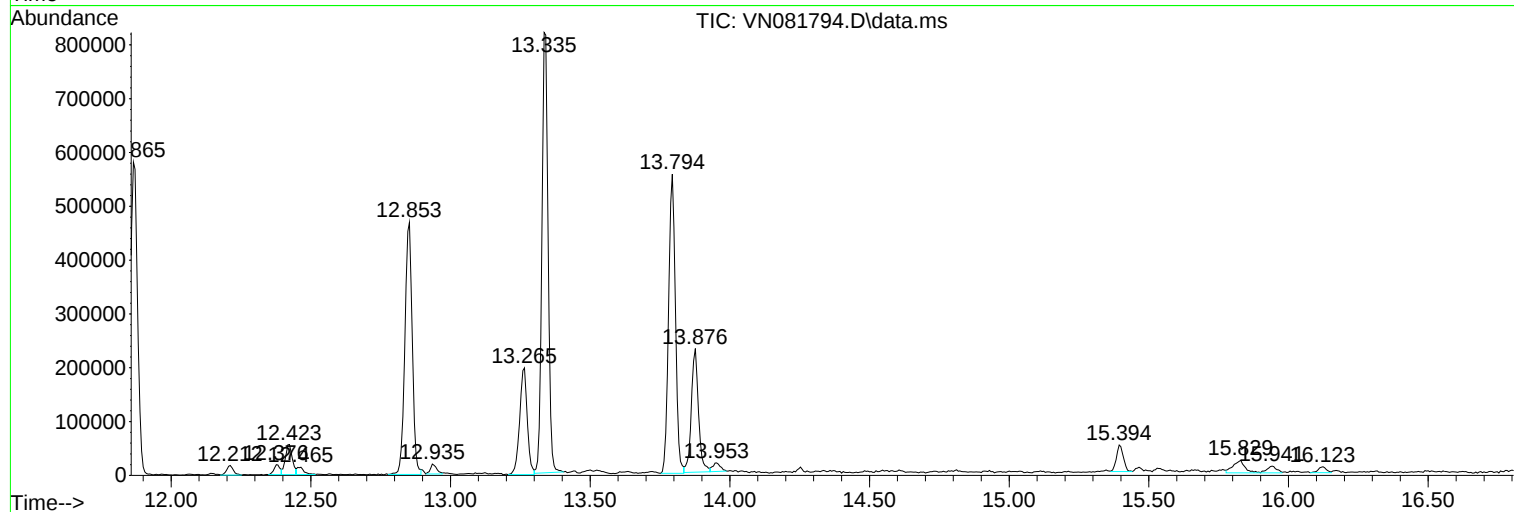
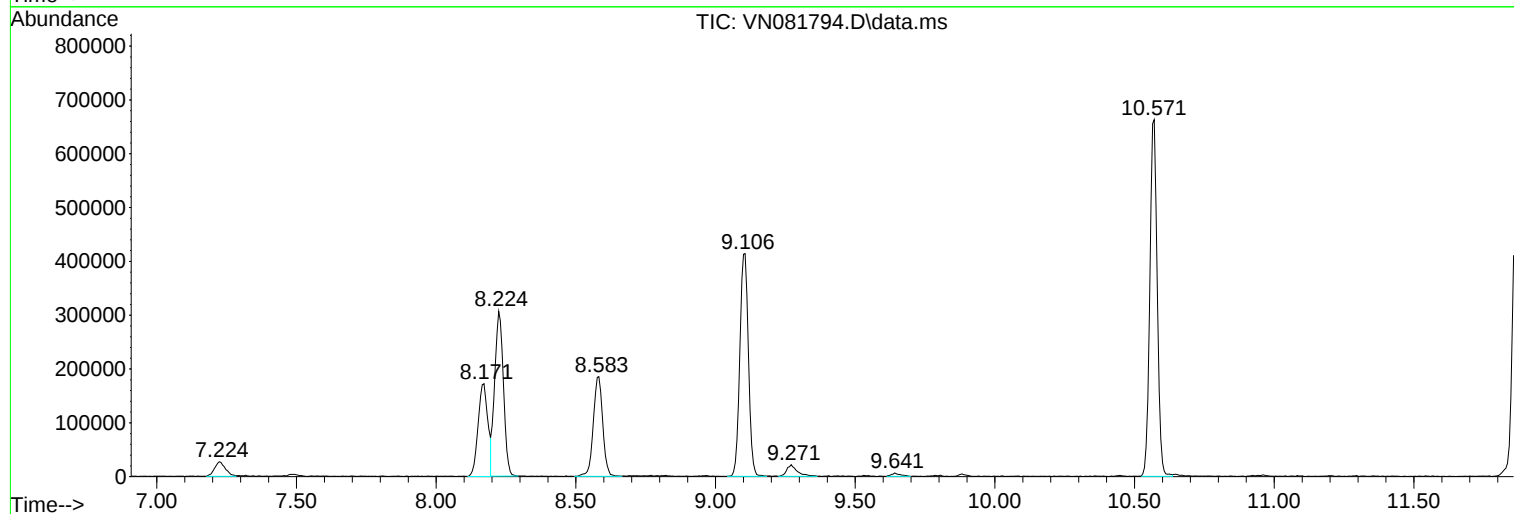
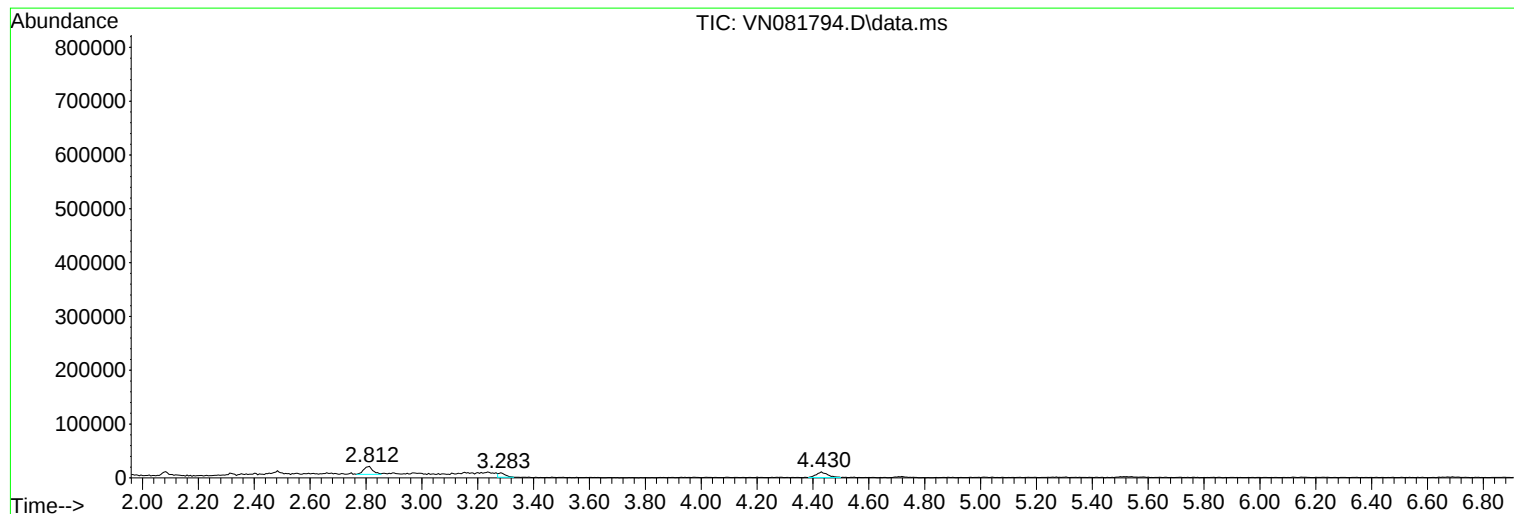
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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



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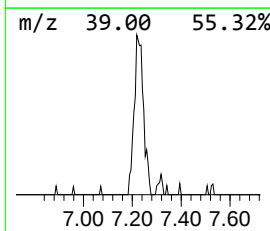
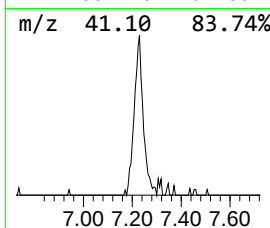
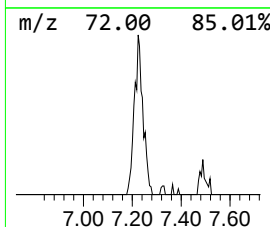
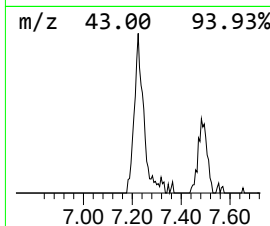
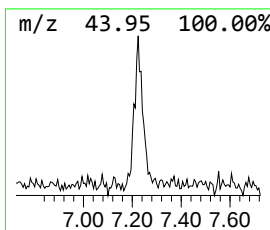
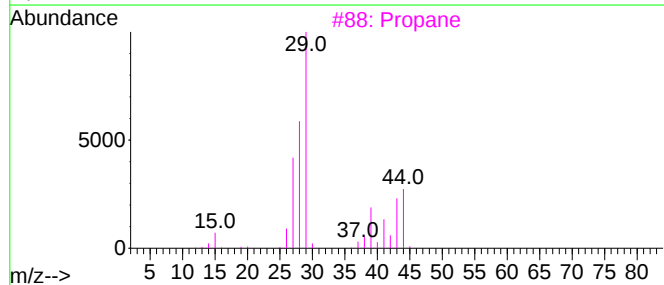
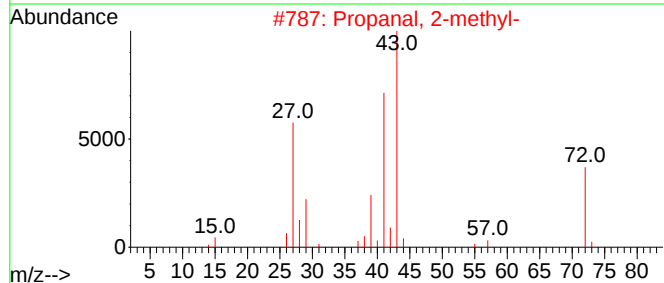
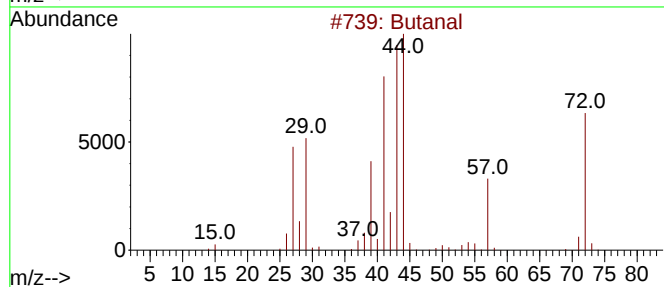
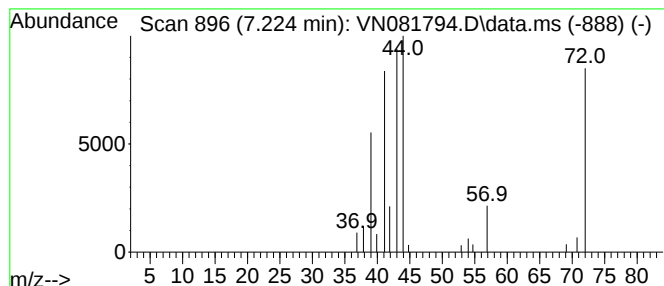
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	5.43 ug/l	72351	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
3			Propane	44	C3H8	000074-98-6	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	17
5			2-Butenal, (E)-	70	C4H6O	000123-73-9	12



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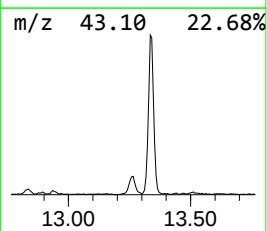
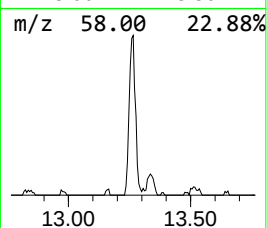
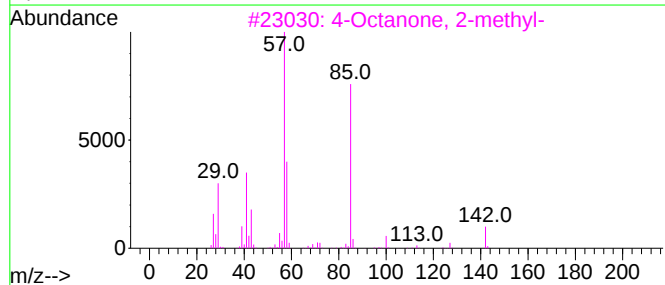
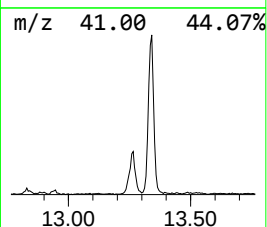
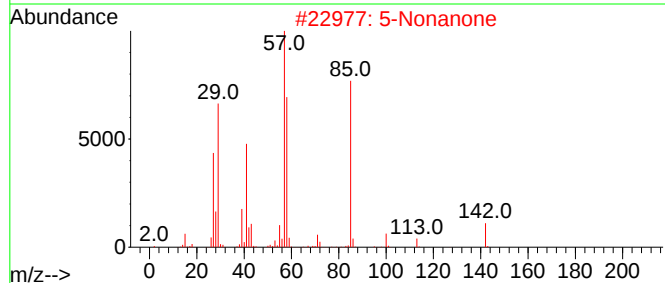
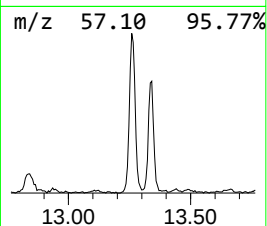
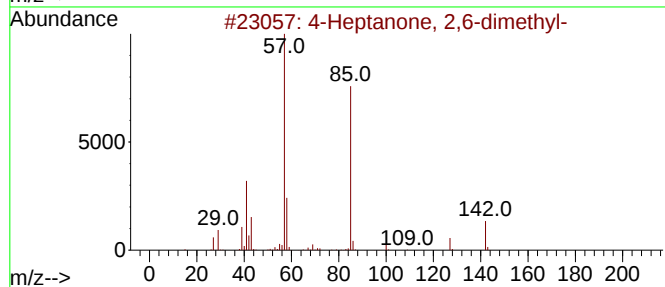
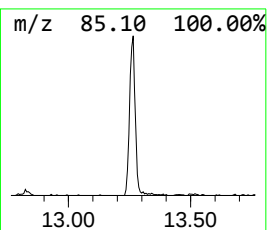
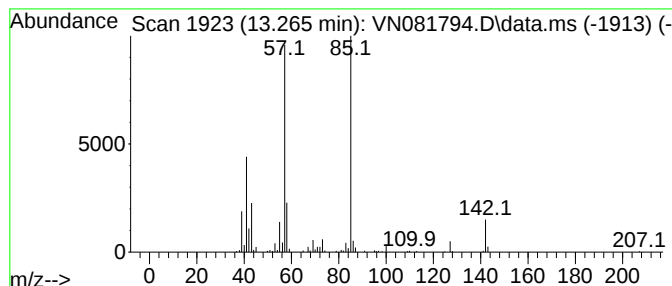
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Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	19.72 ug/l	374245	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			5-Nonanone	142	C9H18O	000502-56-7	64
3			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	59
4			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	50
5			1-Propoxypropan-2-yl 3-methylbut...	202	C11H22O3	1000367-12-6	45



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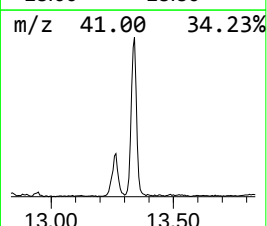
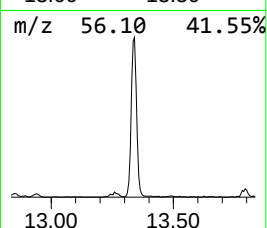
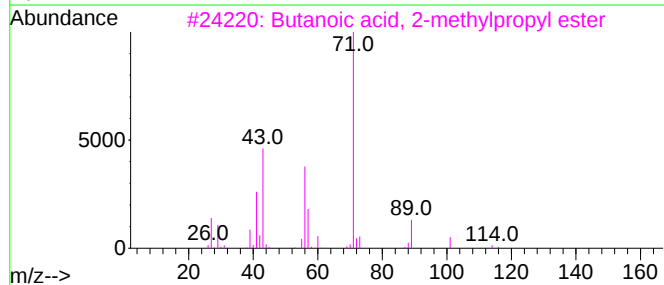
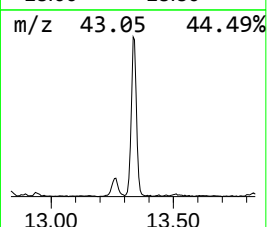
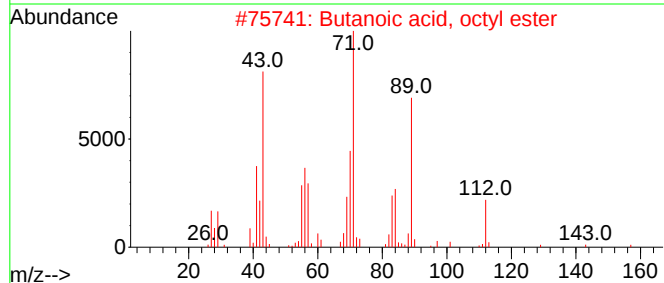
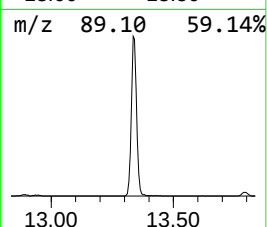
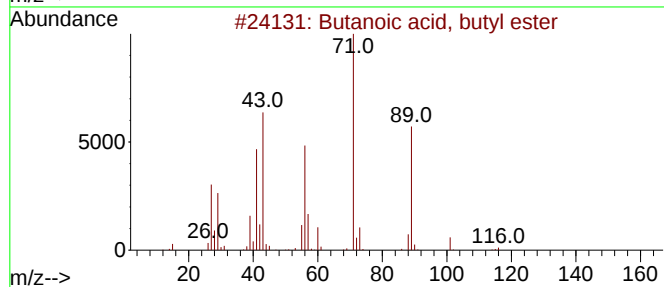
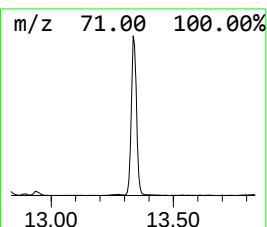
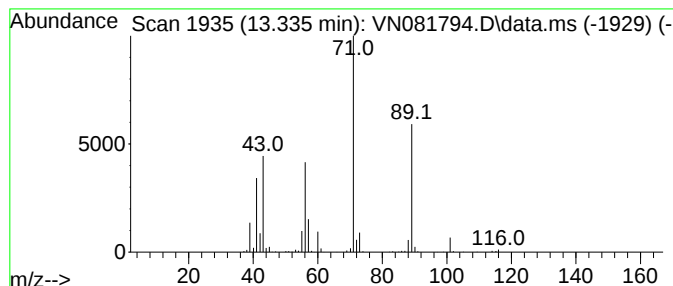
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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	66.32 ug/l	1258360	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, octyl ester	200	C12H24O2	000110-39-4	78
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
4			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	50
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	45



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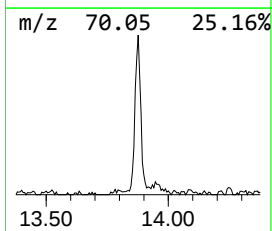
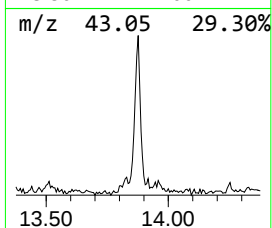
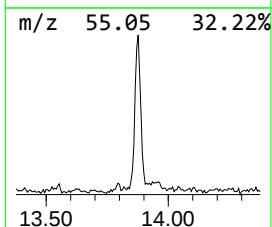
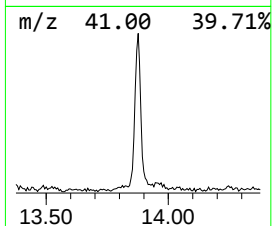
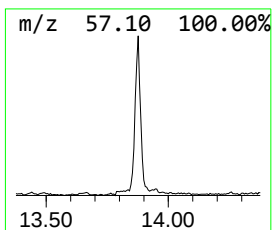
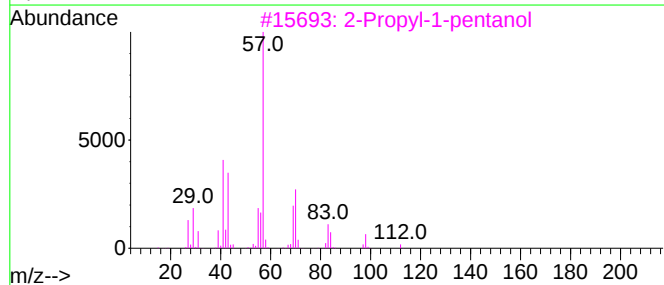
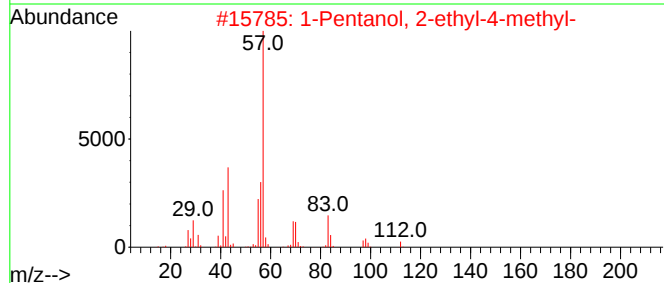
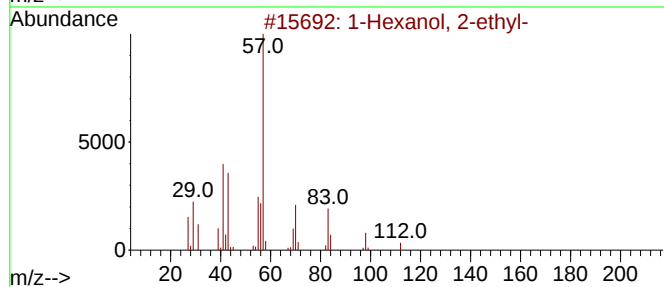
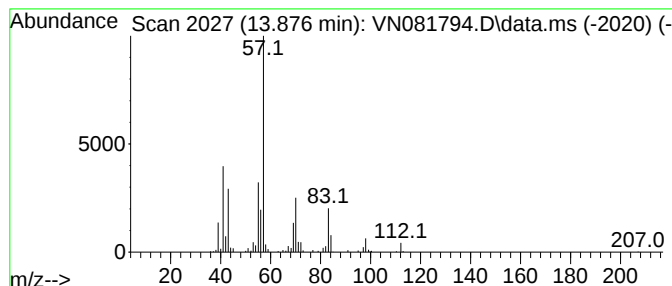
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	21.50 ug/l	407932	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	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	40
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	5.4	ug/l	72351	1	8.224	666122	50.0
4-Heptanone, 2,...	13.265	19.7	ug/l	374245	4	13.794	948725	50.0
Butanoic acid, ...	13.335	66.3	ug/l	1258360	4	13.794	948725	50.0
1-Hexanol, 2-et...	13.876	21.5	ug/l	407932	4	13.794	948725	50.0