

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120623\
 Data File : VN080397.D
 Acq On : 06 Dec 2023 19:31
 Operator : JC\MD
 Sample : 05650-04 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 50197

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\82N111623W.M
 Title : SW846 8260

Signal : TIC: VN080397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	51	57	68	rVB	15150	34323	3.26%	0.467%
2	4.430	413	421	422	rBV2	9303	16632	1.58%	0.226%
3	7.429	925	931	935	rVB2	5942	11554	1.10%	0.157%
4	8.171	1046	1057	1061	rBV	168249	394258	37.49%	5.360%
5	8.223	1061	1066	1077	rVB	228745	518919	49.35%	7.055%
6	8.582	1118	1127	1136	rBV	152947	347720	33.07%	4.727%
7	9.100	1204	1215	1225	rBV	341243	718412	68.32%	9.767%
8	9.653	1303	1309	1316	rVB4	10065	18971	1.80%	0.258%
9	10.570	1457	1465	1475	rBV	560198	1051591	100.00%	14.297%
10	11.864	1678	1685	1697	rBV	567053	995096	94.63%	13.529%
11	12.853	1845	1853	1860	rBV	474727	804686	76.52%	10.940%
12	12.953	1863	1870	1878	rBV	386573	651230	61.93%	8.854%
13	13.182	1900	1909	1919	rBV	304184	520651	49.51%	7.078%
14	13.705	1992	1998	2006	rVV2	103954	167327	15.91%	2.275%
15	13.794	2006	2013	2021	rVB	610484	1035267	98.45%	14.075%
16	14.105	2061	2066	2071	rBV4	10549	20087	1.91%	0.273%
17	14.958	2208	2211	2216	rVB5	13118	19441	1.85%	0.264%
18	15.435	2288	2292	2297	rBV4	7517	15123	1.44%	0.206%
19	15.641	2323	2327	2332	rVB4	8334	14133	1.34%	0.192%

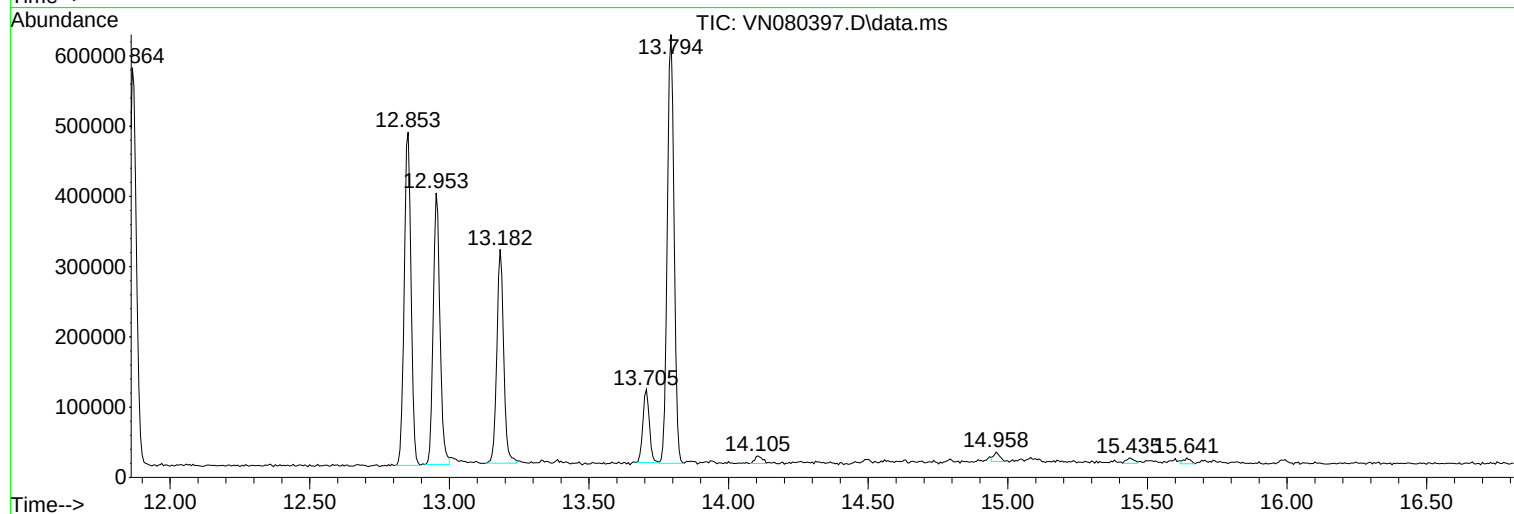
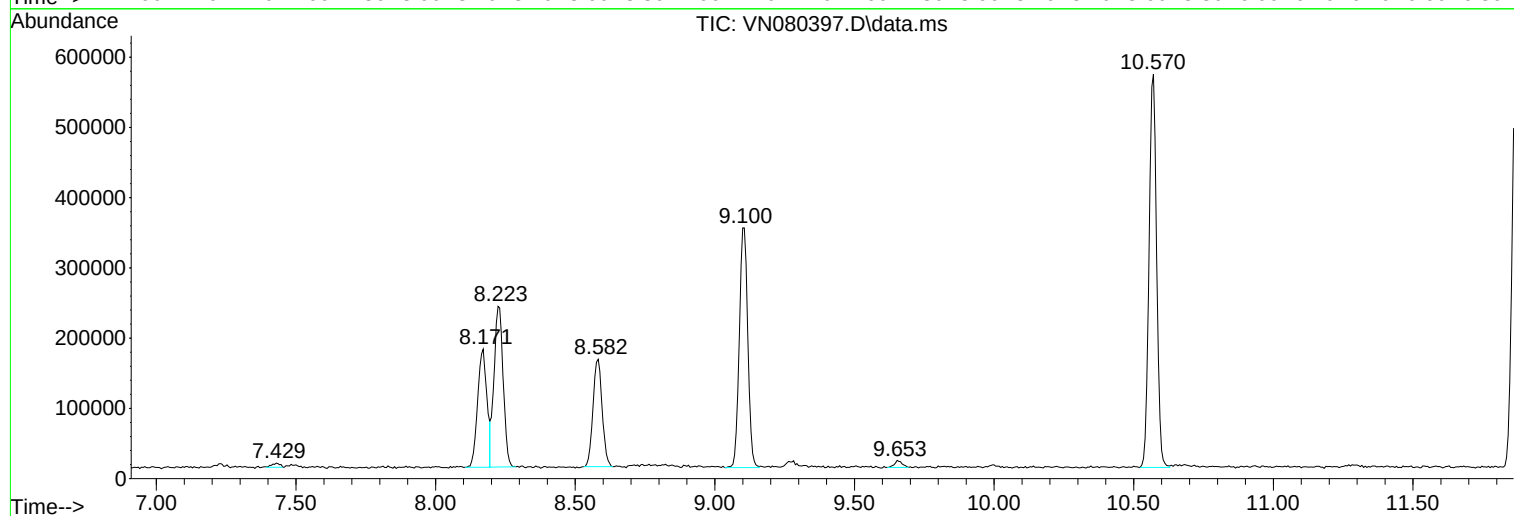
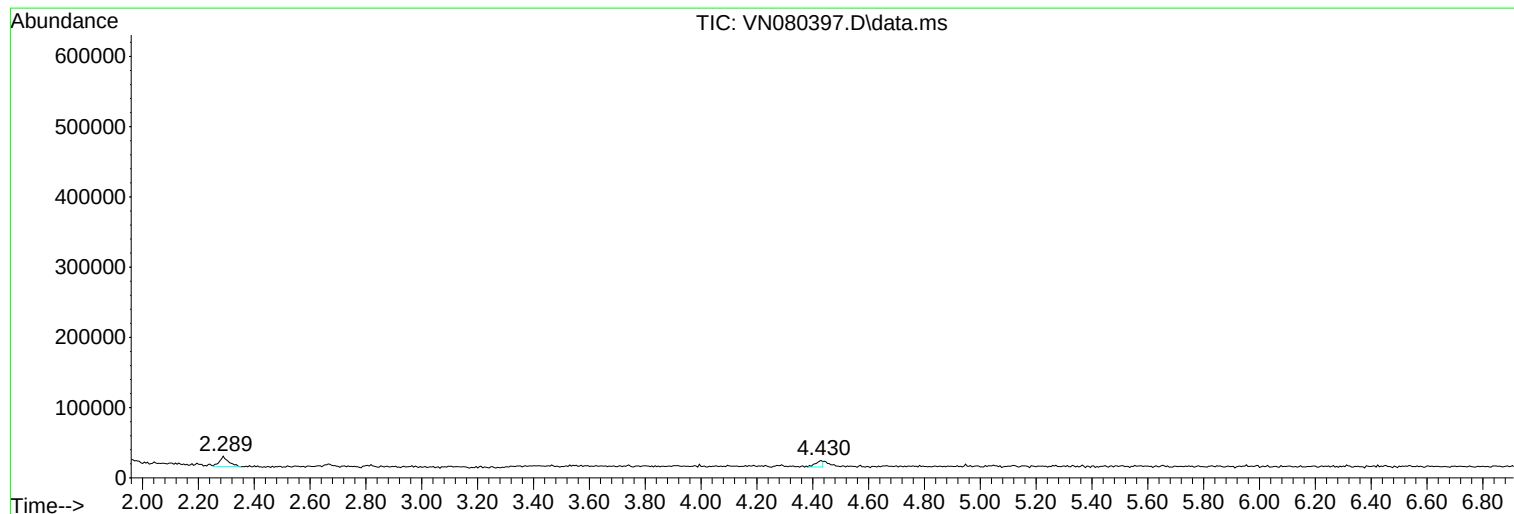
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Quant Title : SW846 8260

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



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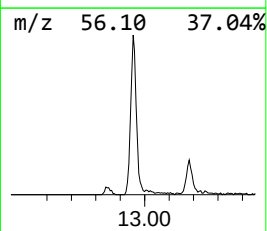
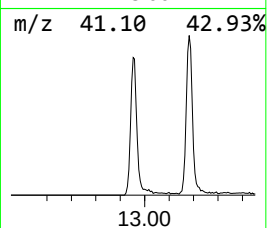
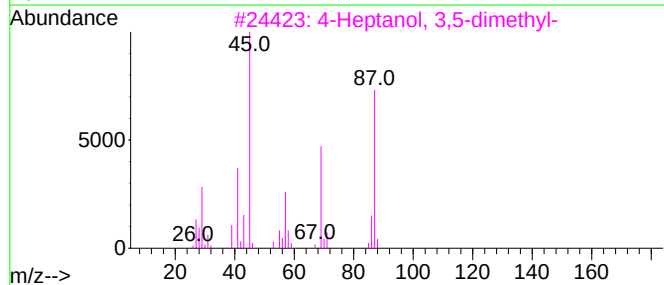
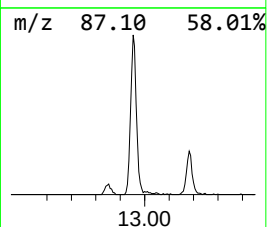
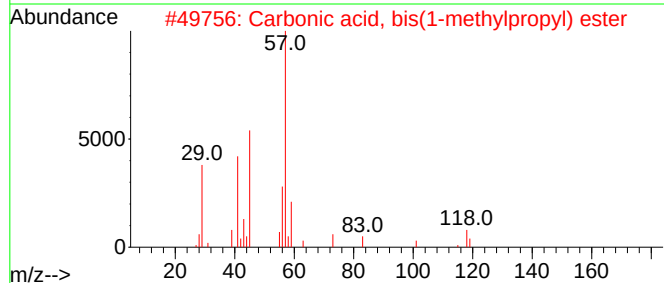
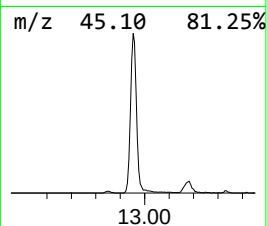
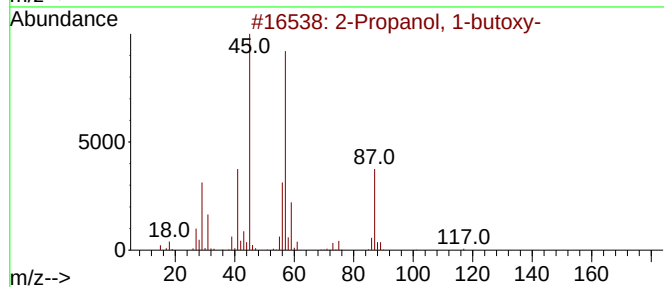
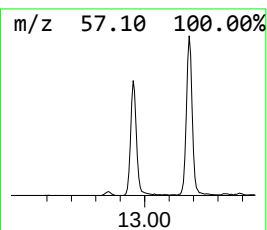
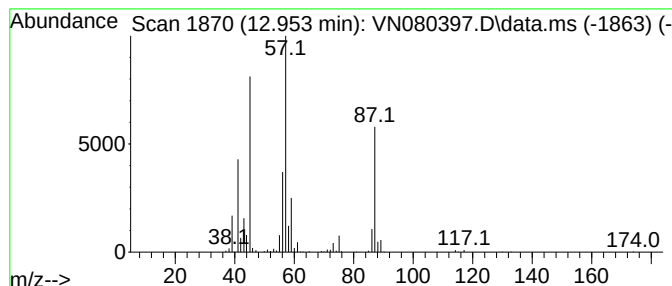
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Propanol, 1-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.953	31.45 ug/l	651230	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-			132	C7H16O2	005131-66-8	90
2	Carbonic acid, bis(1-methylpropy...			174	C9H18O3	000623-63-2	53
3	4-Heptanol, 3,5-dimethyl-			144	C9H20O	019549-79-2	53
4	(Methylthio)-acetonitrile			87	C3H5NS	035120-10-6	50
5	Propane, 1,1'-[ethylidenebis(oxy...			146	C8H18O2	000105-82-8	50



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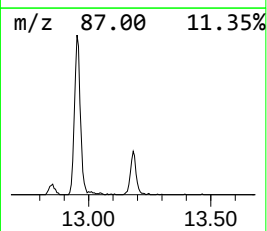
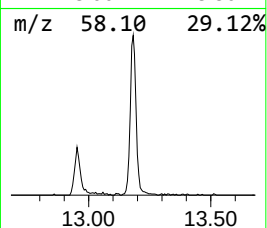
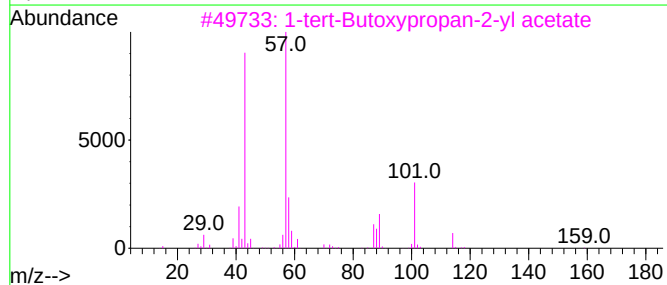
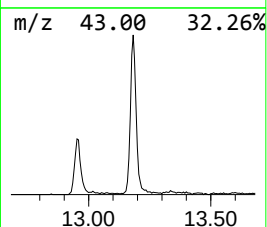
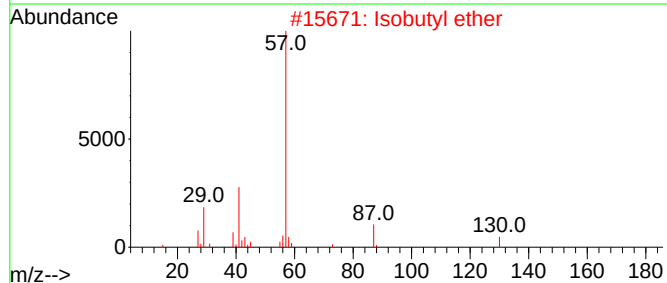
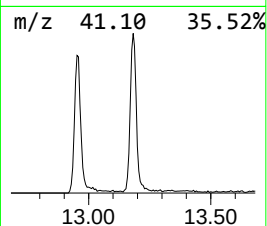
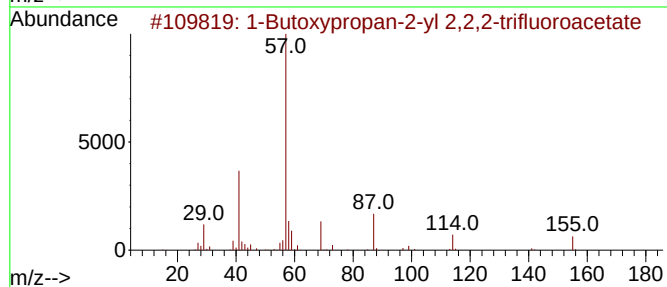
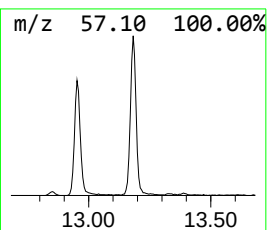
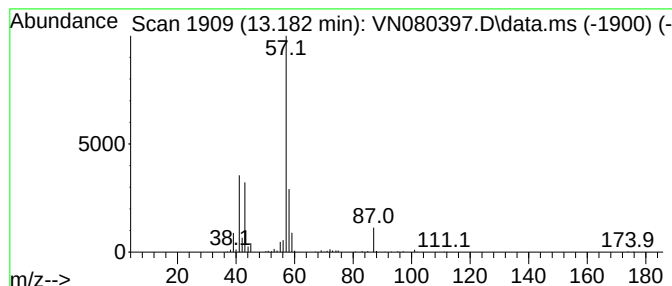
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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Butoxypropan-2-yl 2,2,2-t... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.182	25.15 ug/l	520651	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butoxypropan-2-yl 2,2,2-triflu...	228	C9H15F3O3	1000367-08-1	64
2			Isobutyl ether	130	C8H18O	000628-55-7	42
3			1-tert-Butoxypropan-2-yl acetate	174	C9H18O3	1000367-07-9	39
4			Di-tert-butyl peroxide	146	C8H18O2	000110-05-4	38
5			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	28



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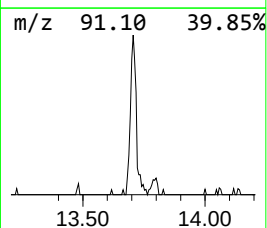
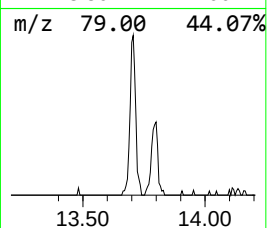
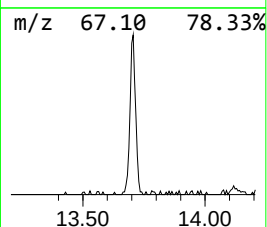
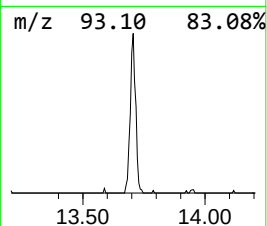
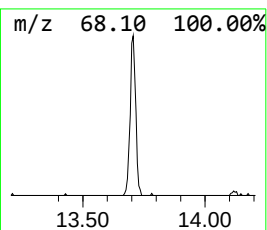
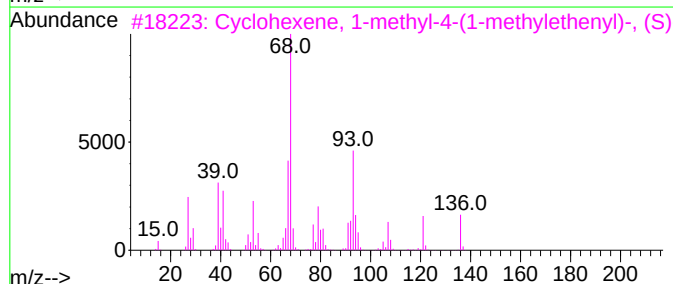
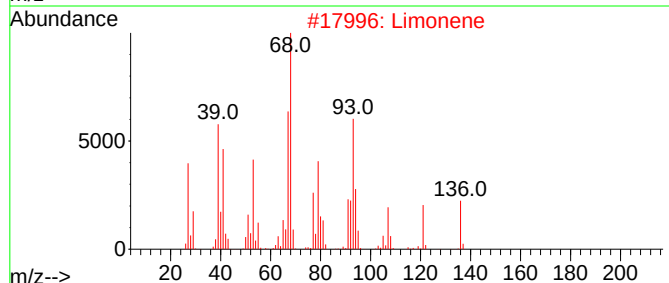
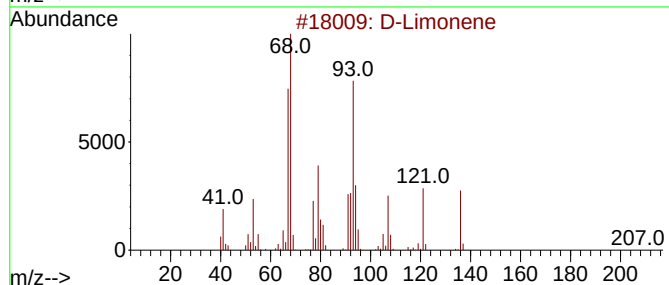
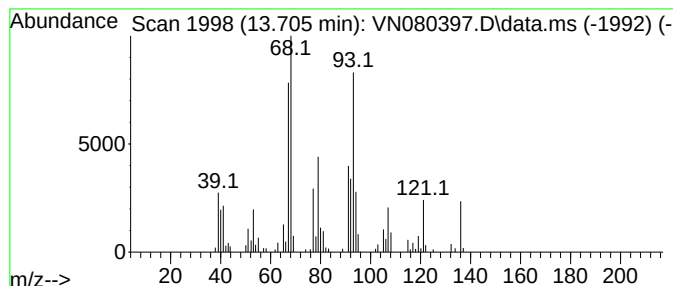
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 D-Limonene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.706	8.08 ug/l	167327	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	97
2			Limonene	136	C10H16	000138-86-3	91
3			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	74
4			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	001461-27-4	49
5			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	45



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 1-b...	12.953	31.4	ug/l	651230	4	13.794	1035270	50.0
1-Butoxypropan-...	13.182	25.1	ug/l	520651	4	13.794	1035270	50.0
D-Limonene	13.706	8.1	ug/l	167327	4	13.794	1035270	50.0