

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
 Data File : VN070375.D
 Acq On : 30 Dec 2021 4:11
 Operator : JC/MD
 Sample : M5007-03RE
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-04RE

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.271	100	105	142	rVB3	189068	376108	7.94%	1.318%
2	4.291	844	858	875	rBV2	27083	74242	1.57%	0.260%
3	5.621	1326	1354	1386	rBV3	90899	330161	6.97%	1.157%
4	7.327	1963	1990	2015	rBV3	159210	435816	9.20%	1.527%
5	8.024	2225	2250	2261	rBV2	646118	1573804	33.23%	5.514%
6	8.086	2261	2273	2297	rVB	1160498	2636978	55.68%	9.239%
7	8.440	2384	2405	2434	rBV	800596	1852698	39.12%	6.491%
8	8.617	2449	2471	2492	rBV	245395	656325	13.86%	2.300%
9	8.968	2583	2602	2637	rBV	1818765	3803302	80.30%	13.326%
10	9.885	2927	2944	2960	rVB3	154619	310058	6.55%	1.086%
11	10.014	2971	2992	3012	rBV	464926	971089	20.50%	3.402%
12	10.443	3135	3152	3191	rVV	2531834	4736205	100.00%	16.594%
13	10.644	3217	3227	3241	rVB3	54518	95649	2.02%	0.335%
14	10.717	3243	3254	3273	rVB3	54654	102530	2.16%	0.359%
15	11.746	3612	3638	3673	rBV	2355296	4330953	91.44%	15.175%
16	12.731	3986	4005	4029	rBV	1750952	3140671	66.31%	11.004%
17	12.905	4060	4070	4086	rVB6	39007	68633	1.45%	0.240%
18	12.980	4086	4098	4106	rBV	61632	106889	2.26%	0.375%
19	13.675	4340	4357	4386	rBV	1636191	2938848	62.05%	10.297%

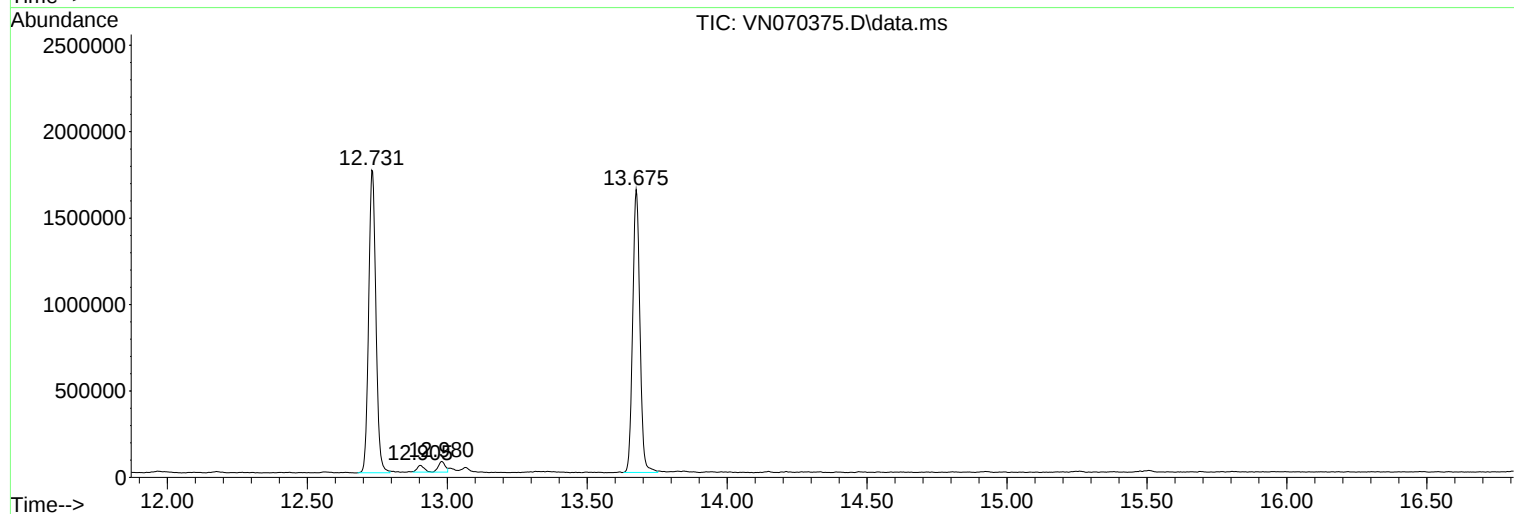
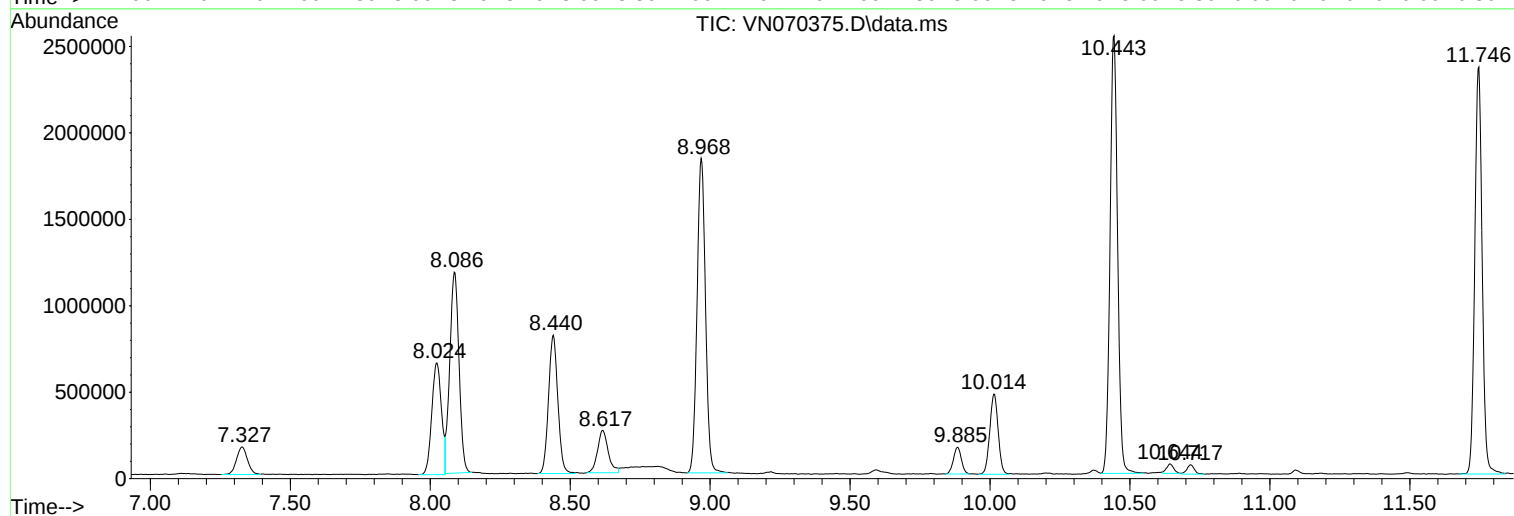
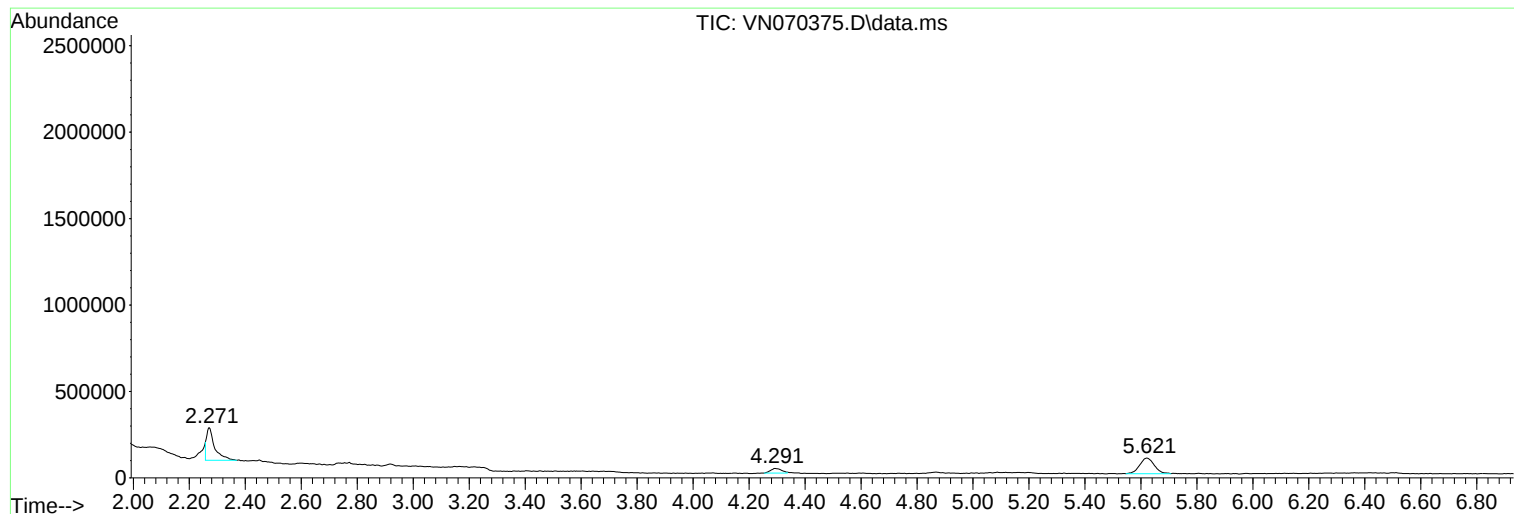
Sum of corrected areas: 28540959

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



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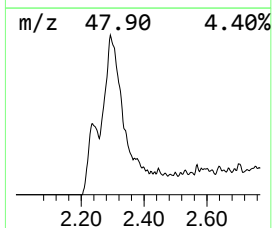
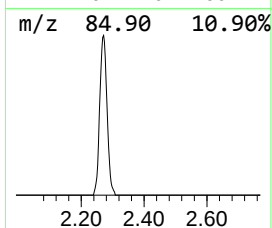
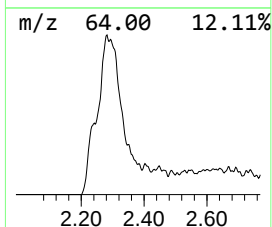
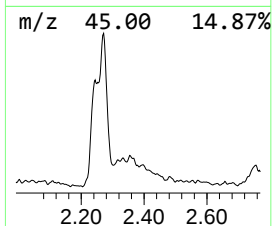
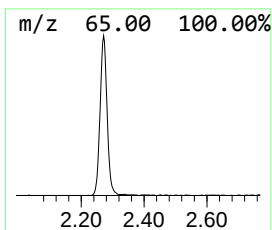
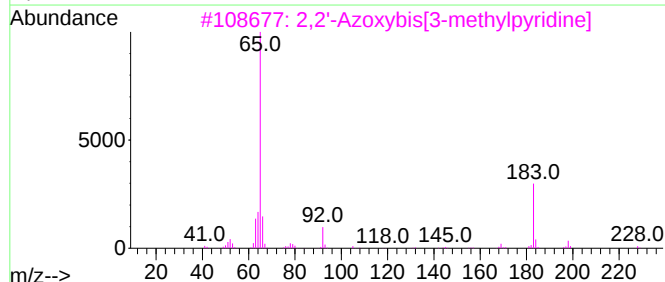
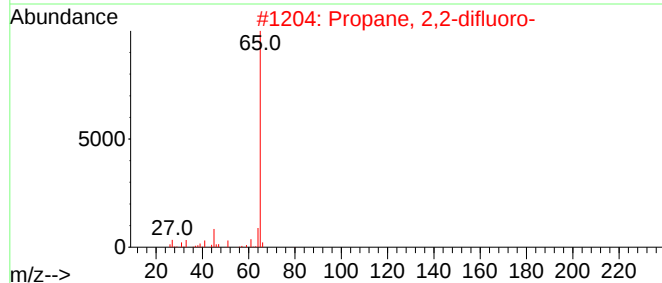
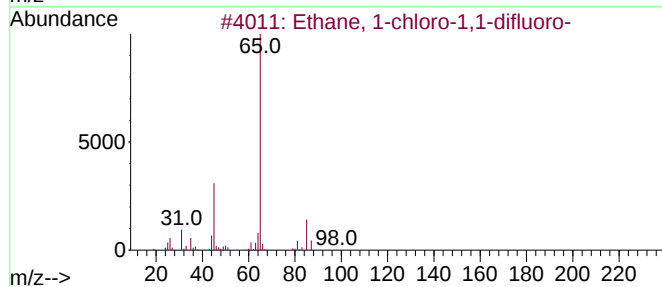
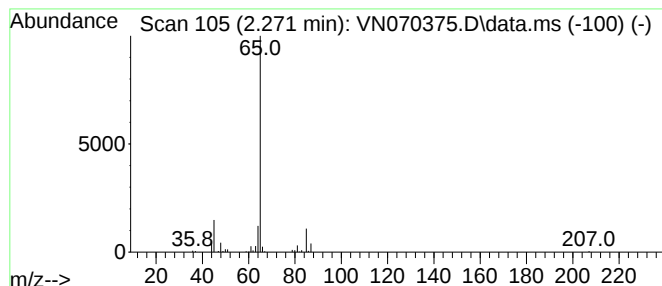
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.271	7.13 ug/l	376108	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	83
2			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	4
3			2,2'-Azoxybis[3-methylpyridine]	228	C12H12N4O	1000213-16-2	4
4			Propane, 1,1,2,2-tetrafluoro-	116	C3H4F4	040723-63-5	2
5			Propane, 1-chloro-2,2-difluoro-	114	C3H5ClF2	000420-99-5	2



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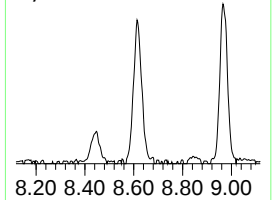
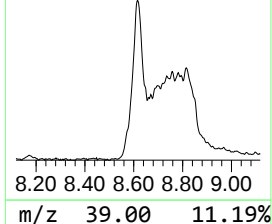
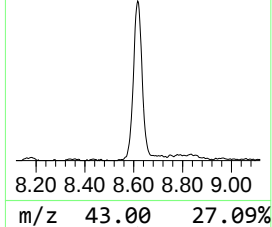
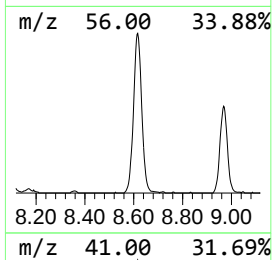
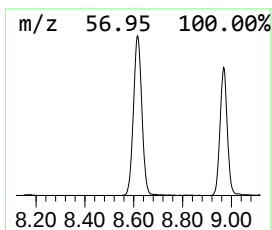
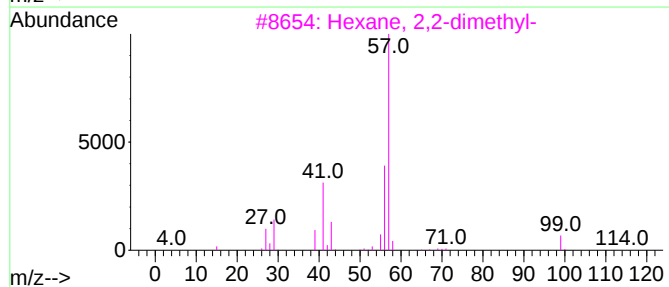
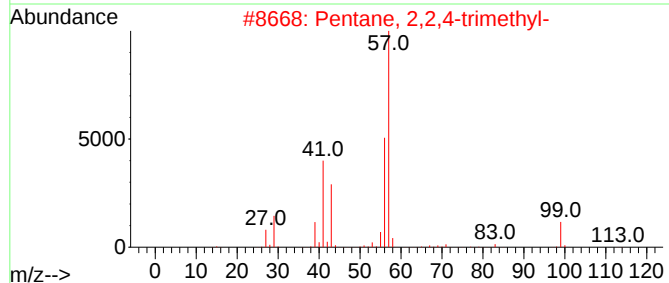
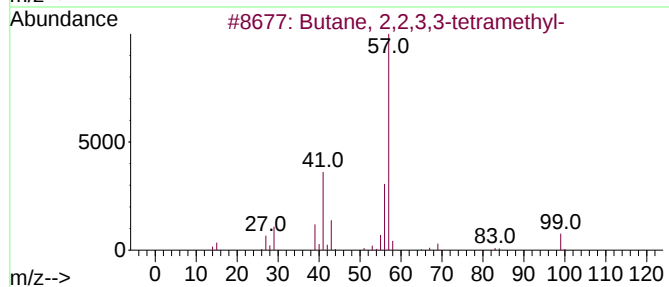
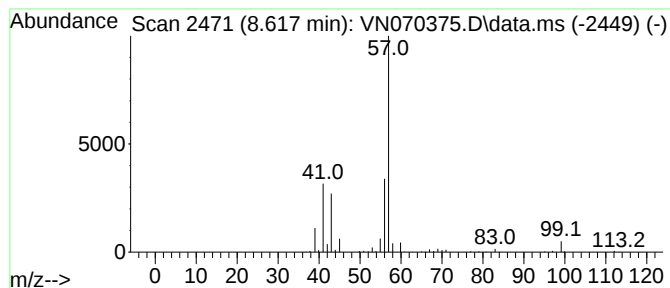
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Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	8.63 ug/l	656325	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	42



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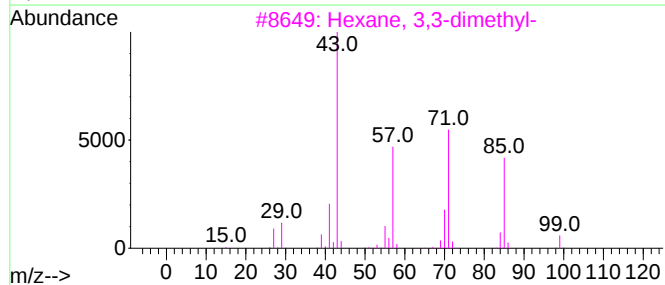
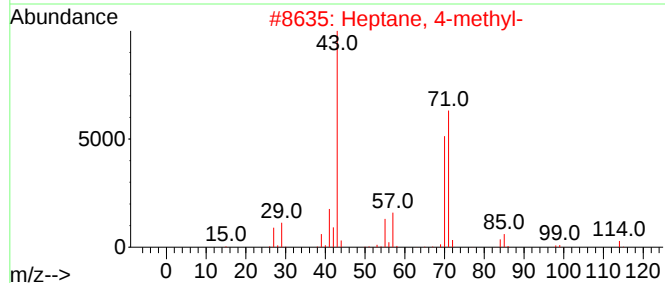
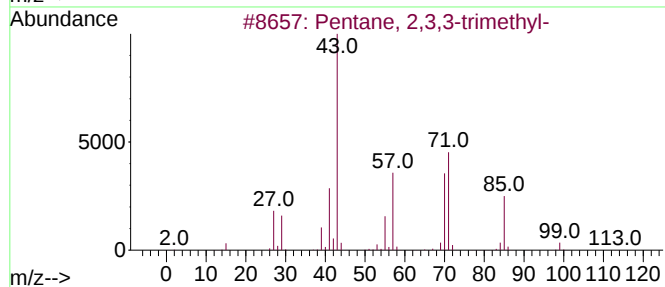
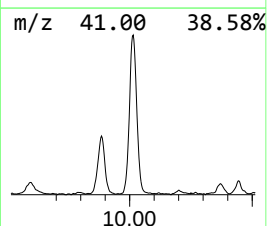
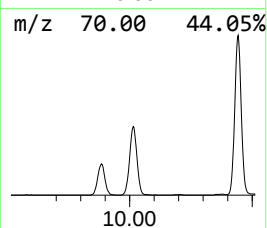
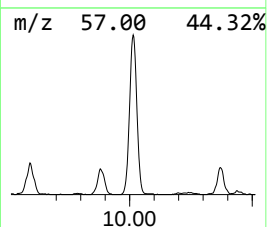
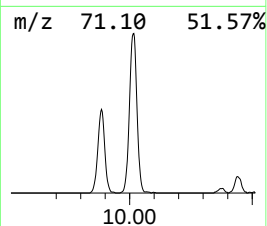
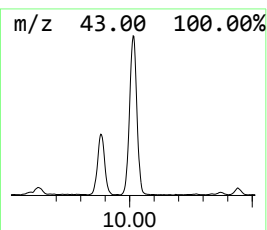
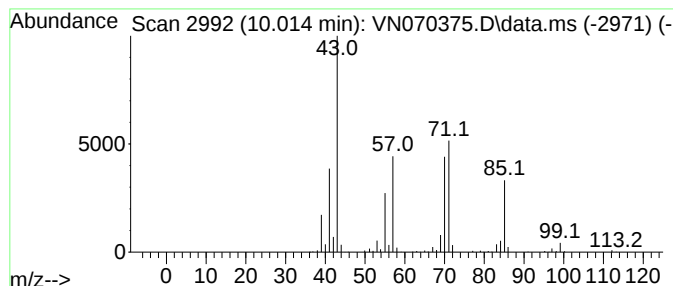
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	12.77 ug/l	971089	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Octane, 4-methyl-	128	C9H20	002216-34-4	59
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1-chlor...	2.271	7.1	ug/l	376108	1	8.088	2636980	50.0
Butane, 2,2,3,3...	8.617	8.6	ug/l	656325	2	8.968	3803300	50.0
Pentane, 2,3,3-...	10.014	12.8	ug/l	971089	2	8.968	3803300	50.0