

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020824\
Data File : VN080958.D
Acq On : 08 Feb 2024 12:58
Operator : JC\MD
Sample : P1373-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1290

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M

Title : SW846 8260

Signal : TIC: VN080958.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	rVB	53759	80246	4.14%	0.549%
2	2.824	138	148	155	rVB	41380	106010	5.47%	0.726%
3	4.430	411	421	431	rBV2	20347	64030	3.30%	0.438%
4	4.718	462	470	482	rVB4	7230	21041	1.09%	0.144%
5	7.224	886	896	907	rBV2	60929	168953	8.72%	1.157%
6	8.165	1045	1056	1061	rBV	292275	706216	36.45%	4.835%
7	8.229	1061	1067	1077	rVB	520132	1171539	60.47%	8.021%
8	8.582	1109	1127	1136	rBV	315901	719713	37.15%	4.927%
9	9.100	1206	1215	1232	rBV	770836	1614132	83.31%	11.051%
10	9.271	1235	1244	1261	rBV4	33734	94068	4.86%	0.644%
11	9.653	1302	1309	1317	rBV8	10845	27248	1.41%	0.187%
12	9.888	1342	1349	1355	rBV2	20190	37473	1.93%	0.257%
13	10.571	1455	1465	1472	rBV	1033594	1901646	98.15%	13.019%
14	10.629	1472	1475	1484	rVB4	15308	28667	1.48%	0.196%
15	11.870	1673	1686	1696	rBV	1020981	1867701	96.40%	12.787%
16	12.206	1737	1743	1753	rVB2	20247	35442	1.83%	0.243%
17	12.423	1774	1780	1790	rVB	77980	126904	6.55%	0.869%
18	12.853	1842	1853	1864	rBV	695286	1300756	67.13%	8.905%
19	12.941	1864	1868	1877	rVB2	27805	52298	2.70%	0.358%
20	13.247	1912	1920	1922	rBV4	38797	70180	3.62%	0.480%
21	13.270	1922	1924	1929	rVV3	39377	56585	2.92%	0.387%
22	13.341	1929	1936	1948	rVB	1299600	1937540	100.00%	13.265%
23	13.688	1985	1995	2001	rBV3	68653	129347	6.68%	0.886%
24	13.794	2005	2013	2021	rBV	943847	1559410	80.48%	10.676%
25	13.876	2021	2027	2037	rBV	265859	482508	24.90%	3.303%
26	13.959	2037	2041	2048	rVB9	19103	34636	1.79%	0.237%
27	14.247	2083	2090	2098	rBV8	16383	29716	1.53%	0.203%
28	15.341	2272	2276	2280	rBV5	12258	22669	1.17%	0.155%
29	15.400	2280	2286	2293	rVB	79051	136683	7.05%	0.936%
30	16.123	2402	2409	2414	rBV4	10379	22857	1.18%	0.156%

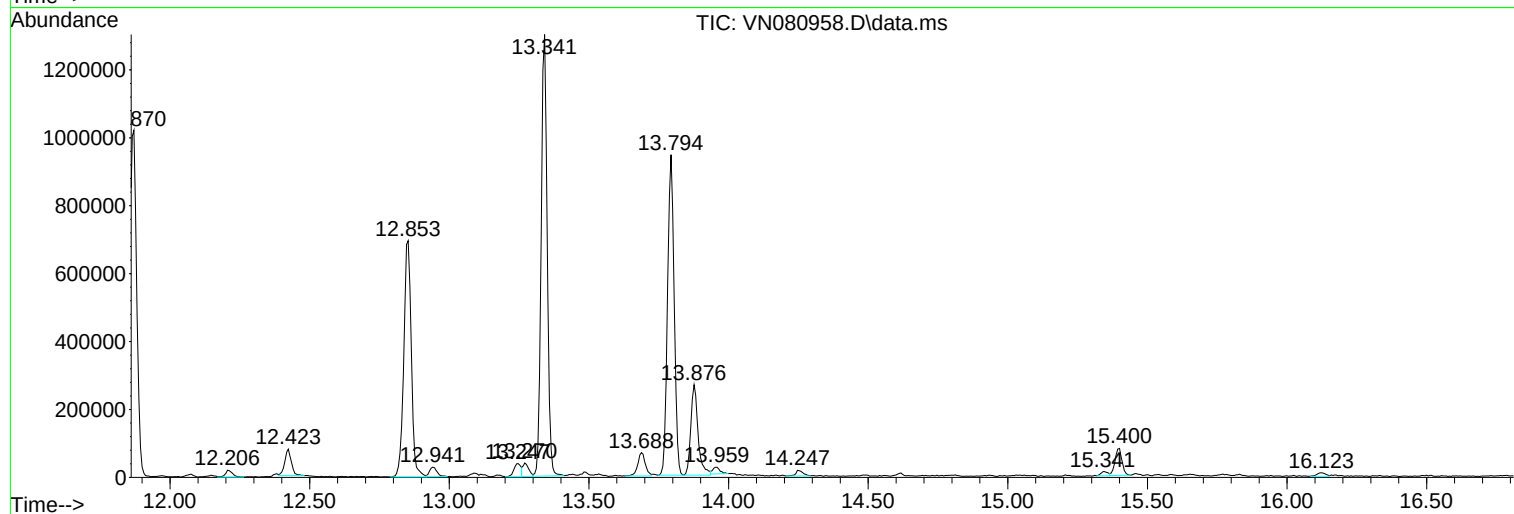
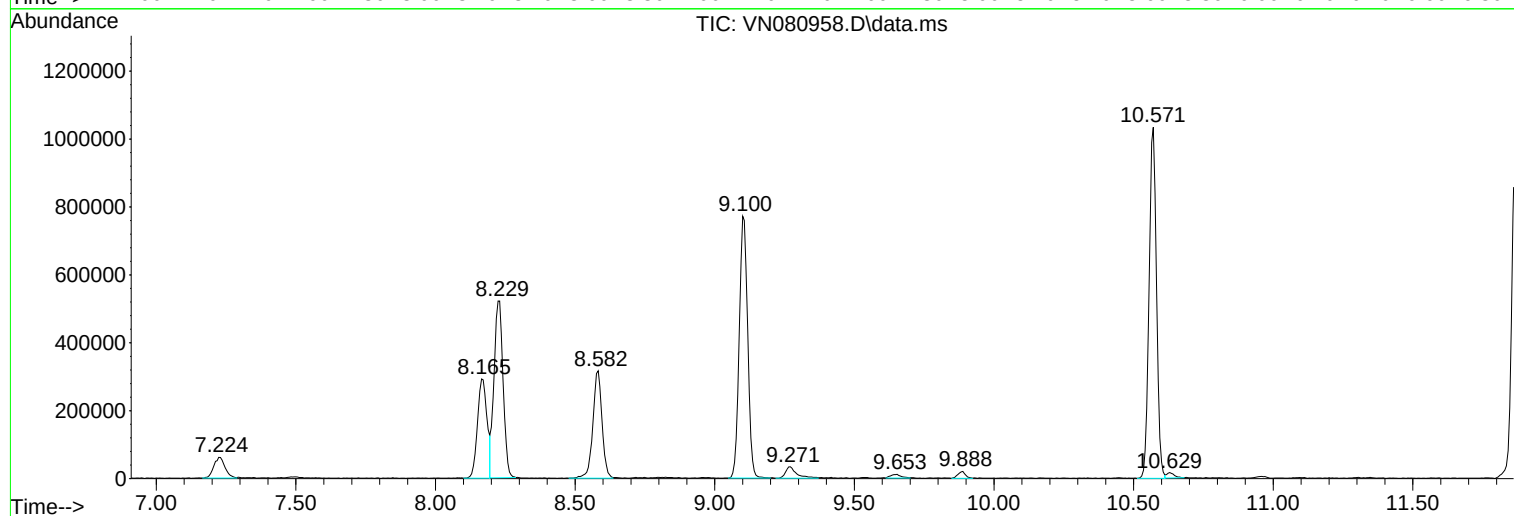
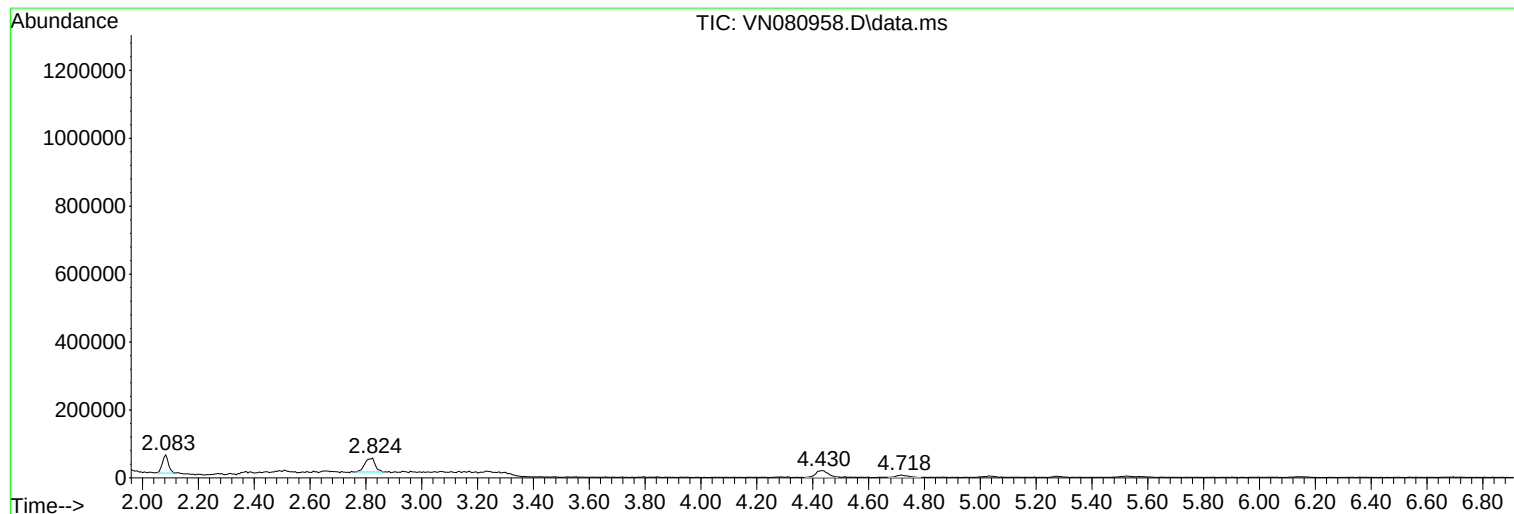
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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



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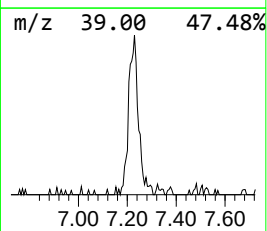
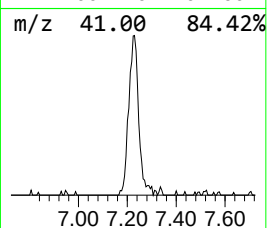
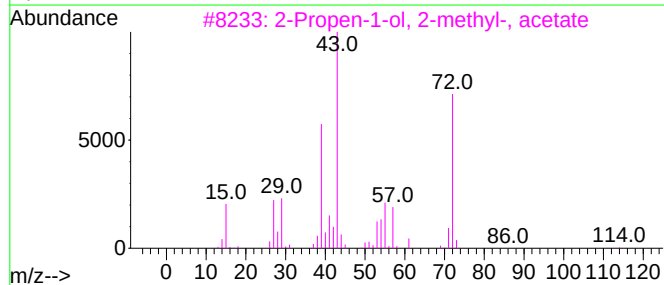
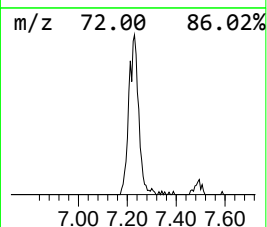
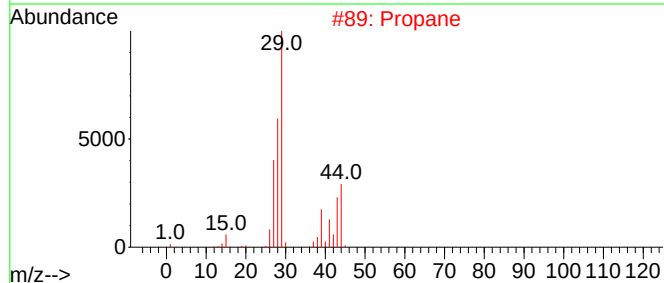
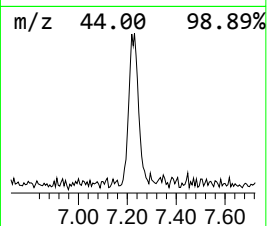
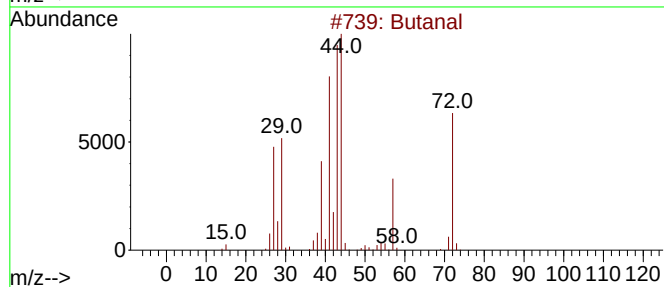
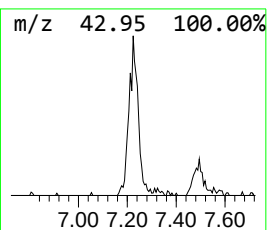
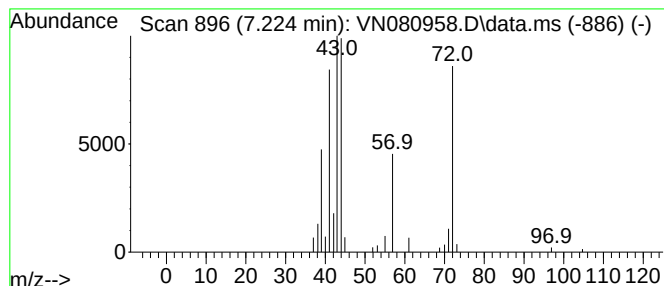
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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	7.21 ug/l	168953	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	43
3			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	40
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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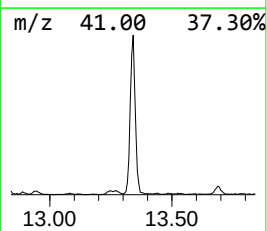
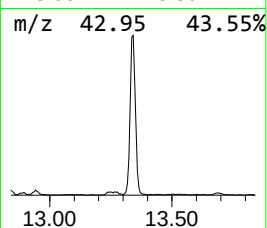
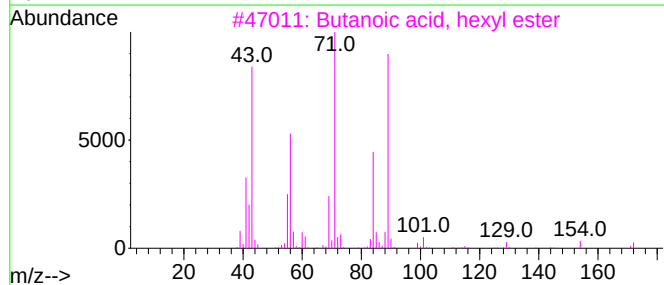
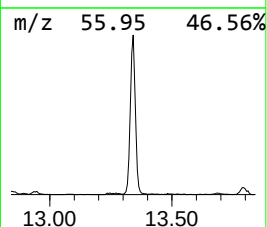
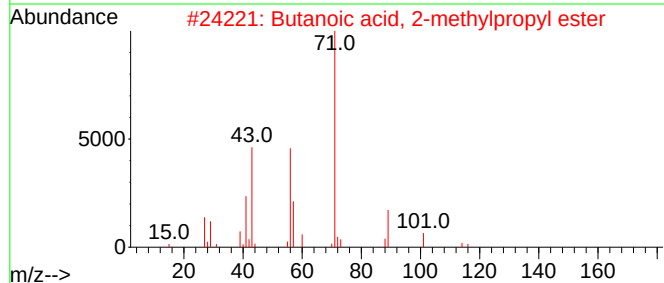
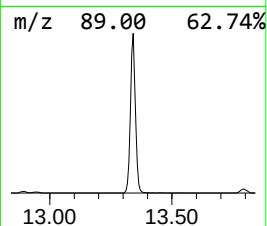
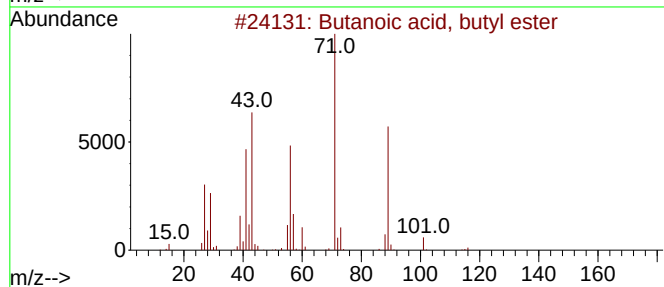
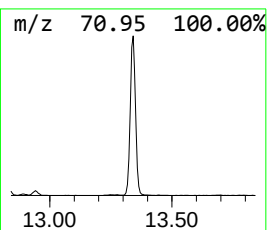
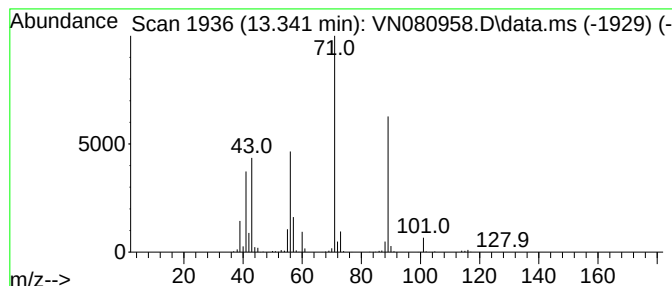
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Peak Number 2 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	62.12 ug/l	1937540	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	64
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
5			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56



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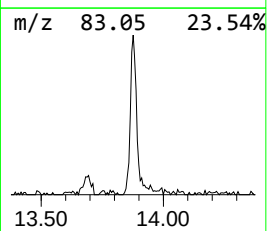
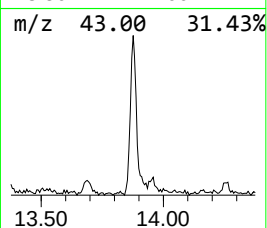
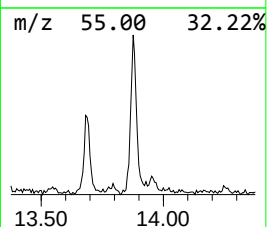
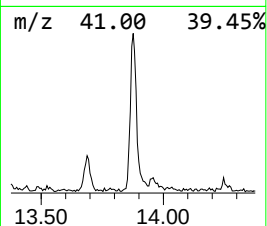
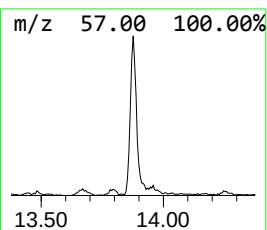
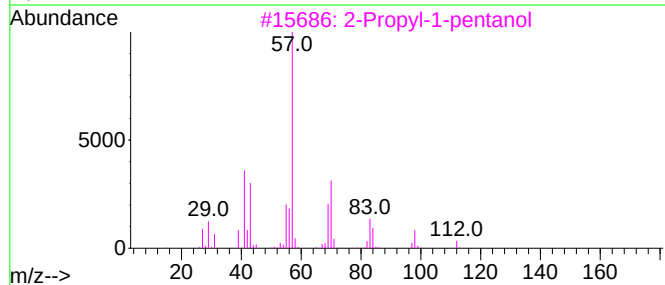
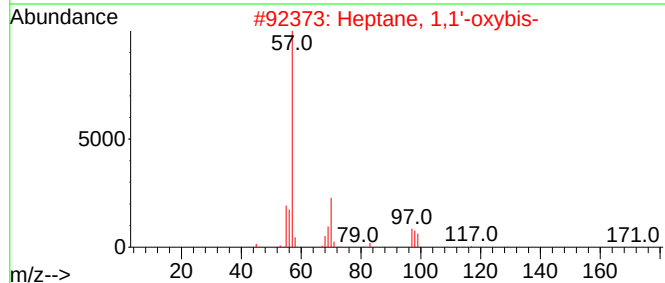
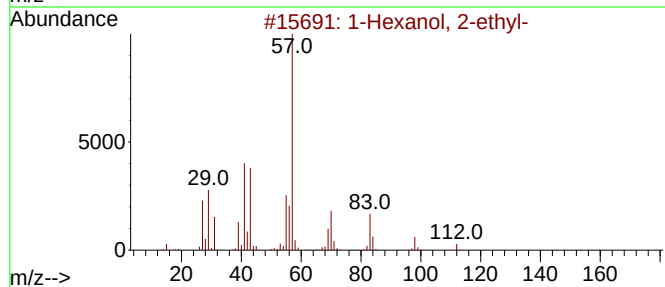
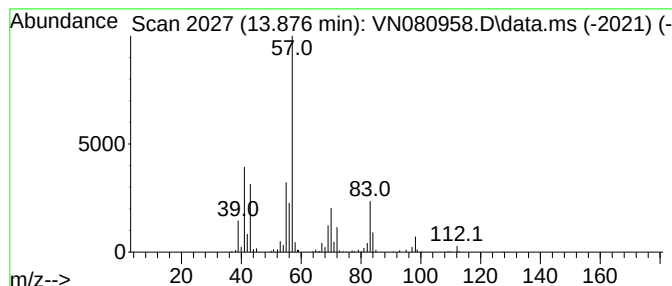
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TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	15.47 ug/l	482508	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			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	43
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	7.2	ug/l	168953	1	8.229	1171540	50.0
Butanoic acid, ...	13.341	62.1	ug/l	1937540	4	13.794	1559410	50.0
1-Hexanol, 2-et...	13.876	15.5	ug/l	482508	4	13.794	1559410	50.0